Supporting Information

One Collision—Two Substituents: Gas-Phase Preparation of Xylenes under Single-Collision Conditions

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Experimental Procedures
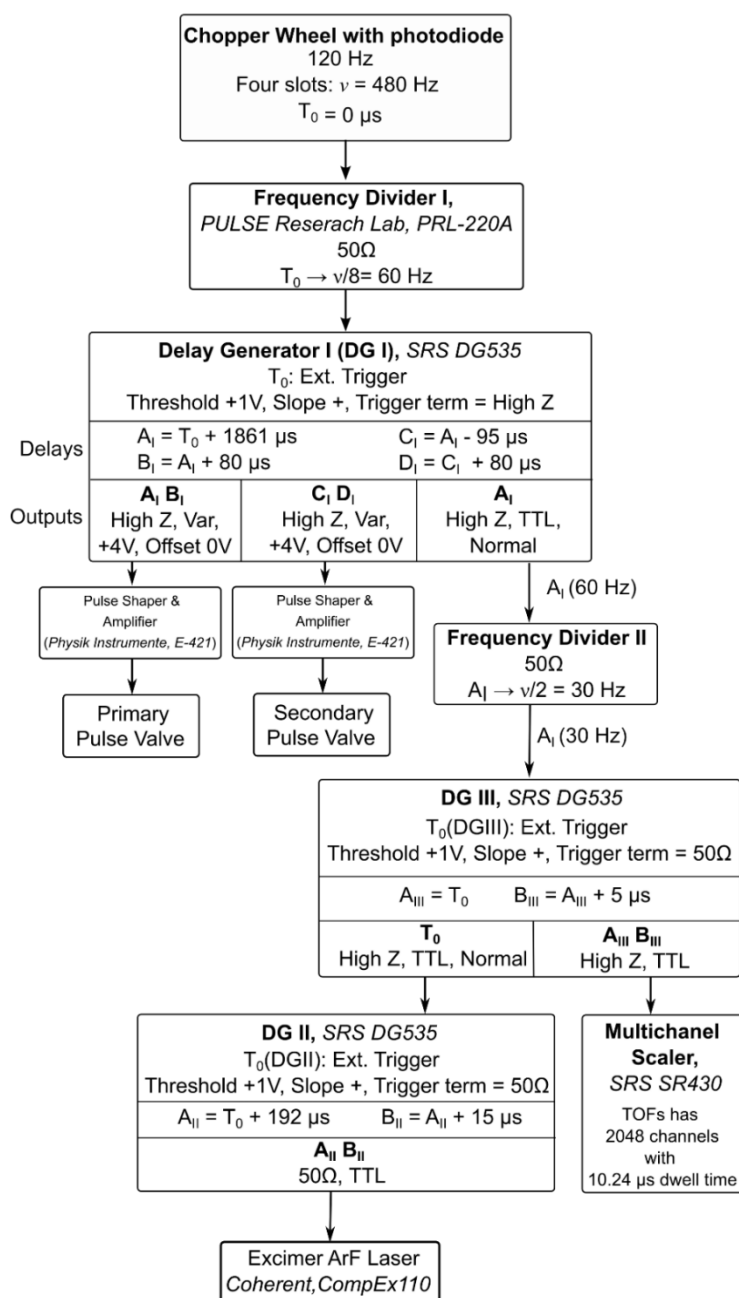
Crossed molecular beams

The gas-phase reactions of the 1-propynyl radical (CH_3CC; X^2A_1) with 2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$; X^1A') and 1,3-pentadiene ($CH_3CHCHCHCH_2$, X^1A') were carried out under single-collision conditions using the crossed molecular beams machine.[1,2]. The crossed beams apparatus consists of two fixed orthogonal source chambers (primary and secondary), the main scattering chamber, and an ultrahigh-vacuum (UHV; 10^{-12} Torr), rotatable, differentially pumped detector. In the primary source chamber, the pulsed supersonic beam of 1-propynyl radical was generated by photodissociation of 1-iodopropyne (CH_3CCI; TCI, 99%+) seeded at a level of 0.5% in helium (99.9999 %, Matheson), using the focused 193 nm output of the excimer laser (Coherent, CompEx110; 20 mJ pulse^{-1}; 30 Hz).[3–5] The secondary molecular beam was produced using 2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$; Sigma, 99%) or 1,3-pentadiene (*cis*- and *trans*- mixture of $CH_3CHCHCHCH_2$; TCI, >96.0%) released by Proch-Trickl pulsed valve[6] at backing pressures of 430 Torr and 350 Torr, respectively. A four-slot chopper wheel located after the skimmer selected a part of the 1-propynyl radical beam with a well-defined peak velocity (v_p) and speed ratio (S) that intersected in the interaction region of the scattering chamber with the secondary beams. The peak velocities (v_p), speed ratios (S), center-of-mass angles (Θ_{CM}), and collision energies (E_C) of the hydrocarbons beams are summarized in Table S1. We should note that it is possible that the propargyl radical (2-propynyl, CH_2CCH) may be produced during generation of 1-propynyl by photodissociation of CH_3CCI via isomerization through hydrogen shift in the 1-propynyl radical in the photolysis zone, too. However, the entrance barrier for the addition of the propargyl radical to the diene moiety was shown to be about 80 kJ mol^{-1},[7] which is well above the collision energy in our experiments (43 ± 2 kJ mol^{-1}). Therefore, even if propargyl is present in the molecular beam, it will not contribute to the reactive scattering signal.

The scattering products of collision events are ionized by electron impact at 80 eV (2 mA) at the entrance of the rotatable detector, filtered according to mass-to-charge (*m/z*) ratios using the QMS (Extrel, QC 150; 1.2 MHz) and then detected using a Daly-type particle ion counter.[8] The pulse scheme of the experiment is represented in Figure S1. Angular resolved time-of-flight (TOF) spectra were recorded in the plane of the reactant beams at discrete laboratory angles, which were integrated and normalized with respect to TOF at Θ_{CM} to extract the laboratory angular distribution (LAD). TOF and LAD were fit using a forward-convolution routine that is constrained by the reactant beam divergences, velocity spreads, and various machine parameters. This is an iterative method where user-defined center-of-mass (CM) translational energy ($P(E_T)$) and angular ($T(\theta)$) flux distributions simulate the measured signal under our experimental conditions.[9,10] CM functions are varied until a suitable fit of the TOF spectra and LAD is achieved. Together, the CM functions represent the reactive differential cross section $I(\theta, u)$, which can be divided into components of the CM scattering angle θ and the CM velocity u, $I(u, \theta) \sim P(u) \times T(\theta)$, which is represented as a flux contour maps (Fig. 2) and reveals an overall image of the reaction outcome.

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Table S1. Peak velocities (v_p) and speed ratios (S) of the 1-propynyl radical (C_3H_3), 2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$), and 1,3-pentadiene

($CH_3CHCHCHCH_2$) beams along with the corresponding collision energies (E_C) and center-of-mass angles (Θ_{CM})

Beam	v_p (m s^{-1})	S	E_C (kJ mol^{-1})	Θ_{CM} (degree)
1-propynyl radical (CH_3CC, X^2A_1)	1722 ± 50	10.3 ± 1.5	–	–
2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$, X^1A')	701 ± 19	5.1 ± 0.5	43 ± 2	35.4 ± 1.2
1,3-pentadiene ($CH_3CHCHCHCH_2$, X^1A')	708 ± 17	5.7 ± 0.5	43 ± 2	35.9 ± 0.9

Figure S1. Pulse sequence for the crossed molecular beam experiment for the reaction of the 1-propynyl radical (CH_3CC; X^2A_1) with 2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$, X^1A') and 1,3-pentadiene ($CH_3CHCHCHCH_2$, X^1A').
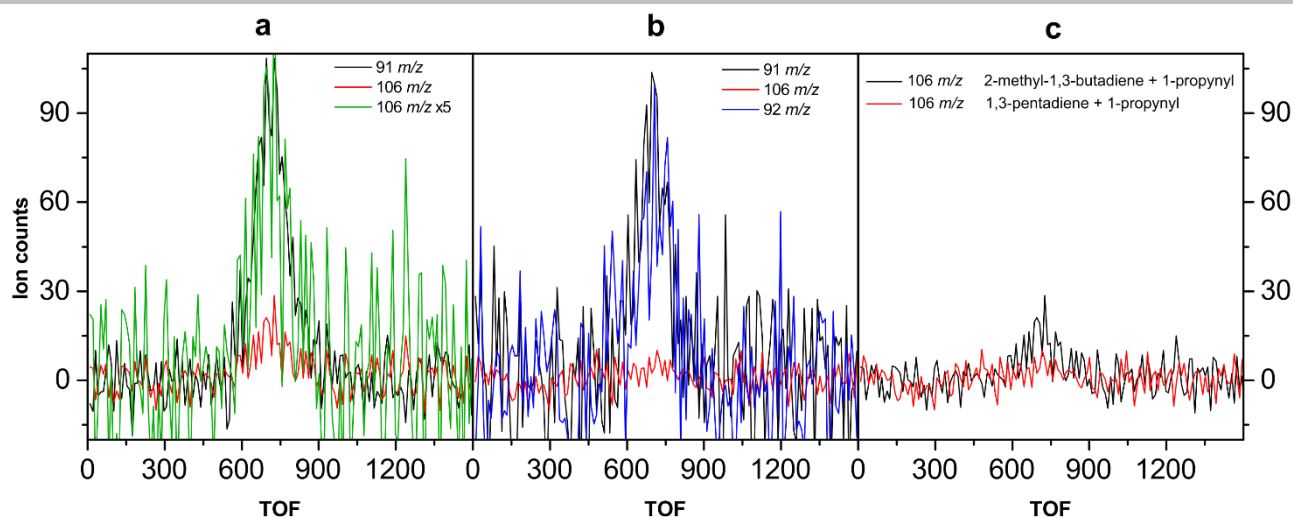
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Figure S2. Time-of-flight (TOF) spectra for the reactions of 1-propynyl radical (CH$_3$CC; X^{2}A$_1$) with (a) 2-methyl-1,3-butadiene (CH$_2$C(CH$_3$)CHCH$_2$, X^{1}A') and (b) 1,3-pentadiene (CH$_3$CHCHCHCH$_2$, X^{1}A') taken at different m/z. On the (c) depicted the direct comparison of the reactive scattering signal recorded at m/z = 106 for the 2-methyl-1,3-butadiene (CH$_2$C(CH$_3$)CHCH$_2$, X^{1}A') and 1,3-pentadiene (CH$_3$CHCHCHCH$_2$, X^{1}A') systems.

Sample preparation

Samples of 1-iodopropyne (CH$_3$CCI; TCI, 99%+), 2-methyl-1,3-butadiene (CH$_2$C(CH$_3$)CHCH$_2$; Sigma, 99%), and 1,3-pentadiene (cis- and trans- mixture of CH$_3$CHCHCHCH$_2$; TCI, >96.0%) were purified by several cycles of freeze-pump-thaw method. 1-iodopropyne (CH$_3$CCI; TCI, 99%+) was then diluted at a level of 0.5% in helium (99.9999%; Matheson) in a Teflon-coated sample cylinder (Swagelok); teflon coating is recommended to prevent sample degradation over time. This mixture was used at backing pressure of 760 Torr in the primary chamber pulsed valve. Neat 2-methyl-1,3-butadiene and 1,3-pentadiene were fed into the secondary chamber pulsed valve at backing pressures of 450 Torr and 400 Torr, respectively.

Electronic structure calculations

Geometry optimization of different structures on the C$_8$H$_{11}$ potential energy surface (PES) accessed by the reactions of the propynyl radical with two C$_5$H$_8$ isomers, 2-methyl-1,3-butadiene (isoprene) and 1,3-pentadiene, was carried out at the density functional ωB97X-D level of theory [11] with the 6-311G(d,p) basis set. Vibrational frequencies for all optimized stationary points were computed at the same ωB97X-D/6-311G(d,p) level. The calculations of frequencies allowed us to characterize all structures as either local minima or transition states and to evaluate zero-point vibrational energy corrections (ZPE). The frequencies were also used for calculations of energy-dependent rate constants. Single-point energies for each stationary point on the PES were rectified using the G3(MP2,CC) model chemistry scheme in which the coupled cluster CCSD(T)/6-311G(d,p) energy is upgraded by a basis set correction to the G3Large basis set evaluated at the Moller-Plesset second-order perturbation theory (MP2) level.[12–14] The resulting G3(MP2,CC)//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) relative energies are known to be typically accurate within 10 kJ mol^{-1} or better.[14] The GAUSSIAN 09[15] and MOLPRO 2015[16] program packages were employed for the electronic calculations.
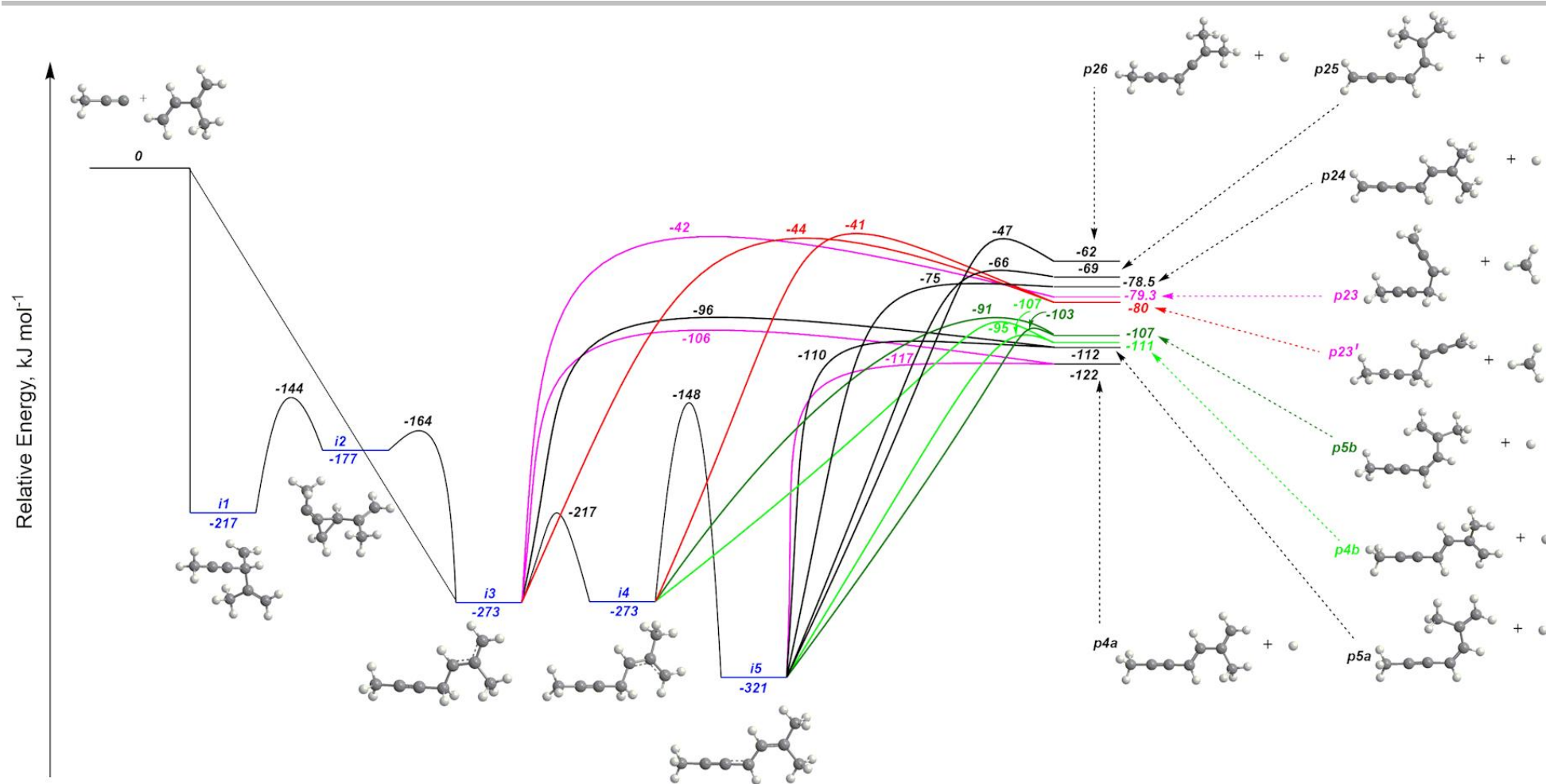
Figure S3. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH_3CC; X^2A_1) radical with 2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$; X^1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part I.
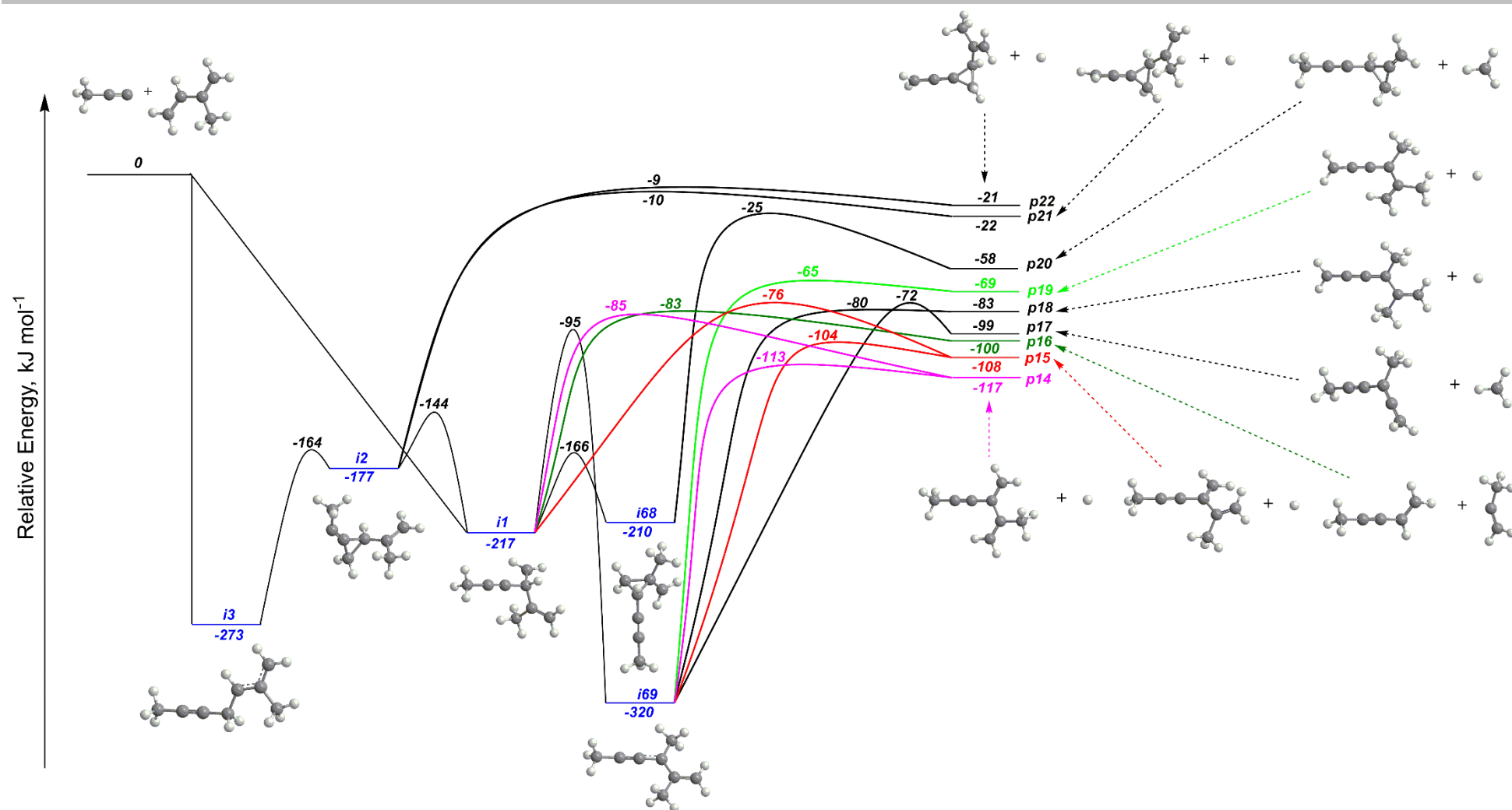
Figure S4. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH₃CC; X²A₁) radical with 2-methyl-1,3-butadiene (CH₂C(CH₃)CHCH₂; X¹A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol⁻¹. Part II.

Figure S5. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) radical with 2-methyl-1,3-butadiene (CH$_2$C(CH$_3$)CHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part III.

Figure S6. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) radical with 2-methyl-1,3-butadiene (CH$_2$C(CH$_3$)CHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part IV.
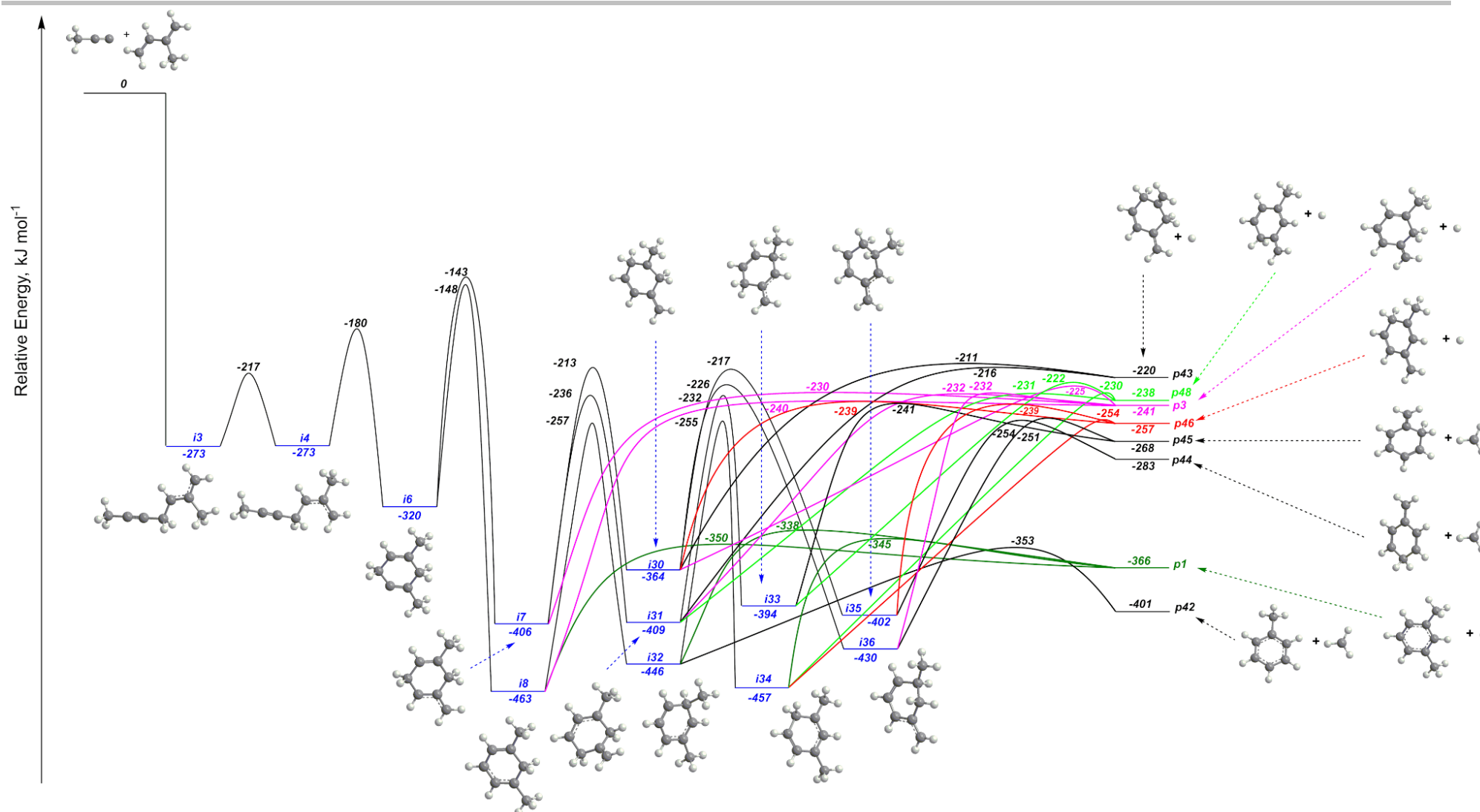
Figure S7. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH_3CC; X^2A_1) radical with 2-methyl-1,3-butadiene ($CH_2C(CH_3)CHCH_2$; X^1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part V.
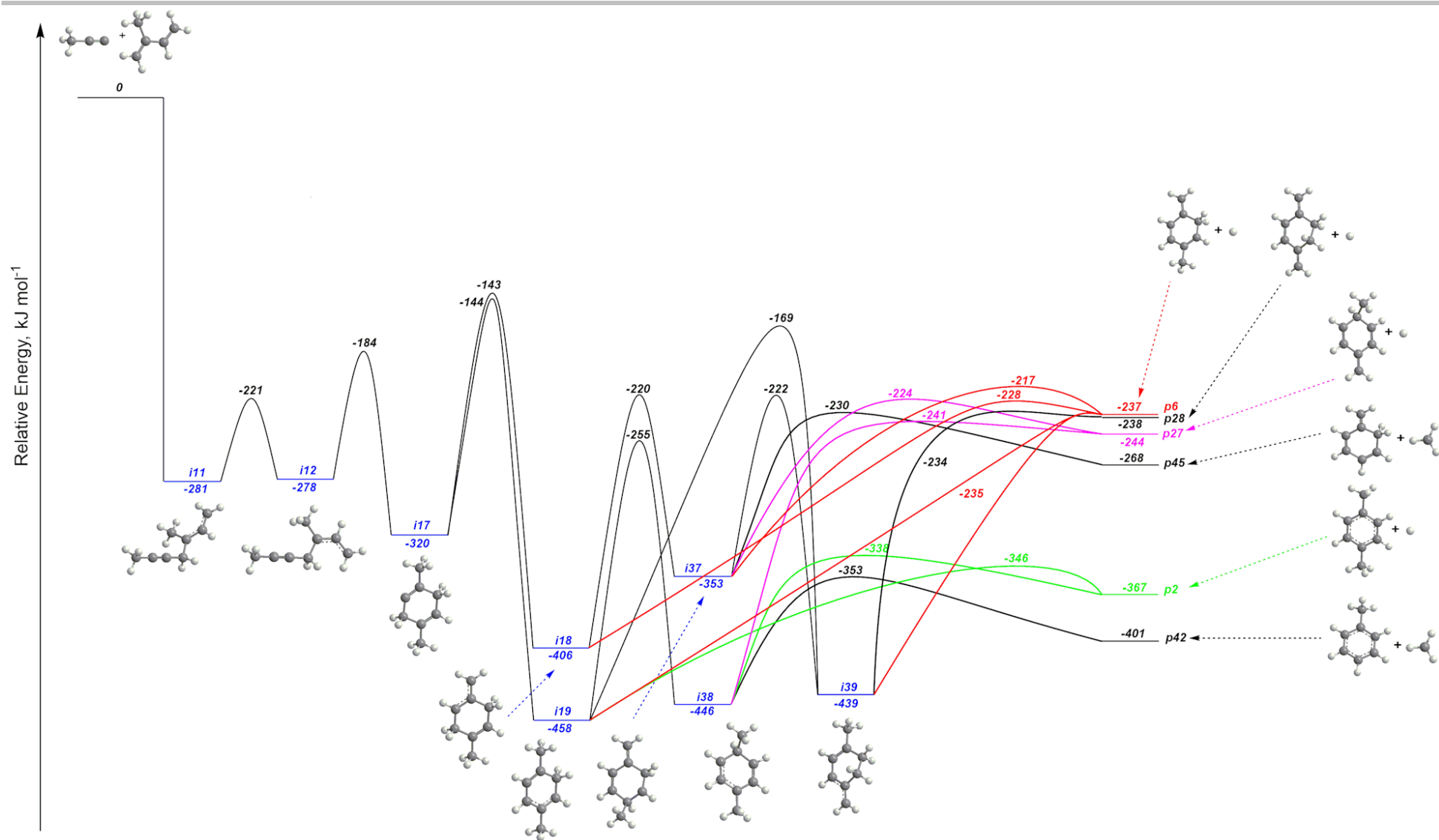
Figure S8. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH₃CC; X²A₁) radical with 2-methyl-1,3-butadiene (CH₂C(CH₃)CHCH₂; X¹A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol⁻¹. Part VI.
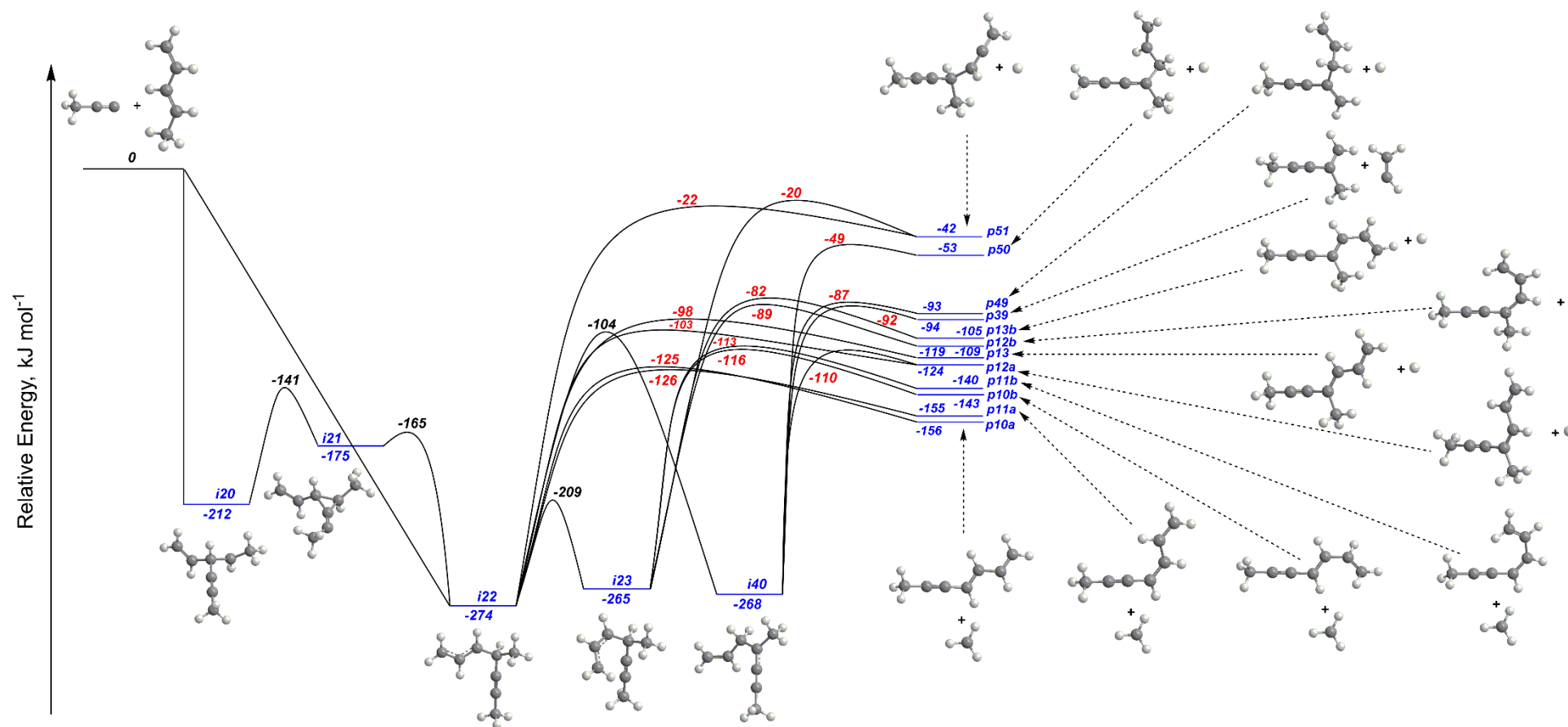
Figure S9. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part I.
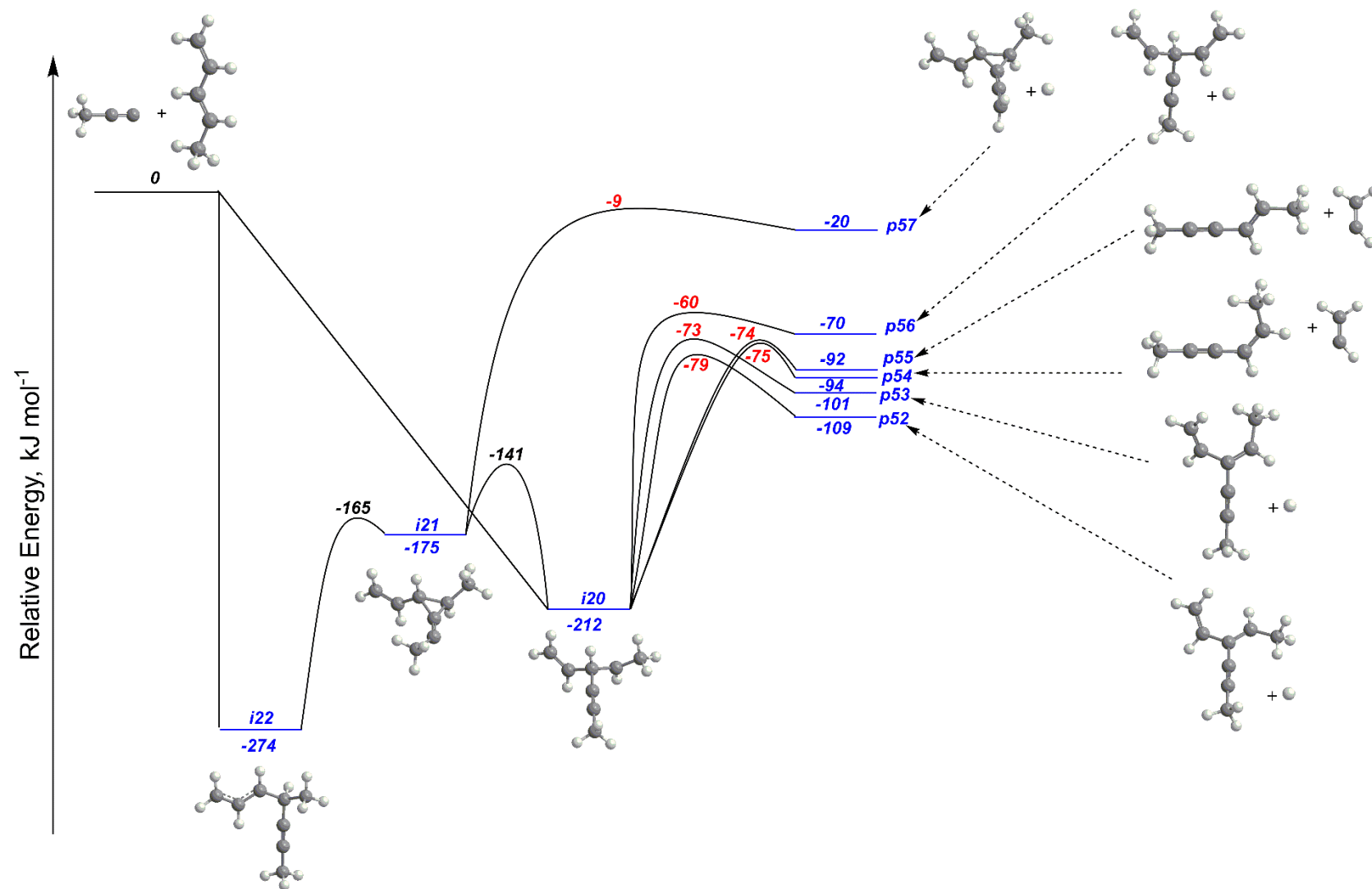
Figure S10. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH_3CC; X^2A_1) with 1,3-pentadiene ($CH_3CHCHCHCH_2$; X^1A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part II.
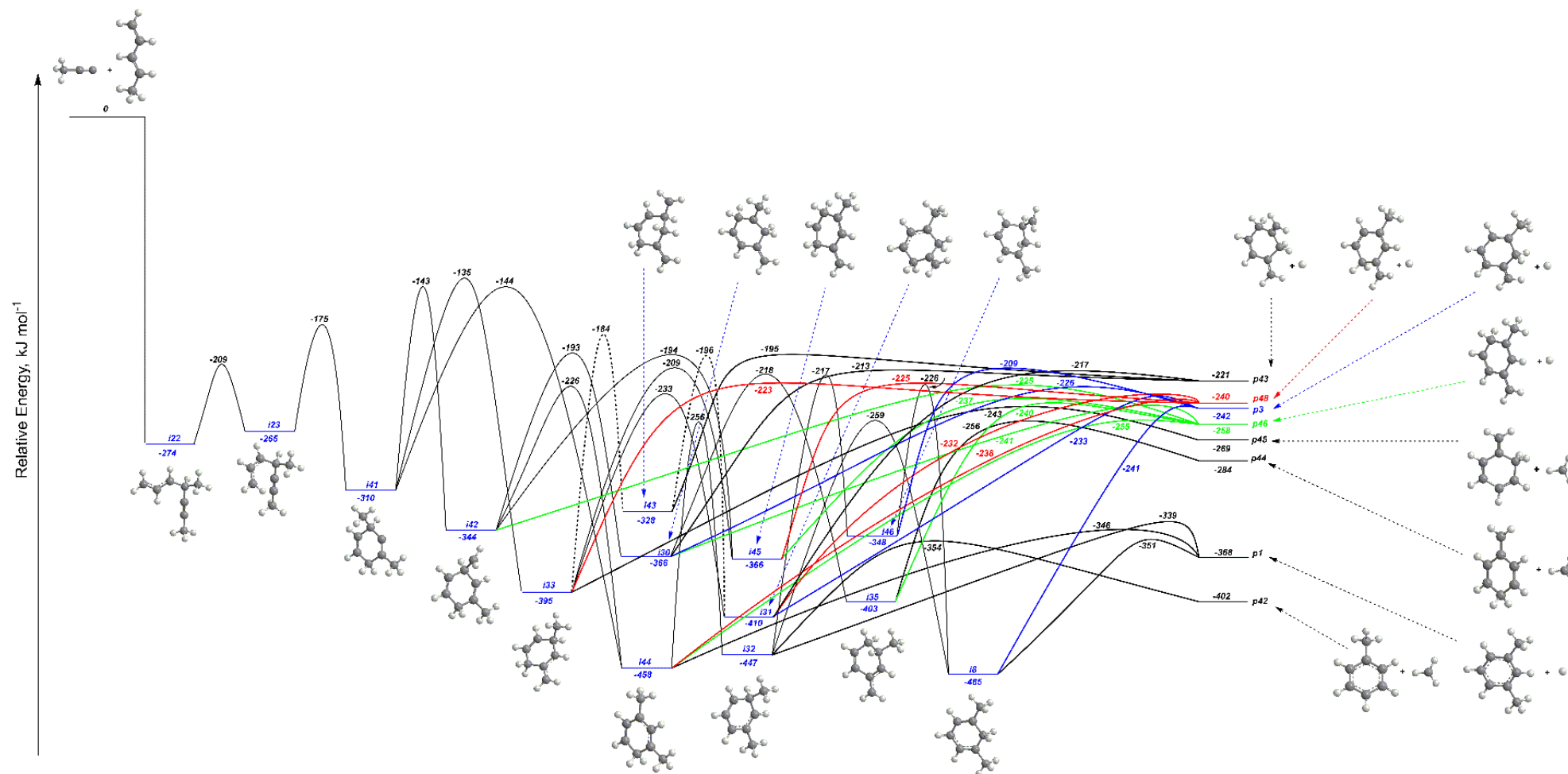
Figure S11. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part III.

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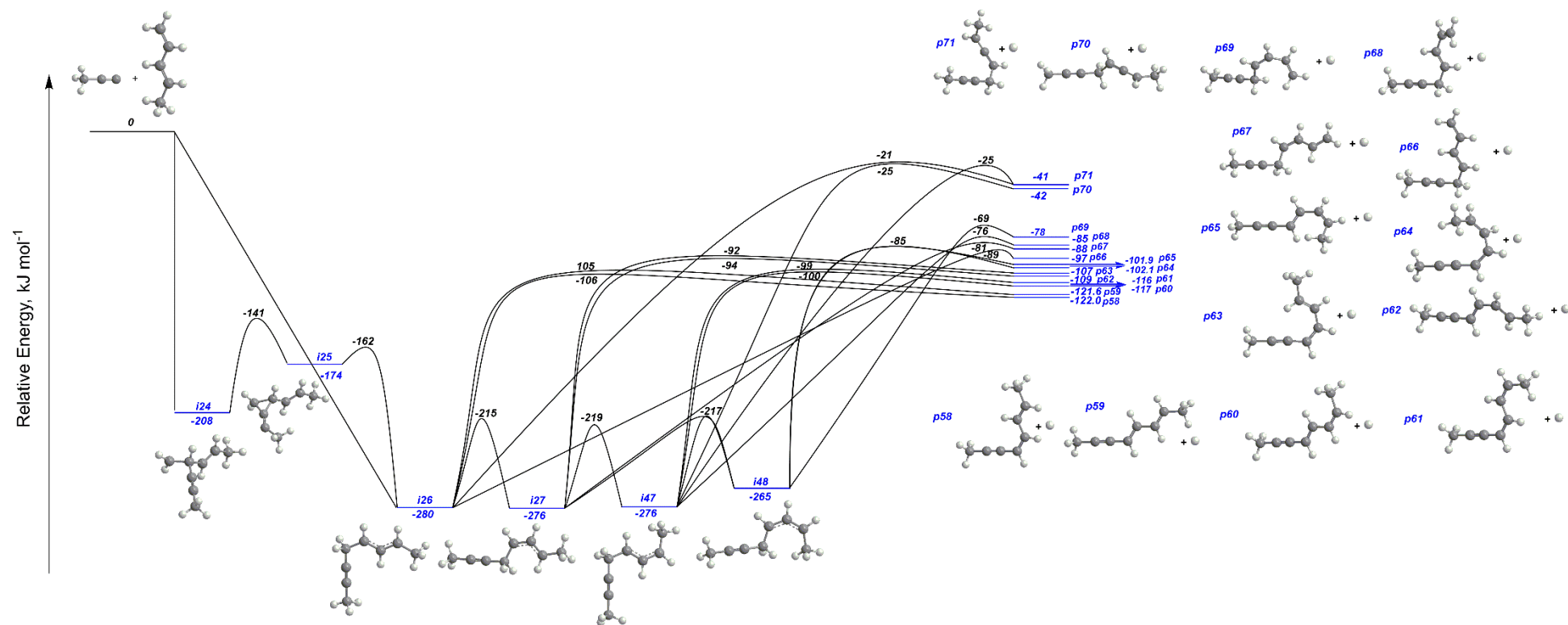
Figure S12. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part IV.
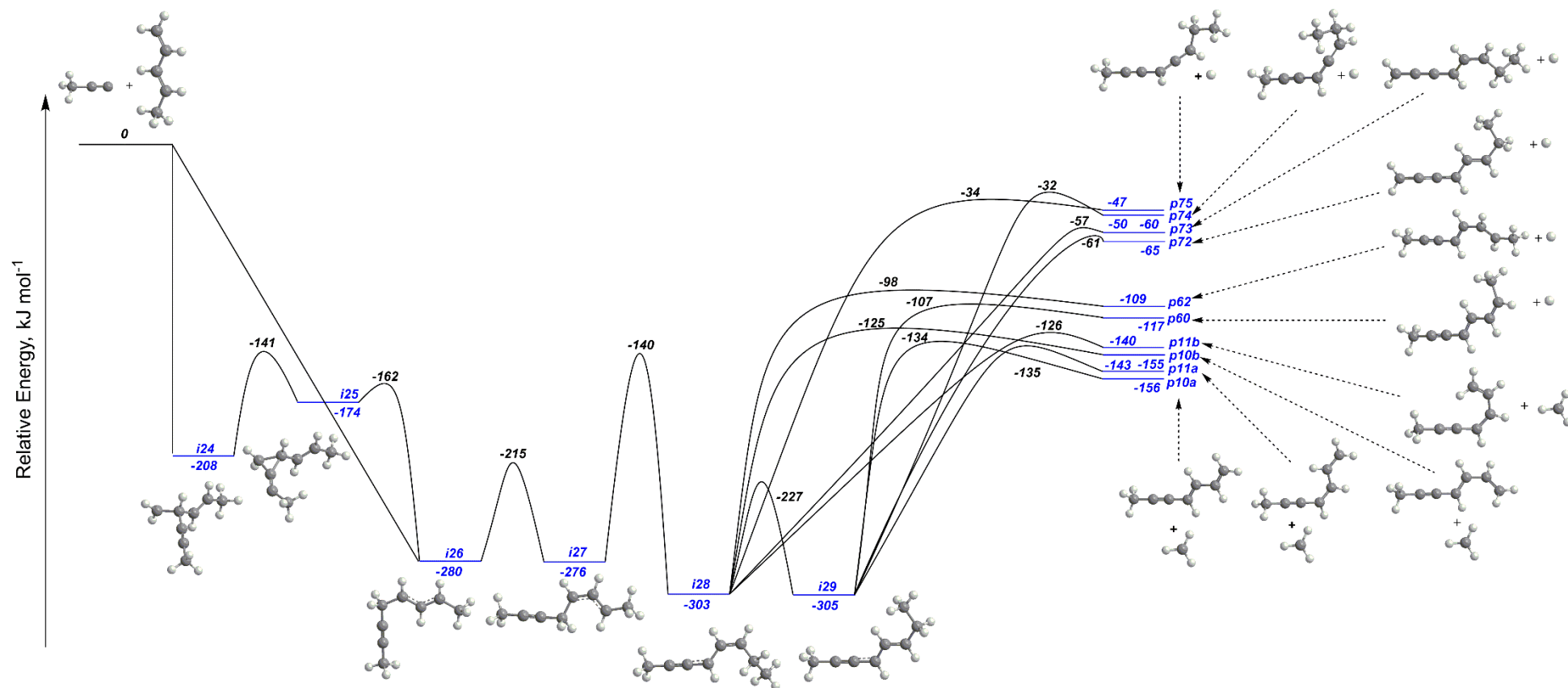
Figure S13. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part V.
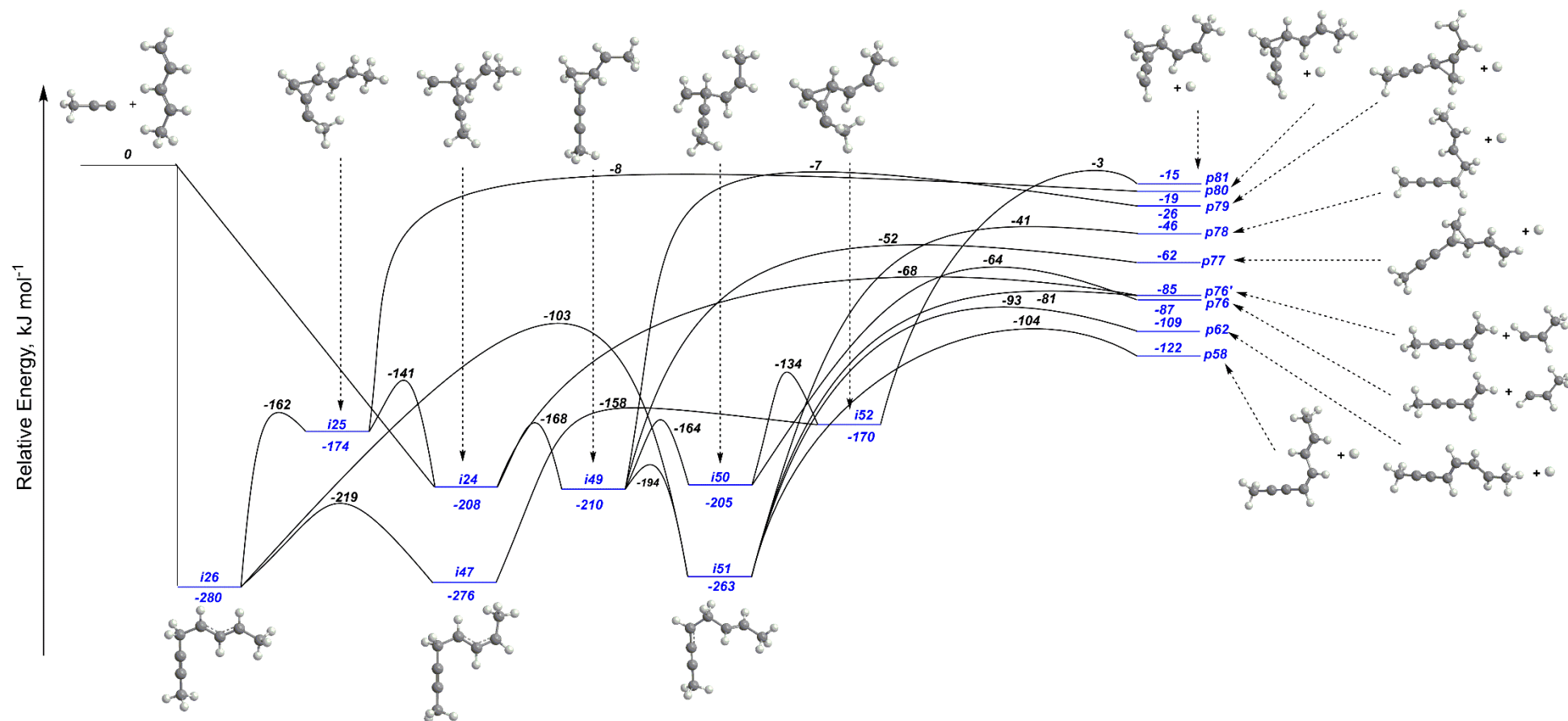
Figure S14. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part VI.
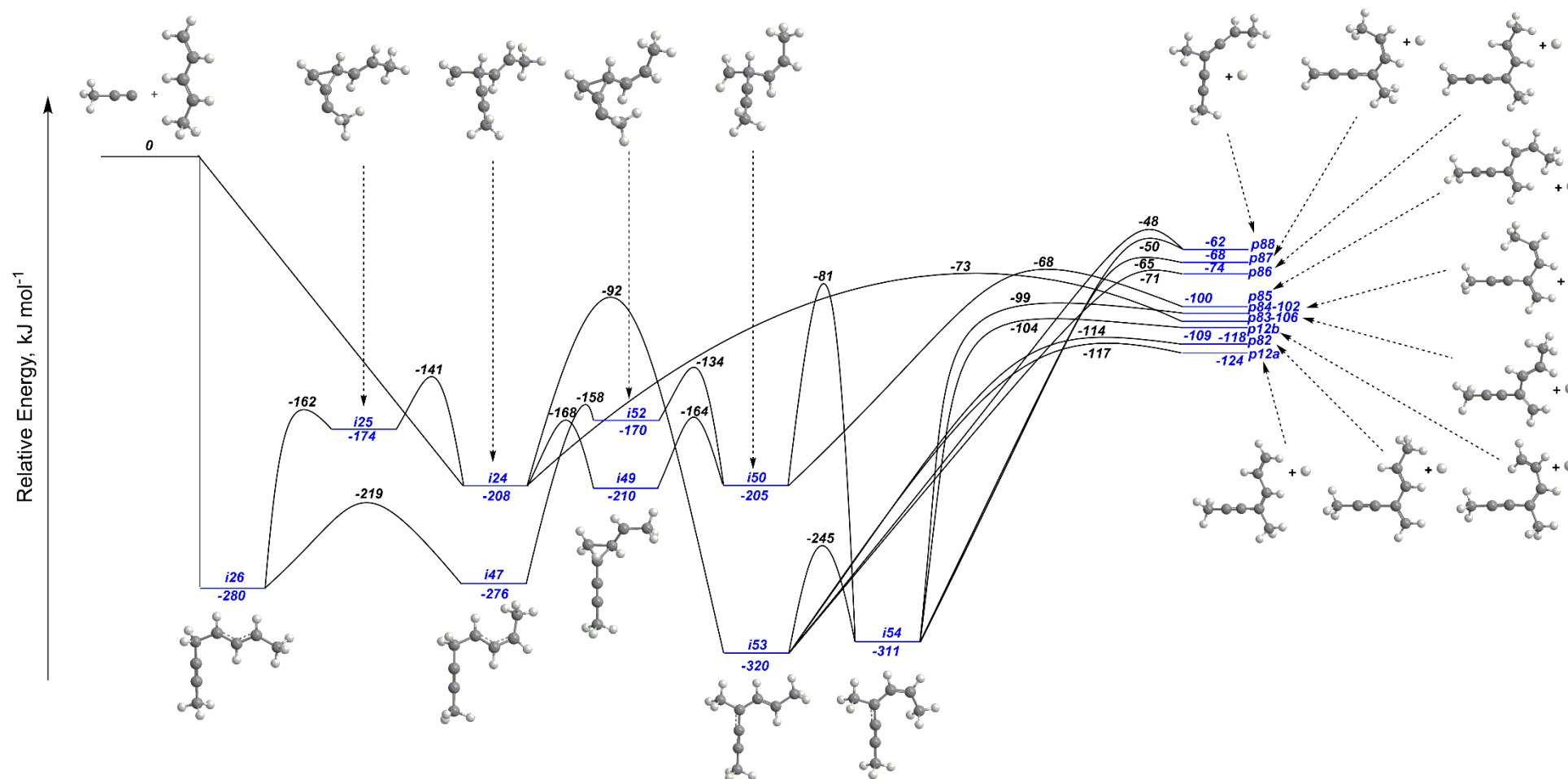
Figure S15. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part VII.
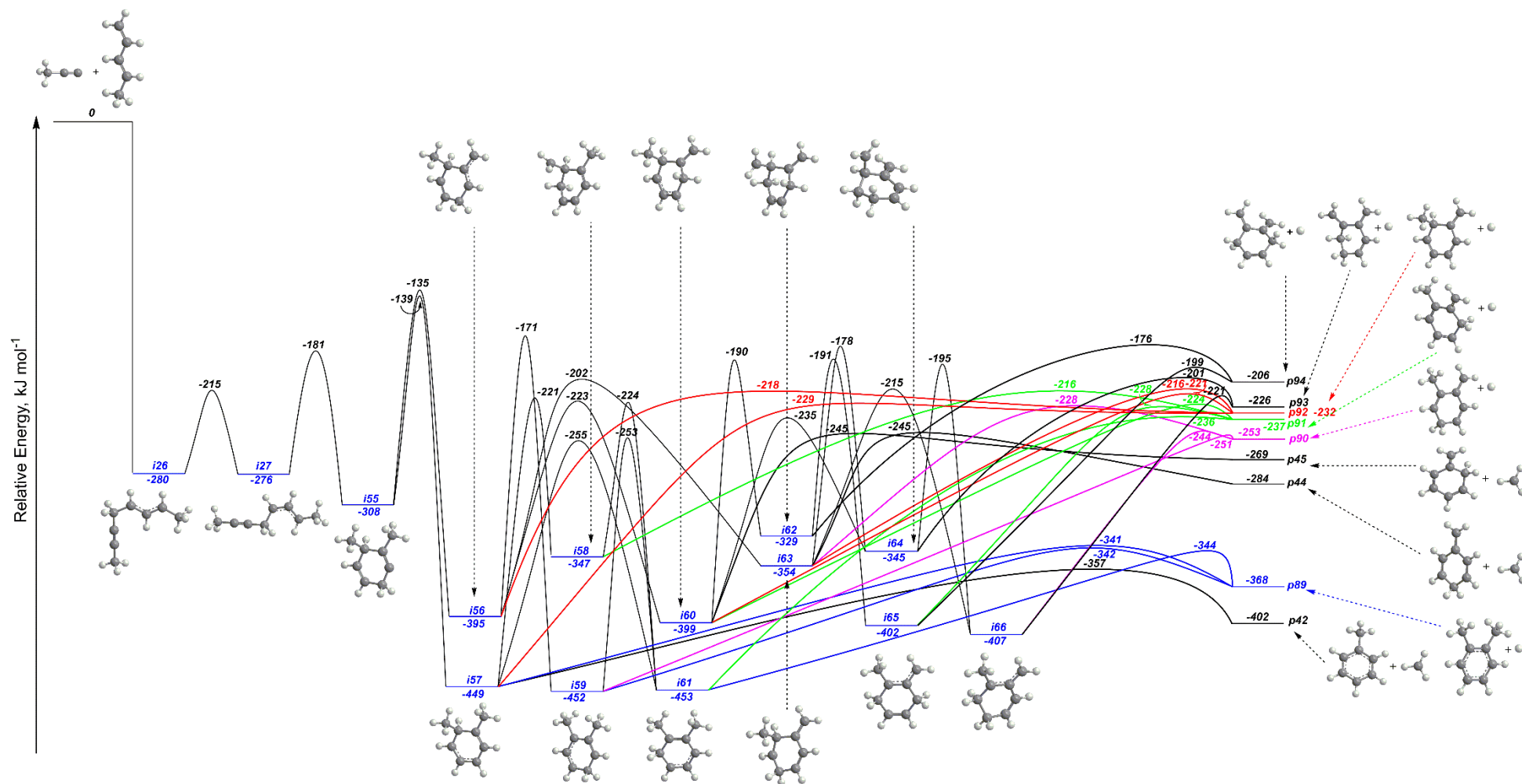
Figure S16. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH$_3$CC; X^{2}A$_1$) with 1,3-pentadiene (CH$_3$CHCHCHCH$_2$; X^{1}A') calculated at the G3(MP2,CC)//ωB97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1}. Part VIII.

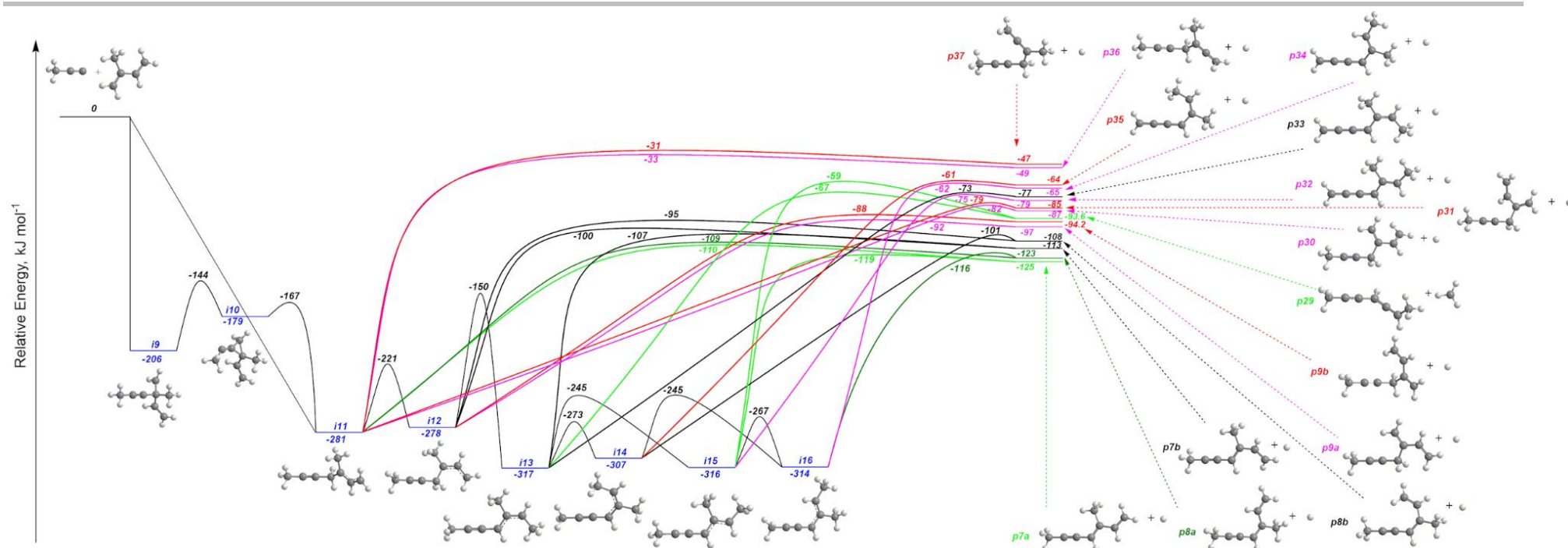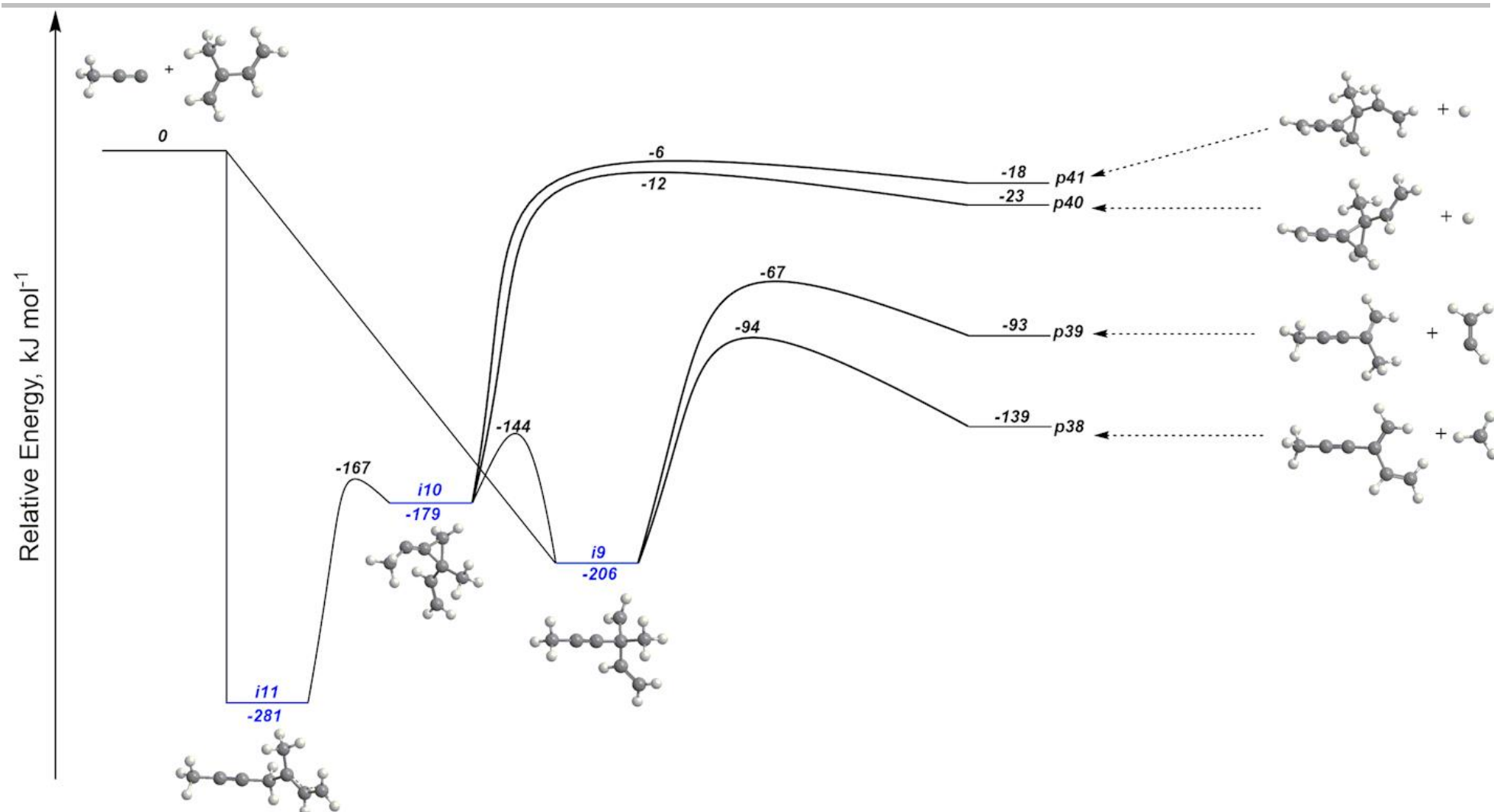### Calculations of energy-dependent rate constants

Rice-Ramsperger-Kassel-Marcus (RRKM) theory[17–19] was employed to compute microcanonical, internal energy-dependent rate constants of all unimolecular reaction steps on the C_8H_{11} PES following the initial association of the H_3CCC radical with the C_5H_8 isomers. We utilized our in-house code Unimol [20] to evaluate the rate constants as functions of the available internal energy of each intermediate or transition state within the harmonic approximation. Unimol is an updated version of our previous software code on energy dependent RRKM calculations of rate constants for multiwell and multichannel unimolecular reactions under single-collision conditions and for solving a system of first-order kinetic equations. [21] The internal energy in these calculations is assumed to be equal to the sum of the collision energy and the chemical activation energy, that is, negative of the relative energy of a species with respect to the reactants. Since the calculations simulate the experimental crossed molecular beams conditions at a zero-pressure limit, only one energy level is considered throughout. With all RRKM rate constants in hand, product branching ratios are then computed by solving first-order kinetic equations within steady-state approximation. The calculated rate constants and product branching ratios depending on the initial reaction intermediate formed by recombination of the reactants are presented in Supporting Information (Tables S9-S10 and S2-S8, respectively).

Table S2. Statistical branching ratios (%) for the reaction of 2-methyl-1,3-butadiene + propynyl with *i1*, *i3*, *i9*, and *i11* as initial intermediates at different collision energies (E_C, kJ·mol^{-1})

	i1		*i3*		*i9*		*i11*	
E_C	0	43	0	43	0	43	0	43
p1	3.7	1.5	3.7	1.5	0.0	0.0	0.0	0.0
p2	0.0	0.0	0.0	0.0	3.7	1.6	3.8	1.7
p3	3.2	1.4	3.2	1.4	0.0	0.0	0.0	0.0
p4a	38.7	33.4	39.0	34.3	0.0	0.0	0.0	0.0
p4b	27.8	31.5	28.0	32.4	0.0	0.0	0.0	0.0
p5a	10.0	10.1	10.1	10.4	0.0	0.0	0.0	0.0
p5b	15.0	18.6	15.1	19.1	0.0	0.0	0.0	0.0
p6	0.0	0.0	0.0	0.0	3.6	1.5	3.6	1.6
p7a	0.0	0.0	0.0	0.0	28.3	22.7	28.7	24.0
p7b	0.0	0.0	0.0	0.0	46.1	47.5	46.7	50.3
p8a	0.0	0.0	0.0	0.0	13.2	13.1	13.4	13.9
p8b	0.0	0.0	0.0	0.0	1.6	2.5	1.6	2.6
p9a	0.0	0.0	0.0	0.0	1.1	2.8	1.2	2.9
p9b	0.0	0.0	0.0	0.0	0.2	0.4	0.1	0.4
p14	0.6	1.6	0.2	0.3	0.0	0.0	0.0	0.0
p15	0.3	1.0	0.1	0.2	0.0	0.0	0.0	0.0
p16	0.1	0.6	0.0	0.1	0.0	0.0	0.0	0.0
p17	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p18	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p19	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p21	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p22	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p23/p23'	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p24	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.0
p25	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p26	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p27	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p29	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.3
p30	0.0	0.0	0.0	0.0	0.2	0.7	0.2	0.7
p31	0.0	0.0	0.0	0.0	0.1	0.2	0.1	0.3
p32	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
p33	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p34	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p35	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p36	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p37	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p38	0.0	0.0	0.0	0.0	1.8	6.5	0.5	1.2
p39	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0
p40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p41	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p42	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p43	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0
p44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p45	0.0	0.0	0.0	0.0	0.1	0.0	0.1	0.0
p46	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0
p48	0.4	0.2	0.4	0.2	0.0	0.0	0.0	0.0

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Table S3. Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene + propynyl with *i1*, *i3* as initial intermediates at different collision energies (E_C, kJ·mol^{-1}) having the energies of *ts*[*i4-i5*] and *ts*[*i6-i7*] increased by 5 kJ·mol^{-1} and the energy of *ts*[*i6-i8*] decreased by 5 kJ·mol^{-1}:
ts[*i4-i5*] := (-148 + 5) kJ·mol^{-1} = -143 kJ·mol^{-1} (reducing the contribution of p4-p5);
ts[*i6-i7*] := (-143 + 5) kJ·mol^{-1} = -138 kJ·mol^{-1} (reducing the contribution of p3);
ts[*i6-i8*] := (-148 - 5) kJ·mol^{-1} = -153 kJ·mol^{-1}.

	i1		i3	
E_C	**0**	**43**	**0**	**43**
p1	8.4	3.6	8.5	3.7
p3	1.9	1.0	1.9	1.0
p4a	37.5	33.1	37.8	34.0
p4b	26.7	30.7	26.9	31.5
p5a	9.6	9.9	9.7	10.1
p5b	14.4	18.1	14.5	18.6

Table S4. Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene + propynyl with *i1*, *i3* as initial intermediates at different collision energies (E_C, kJ·mol^{-1}) having the energies of *ts*[*i4-i5*], *ts*[*i6-i7*], *ts*[*i5-p4a/p4b*], and *ts*[*i5-p5a/p5b*] increased by 5 kJ·mol^{-1} and the energy of *ts*[*i6-i8*] decreased by 5 kJ·mol^{-1}:
ts[*i4-i5*] := (-148 + 5) kJ·mol^{-1} = -143 kJ·mol^{-1} (reducing the contribution of p1-p4);
ts[*i6-i7*] := (-143 + 5) kJ·mol^{-1} = -138 kJ·mol^{-1} (reducing the contribution of p3);
ts[*i6-i8*] := (-148 - 5) kJ·mol^{-1} = -153 kJ·mol^{-1};

ts[*i5-p4a/p4b*] := (-117 + 5) kJ·mol^{-1} = -112 kJ·mol^{-1};
ts[*i5-p5a/p5b*] := (-110 + 5) kJ·mol^{-1} = -105 kJ·mol^{-1}.

	i1		i3	
E_C	**0**	**43**	**0**	**43**
p1	14.1	4.8	14.2	4.9
p3	3.1	1.3	3.1	1.4
p4a	35.8	33.4	36.0	34.3
p4b	23.6	29.4	23.8	30.2
p5a	8.7	9.6	8.8	9.8
p5b	12.6	17.3	12.7	17.7

Table S5. Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene + propynyl with *i9*, *i11* as initial intermediates at different collision energies (E_C, kJ·mol^{-1}) having the energies of *ts*[*i12-i13*] and *ts*[*i17-i18*] increased by 5 kJ·mol^{-1} and the energy of *ts*[*i17-i19*] decreased by 5 kJ·mol^{-1}:
ts[*i12-i13*] := (-150 + 5) kJ·mol^{-1} = -145 kJ·mol^{-1} (reducing the contribution of p7-p8);
ts[*i17-i18*] := (-143 + 5) kJ·mol^{-1} = -138 kJ·mol^{-1} (reducing the contribution of p6);
ts[*i17-i19*] := (-144 - 5) kJ·mol^{-1} = -149 kJ·mol^{-1}.

	i9		i11	
E_C	**0**	**43**	**0**	**43**
p2	8.6	3.7	8.7	3.9
p6	2.1	1.0	2.1	1.1
p7a	27.2	22.2	27.5	23.4
p7b	43.2	43.5	43.8	46.0
p8a	13.5	14.3	13.6	15.1
p8b	1.7	2.7	1.7	2.8
p9a	1.3	3.5	1.4	3.7
p9b	0.2	0.5	0.2	0.5

Table S6.
Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene +propynyl with *i9*, *i11* as initial intermediates at different collision energies (E_C, kJ·mol^{-1}) having the value of *ts*[*i12-i13*], *ts*[*i17-i18*], *ts*[*i15-p7a/p7b*], and *ts*[*i16-p8a/p8b*] increased by 5 kJ·mol^{-1} and the value of *ts*[*i17-i19*] decreased by 5 kJ·mol^{-1}:
ts[*i12-i13*] := (-150 + 5) kJ·mol^{-1} = -145 kJ·mol^{-1} (reducing the contribution of p7-p8);
ts[*i17-i18*] := (-143 + 5) kJ·mol^{-1} = -138 kJ·mol^{-1} (reducing the contribution of p6);
ts[*i17-i19*] := (-144 - 5) kJ·mol^{-1} = -149 kJ·mol^{-1};

ts[*i15-p7a/p7b*] := (-119 + 5) kJ·mol^{-1} = -114 kJ·mol^{-1};
ts[*i16-p8a/p8b*] := (-116 + 5) kJ·mol^{-1} = -111 kJ·mol^{-1}.

	I9		i11	
E_C	**0**	**43**	**0**	**43**
p2	9.7	3.9	9.9	4.1
p6	2.4	1.1	2.4	1.2
p7a	17.0	15.7	17.2	16.6
p7b	54.1	51.1	54.8	54.1
p8a	10.6	12.3	10.7	13.0
p8b	2.0	3.0	2.0	3.1
p9a	1.5	3.7	1.5	3.9
p9b	0.2	0.5	0.2	0.6

Table S7.
Statistical branching ratios (%) for major products of the reaction of 2-methyl-1,3-butadiene+propynyl with *i9*, *i11* as initial intermediates at different collision energies (E_C, kJ·mol^{-1}) having the value of *ts*[*i12-i13*], *ts*[*i17-i18*], *ts*[*i15-p7a/p7b*], *ts*[*i16-p8a/p8b*], *ts*[*i11-p7a/p7b*], *ts*[*i10-p8a/p8b*], and *ts*[*i13-p7a/p7b*] increased by 5 kJ·mol^{-1} and the value of *ts*[*i17-i19*] decreased by 5 kJ·mol^{-1}:
ts[*i12-i13*] := (-150 + 5) kJ·mol^{-1} = -145 kJ·mol^{-1} (reducing the contribution of p7-p8);
ts[*i17-i18*] := (-143 + 5) kJ·mol^{-1} = -138 kJ·mol^{-1} (reducing the contribution of p6);
ts[*i17-i19*] := (-144 - 5) kJ·mol^{-1} = -149 kJ·mol^{-1};

ts[*i15-p7a/7b*] := (-119 + 5) kJ·mol^{-1} = -114 kJ·mol^{-1};
ts[*i16-p8a/8b*] := (-116 + 5) kJ·mol^{-1} = -111 kJ·mol^{-1};

ts[*i11-p7a/p7b*] := (-110 + 5) kJ·mol^{-1} = -105 kJ·mol^{-1};
ts[*i11-p8a/p8b*] := (-109 + 5) kJ·mol^{-1} = -104 kJ·mol^{-1};
ts[*i13-p7a/p7b*] := (-107 + 5) kJ·mol^{-1} = -102 kJ·mol^{-1}.

	i9		*i11*	
E_C	0	43	0	43
p2	14.4	5.1	14.5	5.4
p6	3.5	1.4	3.6	1.5
p7a	24.8	20.5	25.1	21.7
p7b	37.2	41.7	37.7	44.1
p8a	11.2	11.5	11.4	12.2
p8b	3.3	4.5	3.3	4.7
p9a	2.2	4.8	2.3	5.0
p9b	0.3	0.7	0.3	0.7

Table S8. Statistical branching ratios (%) for the reaction of 1,3-pentadiene + propynyl with *i1*, *i3*, *i18*, and *i20* as initial intermediates at different collision energies (E_C, kJ·mol^{-1})

	i20		*i22*		*i24*		*i26*	
E_C	0	43	0	43	0	43	0	43
p10a	19.0	18.2	19.0	18.4	17.5	13.2	17.9	14.1
p11a	66.7	63.4	66.8	64.4	49.6	36.7	50.6	39.1
p10b	6.0	7.2	6.1	7.3	10.6	10.1	10.9	10.7
p11b	6.0	7.7	6.0	7.8	8.6	7.8	8.7	8.3
p12a	0.4	0.6	0.4	0.6	0.1	0.2	0.0	0.1
p13a	0.1	0.3	0.1	0.3	0.0	0.0	0.0	0.0
p12b	0.0	0.1	0.0	0.1	0.0	0.1	0.0	0.0
p13b	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p39	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.0
p49	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p50	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p51	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p52	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0
p53	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p54	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0
p55	0.1	1.2	0.0	0.2	0.0	0.0	0.0	0.0
p56	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0
p57	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p42	0.0	0.0	0.0	0.0	0.8	0.6	0.8	0.6
p1	0.8	0.3	0.8	0.3	0.0	0.0	0.0	0.0
p44	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p45	0.3	0.1	0.3	0.2	0.2	0.1	0.2	0.1
p46	0.4	0.2	0.4	0.2	0.0	0.0	0.0	0.0
p3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p48	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p43	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p58	0.0	0.0	0.0	0.0	4.1	9.1	3.0	6.9
p59	0.0	0.0	0.0	0.0	3.7	8.2	3.7	8.7
p60	0.0	0.0	0.0	0.0	1.3	3.0	1.3	3.2
p61	0.0	0.0	0.0	0.0	0.6	1.5	0.6	1.6
p62	0.0	0.0	0.0	0.0	1.8	5.7	1.0	3.1
p63	0.0	0.0	0.0	0.0	0.3	1.1	0.3	1.2
p64	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
p65	0.0	0.0	0.0	0.0	0.1	0.3	0.1	0.3
p66	0.0	0.0	0.0	0.0	0.2	0.6	0.2	0.6
p67	0.0	0.0	0.0	0.0	0.1	0.4	0.1	0.4
p68	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
p69	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p70	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p71	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p72	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p73	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p74	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p75	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p76	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p76'	0.0	0.0	0.0	0.0	0.1	0.7	0.0	0.3
p77	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p78	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p79	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p80	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

p81	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p82	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.1
p83	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p84	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0
p85	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p86	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p87	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p88	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p89	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p90	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p91	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p92	0.0	0.0	0.0	0.0	0.3	0.2	0.3	0.2
p93	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
p94	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S9. RRKM calculated rate constants ($k(E)$, s^{-1}) of the reaction of 2-methyl-1,3-butadiene + propynyl as functions of the internal energy (E, kJ mol^{-1}) of the intermediate states for unimolecular reaction steps at different collision energies (E_C, kJ mol^{-1})

E_C	0		43		E_C	0		43	
Reaction step	$k(E)$	E	$k(E)$	E	Reaction step	$k(E)$	E	$k(E)$	E
i4 – p23'	3.89E-01	273	1.62E+02	316	*i8 – p3*	6.02E+07	463	2.44E+08	506
i4 – p4b	3.26E+03	273	6.22E+04	316	*i33 – p45*	2.44E+09	394	7.19E+09	437
i11 – p36	1.38E-02	281	1.05E+01	324	*i33 – p48*	3.26E+07	394	1.16E+08	437
i11 – p7a	8.99E+04	281	1.18E+06	324	*i35 – p44*	2.19E+09	402	5.85E+09	445
i3 – p23'	7.10E-01	273	2.20E+02	316	*i35 – p46*	1.10E+08	402	3.38E+08	445
i3 – p1	2.24E+04	273	3.03E+05	316	*i36 – p45*	3.41E+08	430	1.07E+09	473
i2 – i1	5.89E+11	177	1.10E+12	220	*i36 – p3*	1.68E+07	430	6.28E+07	473
i1 – i2	7.02E+08	217	1.99E+09	260	*i30 – p46*	2.22E+09	364	5.75E+09	407
i12 – p7b	3.88E+04	278	6.83E+05	321	*i31 – p48*	1.35E+08	409	4.74E+08	452
i2 – p21	5.72E-01	177	3.24E+03	220	*i1 – i69*	3.93E+06	217	3.33E+07	260
i3 – i2	7.03E+06	273	2.31E+07	316	*i69 – i1*	7.71E+02	320	1.58E+04	363
i2 – i3	6.74E+12	177	8.58E+12	220	*i12 – i13*	1.15E+07	278	4.96E+07	321
i9 – p39	1.84E+05	206	5.92E+06	249	*i13 – i12*	3.15E+05	317	1.76E+06	360
i9 – p38	2.47E+07	206	2.62E+08	249	*i12 – p9a*	4.17E+04	278	9.60E+05	321
i2 – p22	3.40E-01	177	2.62E+03	220	*i19 – i39*	5.26E+02	458	3.92E+03	501
i10 – p41	3.94E-02	179	8.87E+02	222	*i39 – i19*	6.52E+03	439	4.58E+04	482
i1 – p14	2.80E+05	217	4.05E+06	260	*i37 – i39*	1.28E+08	353	3.33E+08	396
i1 – p16	4.83E+05	217	8.22E+06	260	*i39 – i37*	8.05E+05	439	3.12E+06	482
i1 – p15	1.15E+05	217	2.38E+06	260	*i11 – p30*	5.31E+03	281	1.80E+05	324
i10 – p40	4.67E-01	179	2.06E+03	222	*i1 – i68*	6.03E+09	217	1.18E+10	260
i11 – i10	1.63E+07	281	5.62E+07	324	*i68 – i1*	8.05E+10	210	1.49E+11	253
i10 – i11	5.15E+12	179	6.42E+12	222	*i13 – p7b*	6.08E+04	317	1.16E+06	360
i11 – i12	3.16E+10	281	5.45E+10	324	*i13 – p29*	5.58E+01	317	5.71E+03	360
i12 – i11	4.29E+10	278	7.27E+10	321	*i69 – p15*	1.20E+04	320	2.65E+05	363
i4 – i3	1.68E+09	273	2.79E+09	316	*i68 – p20*	1.05E+01	210	1.12E+04	253
i3 – i4	3.23E+09	273	5.40E+09	316	*i39 – p6*	6.66E+07	439	2.58E+08	482
i4 – i6	2.12E+06	273	5.36E+06	316	*i39 – p28*	3.55E+07	439	1.36E+08	482
i6 – i4	9.44E+07	320	3.61E+08	363	*i13 – i14*	5.45E+10	317	7.46E+10	360
i6 – i8	1.02E+06	320	5.66E+06	363	*i14 – i13*	6.44E+10	307	8.28E+10	350
i8 – i6	5.48E+01	463	5.89E+02	506	*i14 – i16*	1.57E+10	307	2.60E+10	350
i6 – i7	1.05E+06	320	6.03E+06	363	*i16 – i14*	8.89E+09	314	1.54E+10	357
i7 – i6	4.50E+02	406	3.99E+03	449	*i69 – p18*	3.08E+01	320	1.59E+03	363
i10 – i9	3.74E+11	179	7.03E+11	222	*i69 – p19*	1.60E+00	320	1.58E+02	363
i9 – i10	2.09E+09	206	5.13E+09	249	*i13 – p33*	1.57E+01	317	1.09E+03	360
i12 – i17	3.17E+07	278	8.06E+07	321	*i4 – p5b*	2.08E+03	273	4.41E+04	316

Reaction step	k(E)	E	k(E)	E	Reaction step	k(E)	E	k(E)	E
i17 – i12	1.87E+08	320	6.79E+08	363	i3 – p23	2.13E-01	273	7.29E+01	316
i17 – i18	8.07E+05	320	4.61E+06	363	i3 – p5a	2.03E+03	273	3.55E+04	316
i18 – i17	4.01E+02	406	3.52E+03	449	i11 – p37	9.99E-03	281	9.11E+00	324
i17 – i19	8.09E+05	320	4.81E+06	363	i12 – p8b	2.07E+04	278	4.25E+05	321
i19 – i17	1.77E+01	458	2.00E+02	501	i12 – p9b	5.32E+03	278	1.37E+05	321
i7 – p3	3.10E+07	406	1.07E+08	449	i14 – p8b	1.70E+03	307	3.57E+04	350
i8 – p1	7.85E+10	463	1.39E+11	506	i14 – p35	7.80E-01	307	9.07E+01	350
i18 – p6	3.47E+07	406	1.23E+08	449	i15 – p29	8.25E-01	316	1.15E+02	359
i19 – p2	8.58E+10	458	1.52E+11	501	i15 – p32	4.11E+01	316	2.62E+03	359
i8 – i32	3.79E+06	463	1.15E+07	506	i15 – p7a	3.34E+04	316	4.59E+05	359
i32 – i8	1.48E+07	446	4.23E+07	489	i11 – p31	1.60E+03	281	5.97E+04	324
i18 – i37	1.30E+06	406	4.49E+06	449	i11 – p8a	1.29E+05	281	1.73E+06	324
i37 – i18	1.13E+08	353	3.05E+08	396	i13 – i15	1.06E+10	317	1.87E+10	360
i19 – i38	2.13E+06	458	6.43E+06	501	i15 – i13	1.05E+10	316	1.86E+10	359
i38 – i19	5.32E+06	446	1.54E+07	489	i15 – i16	4.35E+10	316	6.26E+10	359
i7 – i30	1.18E+06	406	4.35E+06	449	i16 – i15	2.92E+10	314	4.13E+10	357
i30 – i7	4.09E+07	364	1.25E+08	407	i69 – p17	1.59E+02	320	1.28E+04	363
i7 – i31	1.03E+07	406	3.03E+07	449	i69 – p14	2.44E+04	320	4.09E+05	363
i31 – i7	3.67E+07	409	1.10E+08	452	i16 – p8a	7.57E+03	314	1.08E+05	357
i38 – p42	6.22E+10	446	9.92E+10	489	i16 – p34	4.12E+00	314	4.95E+02	357
i38 – p2	6.87E+09	446	1.21E+10	489	i4 – i5	2.52E+06	273	1.06E+07	316
i37 – p45	4.66E+09	353	1.23E+10	396	i5 – i4	3.80E+05	321	2.28E+06	364
i37 – p6	1.78E+08	353	5.39E+08	396	i5 – p24	1.76E+01	321	1.13E+03	364
i32 – p42	3.02E+11	446	4.82E+11	489	i5 – p4b	3.22E+04	321	6.46E+05	364
i32 – p1	3.05E+10	446	5.37E+10	489	i5 – p4a	4.35E+04	321	6.48E+05	364
i30 – i36	6.10E+07	364	1.61E+08	407	i5 – p25	2.23E+00	321	2.17E+02	364
i36 – i30	3.26E+06	430	1.16E+07	473	i5 – p5a	1.16E+04	321	2.08E+05	364
i30 – p3	1.27E+09	364	3.82E+09	407	i5 – p5b	1.73E+04	321	3.77E+05	364
i30 – i35	2.62E+07	364	7.61E+07	407	i5 – p26	9.14E-02	321	3.00E+01	364
i35 – i30	7.52E+06	402	2.61E+07	445	i38 – p27	1.02E+07	446	3.76E+07	489
i31 – i33	1.14E+07	409	3.55E+07	452	i37 – p27	6.15E+08	353	1.73E+09	396
i33 – i31	3.12E+07	394	9.08E+07	437	i34 – p1	1.59E+10	457	2.80E+10	500
i31 – p3	1.02E+08	409	3.52E+08	452	i34 – i32	3.32E+06	457	1.00E+07	500
i19 – p6	1.18E+07	458	4.91E+07	501	i32 – i34	2.40E+07	446	6.95E+07	489
i30 – p43	1.59E+08	364	5.47E+08	407	i34 – p48	2.32E+07	457	9.49E+07	500
i31 – p43	3.53E+07	409	1.44E+08	452	i34 – p46	6.91E+07	457	2.39E+08	500

Table S10. RRKM calculated rate constants ($k(E)$, s^{-1}) of the reaction of 1,3-pentadiene+propynyl as functions of the internal energy (E, kJ mol^{-1}) of the intermediate states for unimolecular reaction steps at different collision energies (E_C, kJ mol^{-1})

E_C	0		43		E_C	0		43	
Reaction step	k(E)	E	k(E)	E	Reaction step	k(E)	E	k(E)	E
i55 – i27	8.48E+08	308	2.98E+09	351	i40 – p39	1.38E+05	268	3.05E+06	311
i27 – i55	7.09E+06	276	1.82E+07	319	i33 – i43	6.87E+05	395	3.32E+06	438
i55 – i56	1.13E+06	308	6.84E+06	351	i43 – i33	2.15E+07	328	7.27E+07	371
i56 – i55	7.70E+02	395	7.32E+03	438	i43 – i31	6.05E+07	328	1.81E+08	371
i55 – i57	1.93E+06	308	1.15E+07	351	i31 – i43	7.09E+05	410	3.23E+06	453
i57 – i55	4.53E+01	449	5.32E+02	492	i64 – p93	3.48E+07	345	1.17E+08	388

i57 – p42	1.96E+11	449	3.10E+11	492	i64 – i66	2.46E+07	345	8.23E+07	388
i57 – p89	1.07E+10	449	1.87E+10	492	i66 – i64	4.63E+05	407	2.10E+06	450
i56 – p92	4.13E+07	395	1.53E+08	438	i62 – i65	4.04E+07	329	1.27E+08	372
i56 – i60	3.05E+07	395	9.68E+07	438	i65 – i62	3.19E+05	402	1.46E+06	445
i60 – i56	3.30E+07	399	1.07E+08	442	i61 – i59	1.20E+07	453	3.65E+07	496
i56 – i63	2.69E+06	395	1.06E+07	438	i59 – i61	1.46E+07	452	4.46E+07	495
i63 – i56	2.86E+07	354	9.22E+07	397	i23 – p13b	1.16E+03	265	3.17E+04	308
i60 – i62	5.91E+05	399	2.68E+06	442	i23 – p10b	1.91E+06	265	1.92E+07	308
i62 – i60	1.61E+07	329	5.01E+07	372	i22 – p10a	7.09E+06	274	6.17E+07	317
i56 – i59	3.76E+04	395	2.08E+05	438	i22 – p13a	5.14E+04	274	8.93E+05	317
i59 – i56	6.71E+02	452	4.69E+03	495	i22 – i40	4.70E+04	274	5.04E+05	317
i57 – i58	6.08E+05	449	2.47E+06	492	i40 – i22	1.63E+04	268	1.68E+05	311
i58 – i57	7.16E+07	347	1.80E+08	390	i50 – i54	4.04E+05	205	4.52E+06	248
i41 – i33	9.35E+05	310	5.72E+06	353	i54 – i50	8.06E+01	311	2.32E+03	354
i33 – i41	7.01E+02	395	6.69E+03	438	i50 – p85	7.34E+03	205	1.77E+05	248
i41 – i23	2.39E+08	310	9.29E+08	353	i26 – p59	3.81E+04	280	5.62E+05	323
i23 – i41	2.65E+07	265	6.82E+07	308	i26 – i47	1.15E+10	280	2.04E+10	323
i41 – i44	1.49E+06	310	8.38E+06	353	i47 – i26	7.24E+10	276	1.25E+11	319
i44 – i41	1.57E+01	458	1.77E+02	501	i27 – p63	6.37E+03	276	1.35E+05	319
i41 – i42	1.99E+06	310	1.08E+07	353	i51 – i49	1.13E+10	263	2.34E+10	306
i42 – i41	8.75E+03	344	5.62E+04	387	i49 – i51	1.15E+12	210	1.43E+12	253
i26 – i27	5.31E+09	280	9.72E+09	323	i28 – i29	4.48E+10	303	8.69E+10	346
i27 – i26	9.48E+09	276	1.69E+10	319	i29 – i28	1.06E+11	305	2.09E+11	348
i23 – i22	3.40E+10	265	5.95E+10	308	i46 – p3	6.65E+08	348	2.09E+09	391
i22 – i23	4.02E+10	274	7.58E+10	317	i46 – i8	1.15E+08	348	2.80E+08	391
i27 – p67	1.29E+03	276	4.27E+04	319	i8 – i46	3.29E+05	465	1.37E+06	508
i27 – p62	5.03E+03	276	9.98E+04	319	i43 – p43	5.34E+07	328	1.76E+08	371
i27 – i28	1.70E+06	276	8.41E+06	319	i20 – p54	2.77E+05	212	6.46E+06	255
i28 – i27	6.42E+05	303	3.90E+06	346	i20 – p53	3.14E+04	212	7.28E+05	255
i27 – p70	8.01E-04	276	1.47E+00	319	i40 – p49	5.80E+04	268	1.48E+06	311
i23 – p11b	1.88E+06	265	2.06E+07	308	i40 – p50	6.66E+00	268	1.30E+03	311
i23 – p12b	8.05E+03	265	1.70E+05	308	i53 – p82	9.31E+03	320	1.51E+05	363
i23 – p51	6.29E-04	265	2.03E+00	308	i53 – p86	1.63E+01	320	1.30E+03	363
i60 – p92	5.28E+07	399	1.93E+08	442	i53 – p88	1.51E-02	320	4.56E+00	363
i60 – p45	1.54E+09	399	4.50E+09	442	i53 – p12a	1.42E+04	320	2.07E+05	363
i60 – p91	2.36E+07	399	8.32E+07	442	i53 – i54	1.06E+10	320	1.93E+10	363
i63 – p92	2.68E+08	354	8.29E+08	397	i54 – i53	2.57E+10	311	4.42E+10	354
i63 – p44	7.35E+09	354	1.68E+10	397	i54 – p87	7.49E+00	311	7.32E+02	354
i63 – p90	2.65E+08	354	7.07E+08	397	i54 – p84	5.35E+03	311	1.28E+05	354
i59 – p89	1.41E+10	452	2.47E+10	495	i54 – p88	6.33E-02	311	1.51E+01	354
i59 – p90	4.21E+07	452	1.46E+08	495	i54 – p12b	7.28E+03	311	1.48E+05	354
i58 – p91	5.93E+07	347	1.71E+08	390	i40 – p12a	1.98E+05	268	2.36E+06	311
i44 – p1	1.57E+10	458	2.76E+10	501	i47 – p60	6.94E+04	276	1.15E+06	319
i44 – i32	3.44E+06	458	1.03E+07	501	i51 – p76'	1.21E+04	263	3.57E+05	306
i32 – i44	1.27E+07	447	3.67E+07	490	i51 – p78	1.56E+00	263	4.72E+02	306
i44 – p48	2.43E+07	458	9.85E+07	501	i51 – p58	2.20E+05	263	2.85E+06	306

i44 – p46	7.19E+07	458	2.47E+08	501	i47 – p68	1.01E+03	276	4.05E+04	319
i42 – p46	2.69E+08	344	6.99E+08	387	i47 – p71	6.29E-03	276	1.10E+01	319
i26 – p58	2.30E+04	280	3.28E+05	323	i47 – p61	3.91E+04	276	6.45E+05	319
i26 – p66	1.58E+03	280	3.96E+04	323	i29 – p10a	5.75E+06	305	5.26E+07	348
i26 – p71	7.43E-05	280	2.39E-01	323	i29 – p72	7.39E+00	305	7.86E+02	348
i57 – p92	1.37E+07	449	5.80E+07	492	i29 – p74	9.01E-03	305	8.60E+00	348
i57 – i61	9.73E+06	449	2.85E+07	492	i49 – p77	6.88E+02	210	4.71E+04	253
i61 – i57	2.07E+06	453	6.09E+06	496	i49 – p79	1.73E-04	210	3.68E+00	253
i60 – i65	3.07E+07	399	8.86E+07	442	i49 – i50	1.72E+10	210	3.30E+10	253
i65 – i60	6.59E+06	402	1.91E+07	445	i50 – i49	1.83E+10	205	3.21E+10	248
i63 – i66	8.10E+07	354	2.26E+08	397	i29 – p60	6.56E+04	305	1.14E+06	348
i66 – i63	1.91E+06	407	6.91E+06	450	i47 – i48	2.88E+10	276	5.04E+10	319
i22 – p12a	1.23E+05	274	1.80E+06	317	i48 – i47	2.21E+10	265	3.54E+10	308
i22 – p51	1.45E-03	274	3.43E+00	317	i50 – i52	7.26E+08	205	2.17E+09	248
i22 – p11a	2.49E+07	274	2.15E+08	317	i52 – i50	3.00E+11	170	6.09E+11	213
i25 – i24	7.76E+11	174	1.48E+12	217	i27 – i48	2.23E+10	276	3.89E+10	319
i24 – i25	3.79E+09	208	1.04E+10	251	i48 – i27	6.05E+10	265	9.65E+10	308
i25 – i26	4.64E+12	174	5.88E+12	217	i50 – p76	2.21E+04	205	7.67E+05	248
i26 – i25	3.31E+06	280	1.22E+07	323	i47 – i52	2.01E+07	276	7.59E+07	319
i21 – i1	8.99E+11	175	1.71E+12	218	i52 – i47	3.84E+12	170	4.87E+12	213
i20 – i21	1.16E+09	212	3.32E+09	255	i52 – p81	5.82E-03	170	5.57E+02	213
i22 – i21	1.03E+08	274	3.47E+08	317	i48 – p69	2.10E+02	265	1.03E+04	308
i21 – i22	5.72E+12	175	7.05E+12	218	i48 – p65	3.06E+03	265	7.62E+04	308
i25 – p80	1.15E-01	174	1.66E+03	217	i48 – p64	1.43E+03	265	3.36E+04	308
i21 – p57	1.73E-01	175	1.77E+03	218	i42 – i30	7.15E+06	344	2.44E+07	387
i63 – i64	4.64E+06	354	1.95E+07	397	i30 – i42	1.30E+07	366	5.07E+07	409
i64 – i63	5.84E+06	345	2.33E+07	388	i42 – i45	6.33E+06	344	2.13E+07	387
i44 – i42	3.92E+05	458	1.60E+06	501	i45 – i42	3.15E+06	366	1.20E+07	409
i42 – i44	1.64E+08	344	3.94E+08	387	i45 – p48	3.17E+08	366	9.47E+08	409
i61 – p89	1.00E+10	453	1.74E+10	496	i45 – p46	1.03E+09	366	2.73E+09	409
i61 – p91	1.25E+07	453	4.99E+07	496	i45 – i33	7.23E+06	366	2.30E+07	409
i58 – i61	1.16E+08	347	2.86E+08	390	i33 – i45	2.48E+06	395	9.15E+06	438
i61 – i58	2.09E+05	453	8.41E+05	496	i51 – p62	1.57E+05	263	2.98E+06	306
i65 – p94	3.88E+06	402	1.85E+07	445	i28 – p11b	1.18E+06	303	1.29E+07	346
i65 – p91	4.42E+07	402	1.53E+08	445	i29 – p11a	1.62E+07	305	1.46E+08	348
i66 – p93	2.53E+07	407	9.59E+07	450	i8 – p1	7.95E+10	465	1.40E+11	508
i66 – p90	1.56E+08	407	4.76E+08	450	i8 – i32	4.03E+06	465	1.22E+07	508
i62 – p94	8.68E+06	329	3.63E+07	372	i32 – i8	1.57E+07	447	4.47E+07	490
i24 – p83	1.47E+05	208	3.21E+06	251	i32 – p42	3.14E+11	447	5.00E+11	490
i24 – i53	3.81E+06	208	3.16E+07	251	i32 – p1	3.19E+10	447	5.60E+10	490
i53 – i24	1.33E+02	320	2.93E+03	363	i30 – p3	1.32E+09	366	3.93E+09	409
i24 – p76'	4.80E+05	208	1.48E+07	251	i30 – i35	2.71E+07	366	7.83E+07	409
i24 – i49	1.43E+11	208	2.48E+11	251	i35 – i30	8.06E+06	403	2.78E+07	446
i49 – i24	5.75E+10	210	1.05E+11	253	i31 – i33	1.18E+07	410	3.66E+07	453
i26 – i51	3.69E+04	280	4.29E+05	323	i33 – i31	3.23E+07	395	9.34E+07	438
i51 – i26	9.92E+05	263	1.02E+07	306	i31 – p3	1.01E+08	410	3.51E+08	453

i20 – p56	5.87E+04	212	3.00E+06	255	i30 – p43	1.65E+08	366	5.65E+08	409
i20 – p52	2.87E+05	212	5.15E+06	255	i31 – p43	3.69E+07	410	1.49E+08	453
i20 – p55	1.07E+06	212	2.71E+07	255	i8 – p3	6.20E+07	465	2.50E+08	508
i28 – p62	2.79E+04	303	6.28E+05	346	i33 – p45	2.52E+09	395	7.40E+09	438
i28 – p10b	1.47E+06	303	1.66E+07	346	i33 – p48	3.40E+07	395	1.20E+08	438
i28 – p75	1.73E-02	303	1.36E+01	346	i35 – p44	2.33E+09	403	6.17E+09	446
i28 – p73	3.91E+00	303	5.28E+02	346	i35 – p46	1.18E+08	403	3.58E+08	446
i32 – i46	2.90E+05	447	1.20E+06	490	i30 – p46	2.29E+09	366	5.90E+09	409
i46 – i32	2.59E+07	348	6.71E+07	391	i31 – p48	1.35E+08	410	4.72E+08	453

Table S11. Natural charge analysis of 1,3-pentadiene
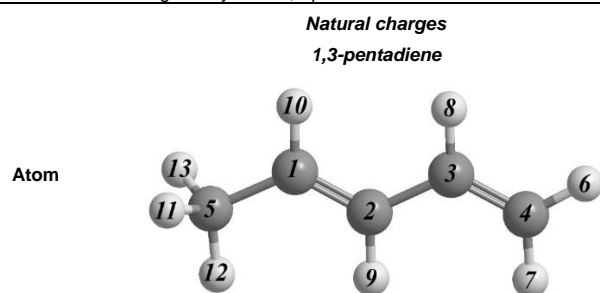
Natural charges
1,3-pentadiene

Atom

	Natural charges
C1	-0.14496
C2	-0.23605
C3	-0.20426
C4	-0.36267
C5	-0.60189
H6	0.18865
H7	0.18054
H8	0.19192
H9	0.19093
H10	0.18309
H11	0.20723
H12	0.20023
H13	0.20724
Total	0

Table S12. Calculated lifetimes for the different initial complecxes in the reaction of the 1-propynyl radical with 2-methyl-1,3-butadiene and 1,3-pentadiene

1-propynyl + 2-methyl-1,3-butadiene				
Initial complex	i1	i3	i9	i11
Lifetime, ns	0.72	98.94	0.253	41.08
1-propynyl + 1,3-pentadiene				
Initial complex	i20	i22	i24	i26
Lifetime, ns	0.46	3.05	0.11	160.59

SUPPORTING INFORMATION

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Author Contributions

R.I.K designed experiments. I.A.M, C.H. and Z.H.Y. performed experiments. A.M.M. and A.A.N. carried out the theoretical calculations. I.A.M, A.M.M. and R.I.K. wrote the manuscript, which was read, revised, and approved by all co-authors.

SUPPORTING INFORMATION

Appendix

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) for all intermediates, transition states, reactants, and products involved in the 2-methyl-1,3-butadiene + 1-propynyl reactions at the ωB97P-D/6-311G(d,p) level.

Reactants
(trans-)2-methyl-1,3-butadiene

C	1.973854	0.006578	0.000167
C	0.833035	-0.680452	-0.000194
H	2.931617	-0.500421	0.000144
H	1.996166	1.091273	0.000490
H	0.874839	-1.767502	-0.000613
C	-0.517629	-0.100332	-0.000109
C	-1.583514	-0.904863	0.000160
C	-0.653664	1.397459	-0.000078
H	-2.593738	-0.510187	0.000344
H	-1.474113	-1.984540	0.000162
H	-1.702903	1.695636	-0.000034
H	-0.172206	1.832714	-0.881248
H	-0.172155	1.832679	0.881081

Frequencies

137.3939	225.5480	297.6232
401.6022	437.5583	541.3986
639.7032	785.0651	801.3264
928.0969	943.5573	972.6251
1015.7076	1028.9680	1076.1723
1094.4048	1327.0370	1340.6146
1418.9358	1443.5148	1464.2737
1488.5355	1511.4583	1691.9826
1743.8405	3047.6580	3110.6408
3139.9049	3154.9701	3160.7078
3172.2382	3243.8763	3253.1487

(trans-)1,3-pentadiene

C	-2.517576	-0.260302	0.000007
C	-1.358229	0.395795	-0.000002
C	-0.049303	-0.246709	-0.000014
C	1.107341	0.417464	0.000001
C	2.462545	-0.214923	0.000005
H	-3.466470	0.262808	0.000021
H	-2.552191	-1.345860	0.000002
H	-1.361331	1.484318	-0.000015
H	-0.039804	-1.336165	-0.000017
H	1.080386	1.506611	0.000000
H	3.038178	0.092906	-0.879154
H	2.394546	-1.305140	-0.000204
H	3.038016	0.092576	0.879387

Frequencies

116.2996	190.2383	201.0248
244.1542	461.6287	488.6761
642.4576	849.5210	915.9246
936.5777	984.1635	995.3123
1043.7708	1067.1296	1108.0483
1212.0422	1294.8272	1324.2103
1340.3223	1416.0599	1455.8048
1478.9669	1493.9892	1700.8253
1765.1114	3034.3836	3092.1631
3126.5166	3148.6404	3151.9411
3155.3764	3164.9185	3248.3316

1-propynyl

C	-1.123766	0.000034	0.000188
C	0.336608	-0.000571	-0.000814
C	1.540300	0.000283	0.000377
H	-1.504993	0.615339	0.817821
H	-1.506845	-1.015014	0.124083
H	-1.507018	0.401203	-0.940410

Frequencies

200.1523	203.0213	952.8370
1014.5159	1022.1101	1413.0112
1478.5078	1483.7864	2276.0322
3059.2654	3134.4920	3139.5728

i1

C	-0.758962	1.919431	0.528457
C	-0.470348	0.764220	-0.383565
C	3.443950	-0.506816	-0.076342

```
C    2.061473   -0.054842   -0.186553
C    0.923441    0.315894   -0.280545
H   -0.050724    2.229783    1.284912
H   -1.726791    2.402361    0.466747
H   -0.642545    1.090388   -1.418866
H    3.712467   -0.683052    0.968230
H    4.131770    0.239729   -0.480999
H    3.593420   -1.439289   -0.626079
C   -1.450322   -0.386128   -0.121123
C   -2.368113   -0.710128   -1.025169
C   -1.323283   -1.075225    1.206641
H   -3.085634   -1.502851   -0.840598
H   -2.433938   -0.197735   -1.979561
H   -2.081776   -1.850640    1.324358
H   -1.428916   -0.354837    2.024213
H   -0.334347   -1.532287    1.306845
```

Frequencies

62.3355	88.5296	92.1546
137.8212	142.456	205.6978
236.3967	270.7907	304.73
394.8174	415.386	472.4497
509.0041	553.334	595.6581
730.2493	772.9026	830.3167
945.1615	973.9402	999.4444
1036.496	1059.139	1063.052
1082.99	1103.893	1179.987
1225.601	1296.75	1338.724
1415.638	1422.269	1450.894
1454.301	1485.637	1487.446
1491.202	1502.671	1744.314
2395.098	3013.603	3043.021
3051.577	3106.876	3122.456
3126.419	3137.852	3149.524
3163.2	3234.671	3285.266

i2
```
C    0.088957    1.885199   -0.037697
C   -0.406246    0.606225   -0.711628
C   -1.424872   -0.285063   -0.097534
C   -2.191137   -1.056100   -0.868731
C   -1.541801   -0.291742    1.402058
C    2.699793   -1.212955    0.013574
C    2.069129    0.105319    0.178716
C    0.973101    0.716611   -0.101416
H    0.304150    2.728003   -0.686831
H   -0.328346    2.150729    0.928573
H   -0.427765    0.637895   -1.797523
H   -2.928126   -1.727845   -0.442200
H   -2.104781   -1.039016   -1.950252
H   -2.210677   -1.085077    1.737670
H   -1.940025    0.660563    1.766914
H   -0.563784   -0.436448    1.870716
H    3.645139   -1.133564   -0.530214
H    2.038569   -1.889785   -0.544397
H    2.914100   -1.670415    0.983494
```

Frequencies

58.4259	79.1364	124.3839
170.9379	201.1269	228.5389
287.535	374.9556	410.005
463.8513	504.2346	552.2834
661.928	743.7214	767.5677
839.4418	904.5862	921.5697
950.4005	1007.409	1031.067

1050.219	1053.467	1061.528
1073.628	1079.342	1099.312
1197.437	1312.846	1353.614
1405.234	1421.246	1451.091
1465.563	1467.507	1482.908
1489.013	1508.134	1726.935
1886.968	3009.831	3042.865
3091.378	3103.092	3115.52
3129.884	3145.227	3150.71
3159.909	3217.702	3237.922

i3
```
C   -0.219178   -0.762535   -0.036247
C    0.731217    0.402709   -0.025376
C    2.117916    0.263898    0.002133
C    2.938576    1.372302    0.005577
C    2.723617   -1.120735    0.029126
C   -4.179704    0.372905    0.024794
C   -2.778365   -0.031910    0.003118
C   -1.626492   -0.368365   -0.014276
H   -0.019313   -1.420339    0.821313
H   -0.038195   -1.387851   -0.922535
H    0.301456    1.398346   -0.045293
H    4.017653    1.277140    0.026709
H    2.522138    2.373181   -0.012599
H    3.813317   -1.075450    0.035535
H    2.414825   -1.704340   -0.843616
H    2.403630   -1.674061    0.917542
H   -4.789725   -0.304072   -0.578413
H   -4.298710    1.382469   -0.376245
H   -4.572598    0.365363    1.044509
```

Frequencies

12.139	41.6526	79.8575
139.3793	185.2888	198.3576
212.7249	290.6685	385.4865
411.5126	481.5263	502.1147
526.9928	573.2427	683.2899
787.9445	794.249	868.9236
913.437	985.5128	1020.547
1058.107	1058.839	1059.573
1127.11	1178.138	1225.088
1260.597	1333.477	1387.695
1420.329	1429.583	1448.205
1467.36	1486.253	1486.785
1493.111	1502.873	1531.551
2399.148	2999.624	3022.179
3042.057	3047.231	3103.054
3119.929	3120.512	3138.996
3153.643	3191.85	3251.341

i4
```
C   -0.265501   -0.850225    0.000735
C    0.733365    0.273520    0.000466
C   -4.171476    0.462940   -0.000520
C   -2.789305   -0.003780    0.000062
C   -1.653809   -0.392444    0.000367
C    2.118721    0.084124   -0.000158
C    2.693760   -1.164429   -0.000707
C    2.994662    1.318918   -0.000025
H   -0.101461   -1.495439    0.874883
H   -0.101243   -1.496067   -0.872897
```

```
H     0.339603    1.284581    0.000941
H    -4.721509    0.051577   -0.850547
H    -4.213403    1.552948   -0.066749
H    -4.686020    0.160047    0.914785
H     3.770639   -1.284059   -0.001217
H     2.099378   -2.070523   -0.000651
H     4.053672    1.055588   -0.002354
H     2.800558    1.933510    0.883204
H     2.797293    1.936090   -0.880716
```

Frequencies

24.205	32.646	42.3382
78.7787	175.5922	206.176
220.5036	293.1935	387.4386
389.6971	481.7588	510.4465
522.4042	577.8029	660.653
780.5432	807.899	900.8756
919.9465	992.1853	1038.82
1059.231	1059.351	1063.149
1112.119	1177.749	1228.634
1253.806	1326.265	1363.637
1416.235	1420.52	1456.891
1483.927	1486.116	1486.893
1491.881	1501.836	1556.408
2399.125	3006.371	3030.671
3047.133	3047.542	3114.581
3119.534	3120.358	3136.001
3159.799	3187.785	3251.928

i5

```
C     0.329285    0.627281    0.000849
C    -0.687063   -0.343321   -0.004445
C     4.286488   -0.306164    0.000848
C     2.868733    0.026023   -0.000469
C     1.688503    0.299665    0.000001
C    -2.040505   -0.123961   -0.005738
C    -2.671484    1.235909   -0.000406
C    -2.999832   -1.276395    0.003105
H    -1.956333    2.045428   -0.143530
H     0.079879    1.683208    0.009222
H    -0.353169   -1.378565   -0.004941
H     4.894092    0.582361   -0.188027
H     4.515625   -1.044883   -0.772123
H     4.589683   -0.725096    0.964807
H    -3.426405    1.308884   -0.790994
H    -3.192478    1.410523    0.948764
H    -3.676001   -1.215360    0.864571
H    -2.485205   -2.238082    0.041366
H    -3.634434   -1.262640   -0.891588
```

Frequencies

57.3121	71.9314	80.3252
111.3967	123.5204	216.7447
229.7661	234.1674	299.5739
382.6394	398.1878	462.5146
492.2241	534.585	735.5088
807.3223	865.337	909.3535
974.8465	1003.23	1041.486
1051.397	1064.58	1080.627
1169.666	1217.376	1235.474
1340.088	1409.761	1420.206
1422.703	1447.866	1471.824

1478.947	1484.302	1486.372
1491.745	1494.175	1558.185
2264.95	3019.955	3031.926
3044.45	3070.462	3083.061
3111.184	3121.671	3134.908
3150.784	3161.347	3186.731

i6
```
C    2.446259  -1.143968  -0.000021
C    1.213355  -0.284680   0.000003
C   -0.093187  -1.039504   0.000041
C   -1.331142  -0.158987  -0.000018
C   -1.164459   1.141704  -0.000034
C    0.067557   1.954922   0.000019
C    1.276773   1.044551  -0.000004
C   -2.661569  -0.858317  -0.000016
H    2.464266  -1.796721  -0.879841
H    2.464263  -1.796759   0.879772
H    3.358361  -0.544343  -0.000004
H   -0.124628  -1.708413   0.872935
H   -0.124621  -1.708540  -0.872750
H    0.098039   2.615576  -0.875648
H    0.098012   2.615506   0.875739
H    2.247438   1.534984  -0.000025
H   -3.484581  -0.143201  -0.000309
H   -2.759159  -1.500949   0.881802
H   -2.758918  -1.501466  -0.881486
```

Frequencies

83.4124	121.4427	151.0743
230.2841	260.2654	262.2348
387.2731	421.2414	465.8643
466.4409	501.5996	698.321
790.8007	848.0587	904.7779
919.3005	931.2447	976.4261
995.1383	1044.843	1070.286
1082.697	1114.454	1173.947
1210.389	1215.058	1235.592
1314.164	1352.909	1403.657
1410.734	1422.706	1466.929
1472.437	1482.859	1485.687
1487.987	1490.797	1767.075
1801.882	3000.338	3023.106
3026.017	3030.247	3036.317
3050.544	3087.34	3093.454
3129.47	3149.598	3167.889

i7
```
C    2.556578  -0.907326   0.000016
C    1.232313  -0.198815  -0.000017
C    0.023567  -1.096718   0.000008
C   -1.316890  -0.388964   0.000016
C   -1.368109   0.991825   0.000012
C   -0.166352   1.875960  -0.000002
C    1.132364   1.126771  -0.000030
C   -2.470638  -1.157830  -0.000003
H    2.651763  -1.553530  -0.879759
H    2.651976  -1.552999   0.880158
H    3.390350  -0.202788  -0.000282
H    0.077003  -1.762202   0.871862
H    0.076981  -1.762237  -0.871818
H   -0.203366   2.549306  -0.869400
H   -0.203330   2.549312   0.869391
H    2.039082   1.726910  -0.000051
H   -2.342062   1.473165   0.000002
H   -3.449940  -0.693278   0.000205
```

H   -2.425451   -2.241071   -0.000302

Frequencies

35.6033	131.2169	194.9589
251.4234	290.3053	413.7416
417.4993	482.0156	482.4788
505.1915	520.2974	706.5145
712.9466	753.4632	815.7129
876.7537	917.6087	924.2151
959.1972	966.0118	1003.715
1062.272	1072.615	1111.714
1167.855	1217.41	1253.425
1256.529	1318.008	1387.098
1391.695	1418.267	1438.983
1460.286	1467.118	1484.861
1489.493	1490.692	1527.866
1787.558	2998.586	3011.166
3020.967	3034.069	3046.575
3090.07	3136.515	3158.248
3158.712	3180.361	3256.985

i8

```
C     2.549259   -0.989396   -0.000009
C     1.268948   -0.215171   -0.000002
C     0.000001   -1.018373    0.000024
C    -1.268949   -0.215172    0.000009
C    -1.223843    1.145347    0.000009
C     0.000001    1.852482    0.000000
C     1.223844    1.145348   -0.000008
C    -2.549260   -0.989395   -0.000017
H     2.613056   -1.641975   -0.879422
H     2.612986   -1.642107    0.879309
H     3.420073   -0.330862    0.000074
H     0.000006   -1.703959    0.867206
H     0.000002   -1.704027   -0.867101
H     0.000000    2.935517    0.000000
H    -2.155453    1.704163    0.000010
H     2.155454    1.704164   -0.000018
H    -3.420069   -0.330855    0.000160
H    -2.612956   -1.642197    0.879237
H    -2.613099   -1.641882   -0.879495
```

Frequencies

105.322	121.3122	146.1784
233.321	271.5806	308.6448
395.1505	463.7989	492.2639
514.9125	529.5915	699.5178
730.1448	864.4786	876.2869
910.5745	921.8337	943.6904
997.9289	1011.912	1041.236
1065.802	1078.291	1128.882
1170.816	1221.361	1244.254
1315.34	1337.058	1398.717
1414.088	1417.337	1444.038
1463.725	1481.334	1481.776
1482.105	1489.225	1570.73
1652.126	2940.093	2940.697
3018.134	3019.617	3069.454

3069.581	3127.566	3127.888
3175.596	3177.772	3220.278

i9

C	-2.349466	1.456940	0.074456
C	-1.357128	0.838970	-0.548699
C	-0.618890	-0.403860	-0.072285
C	-0.780118	-1.488487	-1.106961
C	-1.100878	-0.901576	1.299025
C	3.421952	0.480963	0.086931
C	1.997423	0.173089	0.035835
C	0.822355	-0.076900	-0.000199
H	-2.812883	2.335208	-0.360467
H	-2.738129	1.121898	1.029701
H	-1.002759	1.223293	-1.503043
H	-0.617658	-2.522130	-0.823742
H	-0.798254	-1.232874	-2.159815
H	-0.528783	-1.783741	1.592995
H	-2.158534	-1.172564	1.252376
H	-0.961138	-0.133140	2.062103
H	3.629661	1.239744	0.845492
H	3.773096	0.860627	-0.875848
H	4.003880	-0.411151	0.331632

Frequencies

74.2628	94.877	98.6481
119.2503	137.3561	275.4394
289.1235	303.7181	316.7995
330.2069	375.8219	464.9857
504.6145	540.4581	574.2549
648.942	731.1389	857.2406
936.5041	962.3061	977.0588
1044.306	1045.609	1054.235
1058.279	1076.676	1208.038
1222.232	1260.374	1342.169
1408.368	1415.409	1446.77
1458.054	1485.35	1489.202
1503.581	1507.71	1734.159
2377.707	3047.892	3051.646
3120.136	3120.838	3135.755
3138.576	3150.791	3153.144
3168.111	3248.123	3268.115

i10

C	2.282923	-1.420854	-0.184144
C	1.342939	-0.631353	-0.694942
C	0.617320	0.435050	0.031652
C	0.109839	1.615377	-0.802451
C	0.993434	0.698066	1.471071
C	-2.718066	-1.072077	0.295561
C	-2.023597	0.094197	-0.270159
C	-0.844923	0.600461	-0.347397
H	2.759623	-2.182486	-0.789947
H	2.611720	-1.336273	0.846166
H	1.049195	-0.762508	-1.734721
H	0.093548	2.585883	-0.315397
H	0.367205	1.639876	-1.857504
H	0.366313	1.485390	1.893569
H	2.040223	1.008973	1.548364
H	0.858444	-0.201351	2.078164
H	-3.458154	-0.766998	1.040430
H	-2.003258	-1.752067	0.778697
H	-3.244078	-1.631634	-0.482965

Frequencies

68.073	101.1221	130.958
146.5619	220.0881	238.1919

287.1907	330.6533	379.4441
449.4175	462.3179	513.3329
618.424	706.5186	754.8261
829.937	927.6966	931.3841
961.2905	983.5208	1035.68
1045.225	1049.868	1051.457
1061.184	1096.538	1127.883
1266.275	1314.308	1348.687
1400.821	1413.518	1452.189
1464.328	1468.334	1483.523
1486.451	1507.938	1719.94
1888.322	3008.385	3045.228
3090.178	3114.856	3115.69
3119.324	3139.556	3157.515
3169.661	3207.498	3250.216

i11
```
C     3.235973   -0.010889    0.892106
C     2.143759   -0.628164    0.324311
C     1.091953   -0.019262   -0.351814
C    -0.042366   -0.858219   -0.890797
C     0.980850    1.458211   -0.558268
C    -3.693774    0.241264    0.684779
C    -2.404724   -0.149402    0.124650
C    -1.345917   -0.478813   -0.335636
H     3.996660   -0.593588    1.396114
H     3.376659    1.062978    0.863189
H     2.089286   -1.711396    0.419214
H    -0.088046   -0.748843   -1.983630
H     0.142357   -1.917558   -0.689885
H     0.575893    1.679112   -1.551084
H     1.940311    1.967175   -0.460191
H     0.286444    1.896556    0.168299
H    -3.857953   -0.235445    1.654308
H    -4.510838   -0.050907    0.020401
H    -3.745288    1.323562    0.827282
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Frequencies

34.819	68.747	96.7725
111.3163	183.563	209.75
264.0643	298.345	363.769
387.0372	401.9712	459.1644
556.307	607.2626	765.8929
778.5052	790.6495	922.224
978.6712	999.7615	1033.143
1054.432	1057.976	1064.623
1167.162	1214.502	1233.966
1246.147	1334.613	1387.951
1420.624	1425.472	1460.904
1471.791	1488.162	1493.054
1495.185	1510.345	1527.466
2396.173	3012.865	3033.23
3050.697	3088.125	3090.098
3121.825	3124.658	3144.968
3147.829	3169.833	3262.73

i12
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C     3.184133   -0.943703    0.091464
```

```
C    2.498508    0.247635    0.089097
H    4.262330   -0.960729    0.188519
H    2.685908   -1.901506   -0.004627
H    3.085235    1.159585    0.179121
C    1.118457    0.413154   -0.023666
C    0.228123   -0.803759   -0.158300
C    0.500722    1.772907   -0.054925
C   -3.822871   -0.094110    0.105443
C   -2.387892   -0.339132    0.009522
C   -1.207815   -0.545575   -0.066230
H    0.436493   -1.295181   -1.119349
H    0.501531   -1.538494    0.608908
H   -0.232929    1.893421    0.749683
H   -0.047495    1.934387   -0.990879
H    1.257943    2.553150    0.041022
H   -4.083126    0.320076    1.082641
H   -4.383456   -1.022438   -0.029097
H   -4.150624    0.613221   -0.660364
```

Frequencies

26.2614	70.2711	89.8777
177.9595	198.6185	230.355
231.3176	285.8393	337.838
396.3709	397.9303	516.3181
536.9574	585.2154	770.4785
797.2951	808.9205	891.0093
974.2147	988.9393	1038.766
1057.198	1061.583	1063.775
1177.003	1231.054	1240.729
1253.808	1309.532	1386.801
1420.152	1423.988	1461.751
1467.615	1477.546	1486.431
1489.702	1508.882	1538.321
2399.24	3012.781	3028.913
3050.574	3053.527	3081.334
3125.02	3127.631	3131.575
3157.56	3167.872	3259.18

i13

```
C    3.172976   -1.027368   -0.003493
C    2.413346    0.259738   -0.002308
C    1.053749    0.430415   -0.000257
C    0.147090   -0.656708    0.003969
C    0.480235    1.827035    0.000113
C   -3.892013   -0.207821   -0.002473
C   -2.444890   -0.367340   -0.000104
C   -1.239764   -0.500860    0.002175
H    3.963177   -1.002803   -0.760345
H    3.666485   -1.187558    0.962424
H    3.023445    1.159681    0.011208
H    0.524726   -1.672680    0.013577
H    2.548882   -1.898459   -0.205396
H   -0.153293    1.986339    0.877132
H   -0.148287    1.987779   -0.880296
H    1.270650    2.579232    0.002406
H   -4.276809   -0.105497    1.016575
H   -4.378515   -1.072790   -0.460526
H   -4.184833    0.684206   -0.562494
```

Frequencies

64.5341	69.7866	86.0206
87.7087	112.8042	208.5106
242.034	248.4229	279.7677
404.3287	439.2814	472.2754
514.5803	549.3286	725.9904
773.4526	806.1686	851.1141

977.34	1042.557	1043.12
1058.236	1060.636	1065.297
1116.821	1219.266	1270.875
1324.015	1407.676	1417.135
1419.842	1426.383	1480.892
1484.602	1485.129	1486.299
1492.927	1498.07	1575.66
2255.682	3034.155	3043.212
3054.467	3090.281	3110.299
3118.54	3120.511	3138.713
3144.408	3161.255	3202.247

i14
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C     0.290475    2.020952   -0.000012
C     1.495583    1.133209    0.000011
C     1.519855   -0.237544    0.000003
C     0.387100   -1.086043   -0.000011
C     2.859440   -0.945050    0.000001
C    -3.563928   -0.137882    0.000001
C    -2.147871   -0.473942    0.000013
C    -0.961543   -0.721896    0.000004
H    -0.341621    1.844215    0.876036
H     0.588231    3.070900   -0.000174
H    -0.341775    1.843974   -0.875896
H     2.460490    1.632651    0.000034
H     0.577928   -2.156442   -0.000031
H     2.963558   -1.583989   -0.881904
H     2.963512   -1.584089    0.881839
H     3.686792   -0.233814    0.000062
H    -4.063368   -0.546429    0.883052
H    -4.062760   -0.543949   -0.884540
H    -3.705663    0.946152    0.001465
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Frequencies

38.7034	58.0788	85.7587
90.0574	120.4387	205.2971
247.2714	249.166	313.3354
355.116	440.7697	470.3567
492.08	571.1115	727.2087
756.1042	827.0024	869.5643
999.3428	1031.419	1044.242
1055.671	1064.386	1089.228
1107.07	1211.894	1238.24
1348.307	1394.642	1416.109
1418.753	1420.557	1480.333
1482.139	1484.034	1487.919
1490.743	1503.025	1581.369
2259.049	3035.691	3039.048
3043.356	3091.527	3107.074
3108.341	3114.092	3127.191
3135.611	3155.905	3167.057

i15
```
C    -3.555834    0.100486   -0.012159
C    -2.262985   -0.646031    0.003057
C    -1.007704   -0.090441    0.007534
C     0.120561   -0.941286    0.008728
C    -0.816172    1.407873    0.008976
C     4.006380    0.251784   -0.009528
C     2.611779   -0.166754   -0.001300
C     1.450843   -0.515407    0.005262
H    -4.080689   -0.047513   -0.964094
```

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H    -4.227146   -0.263875    0.772740
H    -3.422218    1.173890    0.129655
H    -2.334075   -1.731338   -0.005372
H    -0.051951   -2.014001    0.009759
H     0.242729    1.665641   -0.004413
H    -1.262779    1.859064    0.899444
H    -1.287914    1.864503   -0.865295
H     4.622987   -0.459202   -0.565677
H     4.403589    0.318117    1.007702
H     4.116259    1.233371   -0.477875
```

Frequencies

59.5974	64.5798	85.6599
89.2758	122.8289	192.8774
247.0468	268.7597	294.1518
386.5907	443.7115	448.1226
478.1843	608.9243	719.4954
792.9951	816.0392	837.0154
961.9144	1035.093	1045.125
1054.221	1057.417	1062.054
1125.472	1213.93	1240.324
1384.898	1414.034	1420.235
1426.165	1439.295	1477.153
1481.874	1485.725	1487.232
1503.867	1505.785	1551.549
2259.316	3028.604	3043.216
3054.317	3080.685	3110.245
3118.154	3120.007	3136.119
3149.584	3163.423	3174.757

i16

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C    -2.389506    1.739908    0.000062
C    -1.159671    0.894326   -0.000008
C    -1.121454   -0.478612   -0.000048
C     0.103572   -1.181178    0.000055
C    -2.395714   -1.294445   -0.000199
C     3.792330    0.532294   -0.000264
C     2.468716   -0.074962    0.000562
C     1.369518   -0.581627    0.000270
H    -2.409126    2.396806   -0.877408
H    -3.309492    1.153517    0.000019
H    -2.409122    2.396635    0.877666
H    -0.209475    1.421364   -0.000085
H     0.078303   -2.266506   -0.000008
H    -2.177641   -2.363537   -0.000425
H    -3.005522   -1.079093   -0.882097
H    -3.005499   -1.079460    0.881804
H     3.975468    1.070030   -0.934892
H     4.569092   -0.228481    0.109861
H     3.896268    1.244499    0.822989
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Frequencies

31.9769	66.4275	82.3036
88.1229	128.8519	199.0461
238.9491	255.6298	309.5971
381.1779	446.9458	459.3498
484.3871	608.7245	715.539
797.4352	801.7105	847.9121
980.1294	1029.141	1038.007
1046.808	1056.918	1057.763
1146.674	1220.435	1256.575
1298.164	1408.959	1417.403

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1421.294	1443.639	1480.114
1482.274	1483.444	1489.69
1500.68	1507.308	1562.146
2280.847	3023.874	3040.662
3046.518	3071.659	3109.044
3110.384	3117.515	3133.174
3136.228	3173.633	3176.081

i17
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C    2.920394   0.065469  -0.000007
C    1.418933   0.061483   0.000005
C    0.690330   1.174779  -0.000003
C   -0.811080   1.231544   0.000007
C   -1.474332  -0.135643   0.000018
C   -0.698980  -1.193118   0.000026
C    0.771528  -1.314573  -0.000006
C   -2.977029  -0.165713  -0.000013
H    3.310992  -0.456830   0.880267
H    3.320348   1.081293   0.000034
H    3.310984  -0.456769  -0.880321
H    1.203612   2.133689  -0.000006
H   -1.160773   1.800001   0.873504
H   -1.160787   1.800000  -0.873486
H    1.118514  -1.878814  -0.875846
H    1.118549  -1.878853   0.875794
H   -3.373117   0.350327   0.881339
H   -3.353853  -1.188928   0.000432
H   -3.373057   0.349517  -0.881872
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Frequencies

63.7905	157.0146	163.0922
228.496	257.1797	270.3686
365.8184	417.3741	428.7065
447.5565	590.7947	704.3292
767.7063	801.4587	909.4865
935.8212	936.3204	960.0613
994.4407	1062.101	1072.815
1077.506	1123.276	1174.23
1199.091	1215.555	1216.587
1323.068	1363.285	1372.302
1410.612	1419.182	1473.308
1474.913	1479.788	1484.587
1492.874	1498.667	1769.293
1802.097	3007.385	3018.71
3030.135	3037.093	3038.79
3043.752	3094.272	3096.199
3135.078	3147.27	3166.344

i18
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C   -2.877528   0.043857  -0.000247
C   -1.376171   0.071144  -0.000036
C   -0.679012   1.202860  -0.000038
C    0.818323   1.291055   0.000287
C    1.529762  -0.047280  -0.000052
C    0.792456  -1.215705  -0.000046
C   -0.698894  -1.273242   0.000313
C    2.916268  -0.064978  -0.000258
H   -3.257642  -0.486902  -0.880318
H   -3.299685   1.050560  -0.000384
H   -3.257865  -0.486744   0.879824
H   -1.212285   2.150832  -0.000233
H    1.147591   1.869995  -0.871717
H    1.147222   1.869309   0.872896
H   -1.047754  -1.851087   0.870151
H   -1.048169  -1.851809  -0.868860
```

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H    3.461815   -1.001717   -0.000437
H    1.324639   -2.163014   -0.000233
H    3.490912    0.854309   -0.000224
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Frequencies

32.6252	153.5709	189.199
245.8089	301.2721	395.0139
431.3302	433.3352	463.8853
536.5198	589.9348	721.328
732.991	766.1395	777.7106
815.7619	911.7521	947.6633
950.4064	984.1298	1004.267
1069.124	1084.533	1106.792
1177.612	1221.373	1239.392
1246.751	1339.659	1345.158
1414.246	1423.053	1432.475
1460.198	1474.305	1480.037
1487.803	1499.26	1527.05
1788.242	2990.066	3003.447
3026.46	3035.137	3051.372
3090.763	3135.365	3154.065
3164.311	3176.584	3253.121

i19

```
C   -2.950150   -0.029540    0.000006
C   -1.444129    0.008453   -0.000008
C   -0.760122    1.181736   -0.000011
C    0.734660    1.252464    0.000006
C    1.421390   -0.081870   -0.000002
C    0.686374   -1.229521   -0.000002
C   -0.724412   -1.220233   -0.000001
C    2.917452   -0.072511    0.000001
H   -3.326172   -0.557698   -0.881343
H   -3.375761    0.975720   -0.000199
H   -3.326162   -0.557335    0.881578
H   -1.301246    2.123479   -0.000021
H    1.083023    1.840363   -0.867336
H    1.083002    1.840336    0.867377
H    1.202403   -2.185722   -0.000005
H   -1.268546   -2.158323   -0.000001
H    3.307051    0.454554   -0.879445
H    3.328985   -1.083778   -0.000011
H    3.307046    0.454531    0.879463
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Frequencies

82.9468	93.9118	146.7413
223.5167	285.8258	293.3116
380.6338	439.5918	442.8224
556.0239	609.5425	722.5785
725.2389	771.15	795.8223
893.2767	940.3589	947.0813
988.6598	1018.376	1051.262
1064.275	1083.699	1132.562
1192.214	1201.929	1226.009
1324.471	1338.469	1378.562
1417.283	1419.706	1439.303
1449.111	1476.679	1483.867
1493.813	1502.522	1594.581
1655.192	2949.82	2951.659

3024.435	3048.341	3074.636
3111.26	3132.17	3137.908
3176.217	3180.537	3203.048

i30

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C   -2.487474   -0.952693   -0.209095
C   -1.171384   -0.267632   -0.083352
C    0.015237   -1.041040    0.394640
C    1.336845   -0.401551    0.027613
C    1.352425    1.062609   -0.025456
C    0.242914    1.802209    0.002934
C   -1.140074    1.220078    0.041835
C    2.436455   -1.120902   -0.201901
H   -2.966310   -1.100032    0.773829
H   -2.382910   -1.944017   -0.661054
H   -3.186371   -0.370877   -0.817844
H   -0.021905   -2.069967    0.023384
H   -0.021213   -1.117714    1.498446
H    2.322653    1.545499   -0.098866
H   -1.635960    1.539484    0.978273
H    0.319877    2.885117   -0.027567
H   -1.744746    1.674330   -0.755471
H    3.383979   -0.643094   -0.428319
H    2.423254   -2.205201   -0.168118
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Frequencies

79.4057	93.8658	176.1463
248.8528	300.3684	311.4142
412.4887	447.0551	479.0285
550.7268	665.3452	706.5412
792.0506	847.4082	871.1036
894.454	922.8413	936.2658
960.6553	1002.119	1009.902
1021.254	1028.195	1168.008
1187.315	1198.469	1241.474
1302.457	1334.236	1342.396
1401.6	1416.749	1430.599
1450.221	1459.394	1469.511
1487.737	1495.112	1700.63
1750.893	2919.809	2927.767
2962.281	3025.068	3060.466
3078.118	3108.928	3153.85
3168.558	3191.707	3240.987

i31

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C   -2.593336   -0.710666   -0.117123
C   -1.230166   -0.114940    0.014043
C   -0.118872   -1.014692    0.489701
C    1.242375   -0.509800    0.081965
C    1.468574    0.959801    0.335176
C    0.291513    1.781073   -0.107108
C   -0.962258    1.218993   -0.251005
C    2.156511   -1.292155   -0.479182
H   -2.920368   -1.162970    0.827817
H   -2.601559   -1.513057   -0.865526
H   -3.335267    0.034680   -0.410917
H   -0.270732   -2.033292    0.118019
H   -0.167766   -1.080958    1.589352
H    2.383658    1.294374   -0.161595
H    1.632160    1.115801    1.414054
H    0.441271    2.837581   -0.297092
H   -1.781954    1.853862   -0.577921
H    3.126360   -0.905903   -0.776126
H    1.968149   -2.345803   -0.658865
```

Frequencies

96.4348	131.4849	180.1724

278.7265	316.9265	384.5447
435.6697	457.2317	477.6432
565.6806	655.0619	688.2445
740.3267	848.5894	888.4527
916.7675	938.4153	941.423
946.8391	991.9668	1010.85
1021.234	1041.957	1159.928
1176.765	1209.453	1239.146
1305.14	1314.646	1352.852
1358.19	1421.729	1453.239
1463.859	1477.486	1481.182
1483.851	1490.352	1527.517
1755.176	2976.726	2981.521
3016.765	3064.256	3076.174
3088.244	3129.688	3148.2
3167.114	3205.381	3233.558

i32

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C     2.228030  -1.105781   0.519544
C     1.259958  -0.388108  -0.447879
C    -0.123747  -0.958546  -0.342887
C    -1.223181  -0.223433  -0.029867
C    -1.092062   1.177006   0.193013
C     0.168234   1.803104   0.080226
C     1.285889   1.094575  -0.231066
C    -2.586964  -0.853125   0.086298
H     2.242174  -2.181775   0.324855
H     1.914401  -0.945959   1.554034
H     3.246137  -0.723800   0.403391
H    -0.223366  -2.027762  -0.513165
H     1.639685  -0.593221  -1.464061
H    -1.968973   1.763433   0.444135
H     0.240769   2.873479   0.244518
H     2.246792   1.593424  -0.312977
H    -2.998449  -0.706450   1.089433
H    -2.549813  -1.925873  -0.111986
H    -3.286300  -0.399656  -0.622476
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Frequencies

85.9816	114.2778	174.0151
248.4061	288.2139	358.7597
417.4039	469.5766	503.6676
560.7307	615.7196	701.1058
749.3744	787.3221	818.1258
874.4487	955.449	970.7935
982.4908	1004.982	1056.894
1065.063	1077.435	1095.725
1144.149	1189.234	1212.73
1289.56	1329.652	1337.855
1378.729	1401.469	1420.146
1449.491	1488.381	1496.472
1501.277	1503.436	1583.228
1641.794	2944.394	3038.905
3041.423	3105.163	3118.466
3127.024	3132.417	3161.83
3170.182	3186.214	3201.231

i33

C	2.275786	-0.980177	0.528621
C	1.260316	-0.356644	-0.447559
C	-0.076138	-1.020382	-0.328735
C	-1.262313	-0.378756	-0.025038
C	-1.277052	1.119996	0.205295
C	0.059596	1.779910	0.047536
C	1.177996	1.131260	-0.249470
C	-2.456834	-1.075926	0.074912
H	2.375645	-2.055297	0.355842
H	1.952535	-0.825460	1.561240
H	3.262342	-0.524128	0.405019
H	-0.100772	-2.096304	-0.486164
H	1.644521	-0.542038	-1.462809
H	-1.667607	1.324655	1.209804
H	-1.993849	1.582090	-0.484671
H	0.087597	2.856960	0.188124
H	2.110366	1.681783	-0.346613
H	-3.386556	-0.570153	0.309672
H	-2.492370	-2.147788	-0.082815

Frequencies

70.0778	132.5585	261.2191
274.4211	343.7674	408.6712
469.8981	481.3361	507.3989
545.5132	575.3951	717.878
752.0301	761.0988	809.9405
861.4819	921.8451	932.5121
974.5356	1014.088	1019.47
1030.787	1057.279	1086.44
1158.529	1203.358	1236.833
1244.765	1311.143	1334.889
1376.46	1408.355	1426.379
1431.08	1471.692	1479.916
1502.55	1508.33	1525.162
1765.876	2988.375	3032.529
3041.537	3058.611	3117.334
3129.72	3156.438	3161.912
3165.402	3186.702	3254.86

i34

C	2.570450	-1.014346	0.010424
C	1.259348	-0.286741	-0.011609
C	0.026741	-0.985166	-0.008752
C	-1.183887	-0.361273	-0.000416
C	-1.273442	1.138380	0.010120
C	0.055862	1.825036	-0.000581
C	1.221995	1.135573	-0.009302
C	-2.479494	-1.109809	-0.000479
H	2.436884	-2.082559	-0.173900
H	3.070146	-0.905901	0.980812
H	3.257644	-0.624536	-0.747730
H	0.052278	-2.072770	-0.015069
H	-1.860856	1.464059	0.886788
H	-1.880307	1.475017	-0.848612
H	0.062994	2.910037	-0.001648
H	2.163158	1.678907	-0.016144
H	-2.323402	-2.190336	-0.010600
H	-3.077502	-0.858476	0.884247
H	-3.086482	-0.843372	-0.874578

Frequencies

102.931	116.0062	130.0723
194.7818	276.2467	301.8438
399.9382	430.1645	486.0878
532.3924	548.824	693.2966
715.9051	871.9445	880.193

929.3859	940.6525	971.4278
994.484	1006.453	1033.661
1045.747	1051.247	1162.291
1191.543	1205.092	1260.657
1282.746	1335.71	1420.465
1425.24	1435.637	1447.421
1455.954	1476.691	1491.096
1493.807	1500.359	1557.749
1650.739	2946.638	2951.201
3015.827	3023.499	3065.289
3079.909	3126.291	3130.617
3164.143	3172.125	3199.686

i35

```
C   -2.457205  -0.960788   0.105921
C   -1.193820  -0.238687  -0.359256
C    0.049324  -1.030566  -0.079215
C    1.307678  -0.424675  -0.014947
C    1.356465   1.047522  -0.122276
C    0.257709   1.791720  -0.003278
C   -1.088735   1.168588   0.244280
C    2.472462  -1.145733   0.145095
H   -2.437213  -1.113060   1.189467
H   -2.549012  -1.940527  -0.370883
H   -3.352344  -0.382517  -0.139219
H   -1.258949  -0.114521  -1.453852
H   -0.023900  -2.112803  -0.015885
H    2.326857   1.511647  -0.267978
H    0.326468   2.874336  -0.042919
H   -1.258229   1.109818   1.329809
H   -1.885397   1.802037  -0.156898
H    3.436644  -0.653350   0.191299
H    2.451802  -2.225341   0.239112
```

Frequencies

127.6151	147.4309	270.0247
276.5751	323.4568	396.2373
447.3198	454.8029	532.2385
556.053	596.9184	691.1269
712.68	765.9744	801.267
877.1029	892.9122	934.0126
957.6913	1007.516	1019.353
1028.981	1077.428	1109.683
1182.438	1193.827	1238.738
1274.452	1314.286	1337.99
1361.483	1374.36	1413.272
1450.093	1452.656	1484.685
1503.243	1512.218	1526.815
1726.102	2959.792	3010.96
3040.424	3090.278	3117.557
3118.17	3159.723	3172.25
3173.394	3196.149	3258.09

i36

```
C    2.513751  -0.845407   0.070056
C    1.168409  -0.266756  -0.365270
C    0.000821  -1.016121   0.288685
C   -1.341075  -0.361894   0.035953
C   -1.351472   1.066167   0.054098
C   -0.151308   1.803890   0.095949
C    1.063436   1.205792  -0.078087
```

WILEY-VCH

```
C    -2.468372   -1.090032   -0.134566
H     2.580614   -1.909749   -0.171391
H     2.649131   -0.733807    1.150399
H     3.342929   -0.334847   -0.427643
H     0.169344   -1.025312    1.374545
H    -0.013436   -2.058013   -0.042450
H    -2.304744    1.583617    0.035868
H    -0.204232    2.880202    0.226282
H     1.079905   -0.391843   -1.456527
H     1.972674    1.799354   -0.079264
H    -3.431080   -0.609278   -0.271519
H    -2.446246   -2.174157   -0.139219
```

Frequencies

123.6878	140.5176	262.392
281.3956	344.6476	413.5174
437.7204	496.6413	525.7228
552.8468	642.6765	701.9464
743.8607	796.0961	865.1197
874.0613	890.187	949.4998
967.8399	979.8493	993.9248
1071.376	1099.735	1118.821
1149.161	1188.727	1219.487
1301.937	1315.957	1332.218
1358.393	1382.296	1419.134
1443.94	1447.65	1469.76
1506.01	1509.943	1556.341
1607.761	2979.765	3027.321
3039.289	3096.958	3113.457
3120.573	3151.993	3171.924
3189.054	3205.065	3245.125

i37
```
C     2.663558   -0.064848    0.570994
C     1.444436    0.063263   -0.355279
C     0.611202    1.252516   -0.011429
C    -0.849291    1.258680   -0.306130
C    -1.513095   -0.059751    0.034632
C    -0.684377   -1.255250   -0.142435
C     0.633115   -1.206786   -0.346785
C    -2.782226   -0.138205    0.436407
H     2.341715   -0.221966    1.603667
H     3.271934    0.842901    0.535081
H     3.294924   -0.907224    0.274737
H     1.110961    2.181417    0.242179
H    -1.351110    2.082442    0.207454
H    -1.005349    1.431649   -1.387151
H    -1.188213   -2.216811   -0.099821
H     1.838149    0.188200   -1.382247
H     1.187059   -2.131519   -0.487822
H    -3.248701   -1.096015    0.642388
H    -3.391305    0.749215    0.571686
```

Frequencies

61.9599	131.7195	233.4363
259.4158	311.59	353.5711
403.8179	426.1038	510.4969
525.0636	614.1826	706.6455
761.5595	791.0572	824.2863
879.2005	922.2864	929.4553
966.1975	988.8026	1013.412
1030.047	1083.365	1099.876
1147.115	1196.878	1211.716

1295.182	1314.052	1328.387
1352.698	1398.606	1408.774
1420.952	1456.891	1468.878
1501.252	1503.6	1698.089
1748.808	2917.162	2930.569
3040.645	3091.397	3118.545
3124.713	3147.072	3157.448
3181.18	3186.243	3234.597

i38
```
C     2.866730   -0.000494    0.300109
C     1.394975    0.001182    0.015549
C     0.670739   -1.215045   -0.107905
C    -0.669020   -1.242660   -0.319999
C    -1.505664   -0.000168   -0.407735
C    -0.669998    1.242916   -0.319723
C     0.670304    1.216204   -0.107456
C    -2.614640   -0.000836    0.668238
H     3.359340   -0.866511   -0.150258
H     3.063841   -0.040511    1.378963
H     3.348700    0.902211   -0.084055
H     1.216349   -2.152130   -0.035509
H    -2.026025   -0.000365   -1.380887
H    -1.184231   -2.193966   -0.414884
H    -1.185813    2.193897   -0.414342
H     1.215021    2.153742   -0.034685
H    -3.247969   -0.887137    0.570981
H    -3.248671    0.884985    0.571277
H    -2.171095   -0.000811    1.666928
```

Frequencies

31.3531	67.0681	218.4332
238.7979	269.1787	350.0759
389.2727	439.6859	492.4607
613.7858	633.2436	745.8777
751.856	759.4227	807.2247
942.67	968.0922	976.7075
980.931	995.0394	1036.044
1041.721	1073.794	1110.352
1184.519	1200.422	1255.272
1276.983	1297.552	1348.657
1401.23	1418.161	1418.94
1480.531	1487.227	1489.014
1498.052	1503.548	1546.347
1637.582	2950.033	3019.086
3038.366	3085.106	3118.126
3120.922	3126.315	3160.648
3161.73	3181.766	3185.399

i39
```
C    -2.872757    0.056986   -0.158564
C    -1.533116    0.064643    0.032183
C    -0.765388   -1.201169    0.349787
C     0.631466   -1.204519   -0.274855
C     1.366386    0.084741   -0.023737
C     0.645012    1.241818    0.088285
C    -0.762061    1.265952    0.015104
C     2.860452    0.049941   -0.006437
H    -3.442563   -0.865196   -0.132753
H    -1.330222   -2.081757    0.035029
H    -3.417254    0.977304   -0.340933
H    -0.656833   -1.259986    1.440250
H     1.209213   -2.052604    0.106266
H     0.552068   -1.351188   -1.362630
```

```
H     1.174592    2.185341    0.189313
H    -1.278642    2.217502   -0.053186
H     3.228059   -0.580079    0.812337
H     3.290818    1.046687    0.109957
H     3.250796   -0.386382   -0.934247
```

Frequencies

98.766	174.162	178.868
297.0049	316.6259	378.5171
420.9092	442.2269	523.253
570.3798	656.4859	729.1508
772.2143	776.4198	792.3128
865.6486	918.1024	943.8353
971.1904	1007.506	1021.067
1051.36	1067.015	1123.081
1191.83	1204.74	1243.794
1315.76	1343.087	1363.326
1371.346	1419.269	1432.643
1451.421	1475.03	1482.619
1487.38	1492.814	1566.819
1613.2	3002.288	3021.155
3034.697	3072.772	3081.711
3103.836	3125.281	3152.584
3172.046	3197.634	3245.294

i68
```
C     1.116717   -0.943323    1.016349
C     0.318192   -0.823835   -0.254107
C    -3.630429    0.263894   -0.123121
C    -2.225788   -0.125761   -0.169021
C    -1.068844   -0.448162   -0.209455
C     1.432770    0.201341    0.066420
C     1.049313    1.553611    0.451373
C     2.697461    0.082740   -0.759303
H     0.608593   -0.698774    1.940938
H     1.839101   -1.749158    1.084182
H     0.573965   -1.520908   -1.046058
H    -3.796250    1.020962    0.647682
H    -4.268357   -0.593860    0.104912
H    -3.952390    0.682472   -1.080018
H     1.676839    2.394274    0.184330
H     0.111397    1.739350    0.958651
H     3.552171    0.488306   -0.210229
H     2.599881    0.634349   -1.698349
H     2.918703   -0.960042   -1.000848
```

Frequencies

89.6418	93.1368	102.7952
182.4453	210.8472	250.0674
264.3337	336.8315	374.0059
381.7653	408.7911	486.927
529.5634	564.0217	716.468
736.2403	799.0308	932.2291
939.7564	949.3797	985.1335
1051.539	1053.718	1056.241
1072.874	1104.281	1122.04
1218.955	1286.946	1334.092
1404.008	1416.104	1430.14
1465.472	1485.011	1487.546
1489.592	1500.212	1509.636

2392.8	3044.392	3046.888
3117.404	3120.045	3120.302
3123.219	3144.059	3165.754
3167.782	3242.562	3276.098

i69

C	-0.882805	2.029523	-0.000115
C	-0.464773	0.584063	-0.000523
C	3.518836	-0.236136	0.000639
C	2.092010	0.053184	-0.000357
C	0.902437	0.290796	-0.000714
C	-1.428552	-0.474914	-0.000060
C	-2.763793	-0.222226	0.000858
C	-0.924841	-1.897568	-0.000456
H	-0.011628	2.683912	-0.001109
H	-1.487034	2.264250	0.883001
H	-1.489099	2.264266	-0.881792
H	3.697796	-1.311762	0.072059
H	4.014059	0.247322	0.847462
H	3.991761	0.127229	-0.916176
H	-3.482647	-1.033182	0.001277
H	-3.163613	0.784327	0.001288
H	-1.754233	-2.606344	-0.000254
H	-0.302939	-2.090296	0.878050
H	-0.303539	-2.090049	-0.879434

Frequencies

40.129	71.4481	93.8393
125.8713	152.882	174.9158
273.1527	286.7731	328.1529
424.1345	436.1929	437.669
550.3512	593.4978	643.0224
653.7907	854.1958	872.9141
967.1359	1018.856	1022.352
1045.887	1052.045	1062.93
1064.522	1166.984	1345.335
1356.536	1395.999	1409.469
1426.39	1437.057	1479.94
1485.906	1486.712	1489.38
1495.139	1502.627	1585.819
2245.934	3030.376	3044.376
3053.966	3086.672	3111.085
3118.196	3123.302	3145.611
3148.55	3172.812	3261.649

Transition states

i4 – p23

C	0.383556	-0.988528	0.741919
C	-0.763990	-0.012557	0.568116
C	3.959812	0.635537	-0.510913
C	2.697998	0.056069	-0.064135
C	1.659956	-0.425439	0.298903
C	-1.836473	-0.314415	-0.121603
C	-2.624221	-1.082719	-0.874622
H	0.167780	-1.906997	0.190192
H	0.465294	-1.262307	1.800630
H	-0.647752	0.954865	1.042841
H	4.625920	0.823033	0.334949
H	3.790218	1.584733	-1.025338
H	4.472588	-0.036564	-1.203487
H	-3.409340	-1.682979	-0.426440
H	-2.603528	-1.004977	-1.956824
C	-3.050661	1.647716	0.104725
H	-3.968566	1.472518	-0.442052
H	-2.327814	2.311113	-0.354675
H	-3.120665	1.653584	1.185865

Frequencies

-524.882	23.1781	36.0978
45.907	83.8396	125.6289
174.7322	199.2855	238.273
300.4985	321.2879	398.3154
440.5207	466.5085	482.4191
524.2345	562.1733	773.0305
797.912	845.1525	869.192
932.4045	1025.18	1032.627
1058.86	1059.967	1116.962
1173.314	1226.303	1312.902
1377.229	1419.662	1420.275
1429.381	1465.667	1472.211
1486.013	1486.377	1947.524
2394.213	3038.418	3046.586
3099.203	3099.804	3119.011
3119.932	3138.218	3194.978
3225.866	3268.168	3268.881

i4 – p4b
```
C     0.255849   -0.562427   -0.218396
C    -0.730317    0.281849    0.169483
C     4.232132    0.341533    0.038179
C     2.813321    0.022433   -0.047805
C     1.641548   -0.241606   -0.111509
C    -2.165739    0.029673    0.027581
C    -2.678960   -1.204660    0.000637
C    -3.035330    1.258633   -0.048725
H     0.006093   -1.444855   -0.800665
H     0.170641   -1.911305    1.323888
H    -0.442404    1.226227    0.624959
H     4.684843   -0.137785    0.910089
H     4.383287    1.419948    0.128420
H     4.762492   -0.003964   -0.852575
H    -3.744752   -1.365565   -0.117612
H    -2.056568   -2.084473    0.121351
H    -4.088927    0.997119   -0.156784
H    -2.746618    1.889214   -0.895198
H    -2.923117    1.862874    0.857458
```

Frequencies

-729.82	51.4711	79.3246
84.1694	104.7347	160.2956
219.2751	239.0138	308.8992
333.2526	348.7458	395.8244
446.6108	515.839	530.3522
538.9378	705.695	808.8473
891.2799	914.1334	934.5635
986.2355	1005.404	1033.058
1057.037	1062.953	1072.805
1199.636	1251.136	1309.968
1352.959	1415.205	1424.917
1446.935	1483.764	1487.596
1487.903	1498.591	1626.718
1709.567	2378.019	3043.752
3051.578	3104.819	3123.344
3126.731	3145.434	3161.124

3169.223	3177.74	3249.524

i11 – p36

C	-3.125400	-1.065683	-0.648438
C	-2.186149	-0.312991	-0.142757
C	-1.078688	0.352103	0.128646
C	-0.056765	-0.237973	1.083702
C	-0.852488	1.756592	-0.352102
C	3.727780	-0.302762	-0.550159
C	2.390825	-0.277021	0.032516
C	1.291435	-0.262801	0.514598
H	-4.101648	-1.156921	-0.188518
H	-2.935989	-1.624501	-1.560303
H	-3.118558	0.349994	1.495891
H	-0.049151	0.361610	2.003563
H	-0.359060	-1.248922	1.366692
H	-0.847092	2.451395	0.495608
H	-1.627552	2.067807	-1.051910
H	0.123057	1.830008	-0.841244
H	3.808142	-1.087895	-1.305869
H	4.482471	-0.491426	0.217252
H	3.962075	0.652065	-1.027197

Frequencies

-704.657	34.575	89.2646
101.4763	102.5042	179.4779
185.1878	204.6773	250.9511
301.4917	352.1747	397.5136
458.751	480.6688	549.3136
595.8821	668.4907	782.3708
788.7337	913.2074	920.776
1010.46	1028.73	1056.378
1060.335	1065.26	1170.315
1193.616	1235.217	1303.704
1359.561	1412.43	1424.204
1464.721	1476.392	1484.701
1490.011	1494.878	1510.306
2021.935	2397.095	3029.333
3040.248	3051.225	3105.759
3107.857	3122.95	3125.746
3147.32	3158.398	3236.924

i11 – p7a

C	-3.525503	0.089437	-0.109800
C	-2.384911	-0.604743	-0.115319
C	-1.047280	-0.035666	-0.009493
C	0.019174	-0.885014	0.001307
C	-0.889322	1.447064	0.128773
C	3.944819	0.241465	-0.090402
C	2.542199	-0.150205	-0.052897
C	1.383654	-0.473319	-0.016106
H	-4.482834	-0.410481	-0.195608
H	-3.544088	1.170203	-0.020477
H	-2.432477	-1.687849	-0.203545
H	-0.160021	-1.943449	-0.166102
H	0.162070	1.727897	0.180142
H	-1.389090	1.801833	1.036121
H	-1.348118	1.964074	-0.719670
H	4.117228	0.998875	-0.859373
H	4.581158	-0.618671	-0.311936
H	4.257889	0.657331	0.870785
H	-0.018694	-1.433884	1.973290

Frequencies

-704.823	71.4255	85.0857
94.0716	151.5305	165.9834
231.1752	252.4304	297.769

302.7745	336.3613	395.6933
437.6017	452.9303	536.9052
597.3534	699.8729	821.9496
836.7278	936.7372	950.4037
991.1049	1032.49	1050.887
1052.84	1059.991	1086.407
1210.51	1243.718	1333.426
1383.279	1411.676	1432.443
1454.098	1481.384	1487.669
1487.812	1493.842	1613.317
1689.621	2374.533	3046.128
3048.384	3105.383	3118.933
3124.808	3157.984	3158.423
3170.009	3173.4	3253.396

i3 – p23
```
C    -0.063821   -1.307824    0.477250
C     0.973988   -0.908148   -0.544928
C     2.054940   -0.190597   -0.241030
C     3.331343    0.024102   -0.032306
C    -3.676713    0.561079   -0.208278
C    -2.402848   -0.104615    0.040381
C    -1.355369   -0.653183    0.249871
H     0.298888   -1.069267    1.480708
H    -0.206240   -2.394349    0.440982
H     0.731314   -1.077113   -1.590571
H     3.743832    1.013769    0.117684
H     4.015834   -0.818666    0.000200
H    -4.425901   -0.149906   -0.565211
H    -3.565027    1.343030   -0.963513
H    -4.057632    1.025128    0.704825
C     1.164106    1.898037    0.203464
H     1.581039    2.054651    1.191279
H     0.093666    1.744086    0.140236
H     1.636467    2.415531   -0.623169
```

Frequencies

-561.957	31.5615	34.2126
56.4336	91.9255	126.9622
181.2839	216.5675	249.7489
286.4341	333.6092	399.6932
449.3654	479.7481	545.1901
572.4651	584.6761	775.9255
817.9212	844.4237	893.0862
908.7114	1018.107	1028.217
1059.345	1060.1	1129.648
1169.973	1225.143	1307.288
1383.471	1417.606	1420.587
1431.37	1469.089	1479.809
1486.016	1486.577	1937.852
2391.046	3039.56	3047.416
3094.835	3096.081	3119.937
3121.113	3143.605	3167.084
3235.989	3263.999	3265.711

i3 – p4a
```
C     0.214521   -0.511480    0.012550
C    -0.732948    0.460508    0.034019
C    -2.167077    0.224855   -0.029929
```

```
C    -3.010035    1.265912    0.016496
C    -2.663044   -1.191645   -0.134634
C     4.227201    0.252158   -0.067516
C     2.795252   -0.013807   -0.036465
C     1.612641   -0.231298   -0.004032
H    -0.068826   -1.541694   -0.180376
H     0.078819   -1.178902    1.934926
H    -0.409596    1.491897    0.140832
H    -4.084568    1.128382   -0.029084
H    -2.643222    2.283492    0.100245
H    -3.752882   -1.225063   -0.155146
H    -2.315667   -1.785617    0.716934
H    -2.289073   -1.672645   -1.043741
H     4.781478   -0.556853    0.414622
H     4.459751    1.183487    0.454489
H     4.584719    0.342302   -1.096629
```

Frequencies

-738.138	51.6053	80.6083
81.8326	140.2837	213.9521
222.6907	227.9622	303.9014
332.506	377.3573	412.9783
455.7929	499.4519	534.9834
537.6267	704.048	819.7433
872.7091	894.5095	931.913
997.7217	1000.326	1045.426
1050.351	1056.558	1070.973
1207.071	1288.507	1310.328
1349.285	1413.788	1418.245
1449.626	1481.304	1486.164
1486.721	1504.927	1617.662
1687.233	2376.425	3045.211
3050.834	3107.324	3121.899
3126.866	3146.821	3157.571
3183.381	3191.311	3248.071

i2 – i1

```
C     0.082894    1.429322    0.998591
C    -0.508883    0.832143   -0.245360
C    -1.626572   -0.171246   -0.138480
C    -2.680834   -0.075577   -0.942579
C    -1.486640   -1.256672    0.890133
C     3.350273   -0.588351   -0.239281
C     1.958078   -0.200671   -0.434606
C     0.859149    0.335176   -0.261449
H     0.463309    2.440283    0.972925
H    -0.026163    0.928113    1.949576
H    -0.702768    1.567820   -1.026079
H    -3.496223   -0.789272   -0.890836
H    -2.762759    0.714832   -1.681426
H    -2.294000   -1.984942    0.803332
H    -1.512668   -0.841662    1.902762
H    -0.530416   -1.775154    0.775172
H     3.772771   -0.122450    0.659363
H     3.962106   -0.289797   -1.094810
H     3.442015   -1.672517   -0.131787
```

Frequencies

-701.408	47.6671	89.1969
109.3249	133.4152	183.1116
239.9172	281.4139	349.7103
381.0386	425.6427	470.0384
537.1517	618.3779	674.9309
719.9661	783.1061	817.6419
945.4904	948.451	1006.605

1034.251	1056.018	1064.238
1075.613	1093.52	1180.812
1224.869	1311.519	1347.088
1414.1	1418.4	1445.464
1463.448	1480.92	1482.66
1488.43	1504.547	1746.288
2093.87	3021.843	3048.979
3090.699	3111.609	3112.647
3113.413	3144.625	3152.517
3180.085	3238.78	3300.162

i12 – p7b

```
C    -3.131748   -1.024745    0.106434
C    -2.515525    0.109439   -0.227262
C    -1.081638    0.381964   -0.086813
C    -0.166314   -0.620042   -0.166164
C    -0.698814    1.807345    0.178028
C     3.886402   -0.131602    0.008157
C     2.439651   -0.293378   -0.050784
C     1.244717   -0.429224   -0.091428
H    -4.199521   -1.143277   -0.035672
H    -2.596308   -1.857882    0.550283
H    -3.113407    0.937617   -0.603697
H    -0.426355   -1.402648    1.732656
H    -0.497871   -1.605020   -0.479756
H     0.382733    1.938323    0.203861
H    -1.114765    2.141036    1.134812
H    -1.113000    2.461449   -0.596473
H     4.307936   -0.011609   -0.993351
H     4.354001   -1.005099    0.469311
H     4.156168    0.748563    0.597019
```

Frequencies

-633.268	72.3244	82.1737
94.3808	107.3674	136.4271
236.8147	244.0919	285.369
287.8809	355.9344	398.1012
426.3269	512.0417	535.8708
557.8188	697.2862	818.3842
846.7278	918.6349	968.386
1008.021	1034.344	1045.698
1058.158	1061.707	1082.442
1199.381	1247.272	1320.376
1359.071	1414.667	1423.422
1464.587	1483.286	1484.842
1485.042	1489.867	1624.565
1706.79	2374.317	3039.961
3047.227	3097.878	3117.138
3123.702	3153.044	3157.3
3163.865	3185.248	3249.64

i2 – p21

```
C     0.121380    1.777412    0.278875
C    -0.486360    0.683930   -0.600192
C    -1.533344   -0.252255   -0.102165
C    -2.453691   -0.722285   -0.941226
C    -1.499556   -0.640558    1.349907
C     3.080314   -0.827660   -0.011088
C     1.997383   -0.080885   -0.038231
C     0.914774    0.599808   -0.103210
H     0.351540    2.724854   -0.196666
H    -0.202851    1.849309    1.311752
```

H	-0.580121	0.943931	-1.650889
H	-3.220441	-1.413135	-0.608250
H	-2.468230	-0.434883	-1.987254
H	-2.243764	-1.408319	1.563721
H	-1.709611	0.220101	1.993095
H	-0.513722	-1.023749	1.629088
H	3.887179	-0.661910	-0.716567
H	3.262056	-1.513278	0.809395
H	2.592573	-2.507953	-1.143443

Frequencies

-546.244	41.9363	81.1754
159.3043	187.4334	195.6447
271.6711	289.4926	319.1018
394.2563	411.7304	477.5827
522.1399	594.8356	652.0954
683.1569	749.1173	790.8776
901.2393	927.8465	931.7804
940.6602	978.393	1012.33
1029.487	1059.362	1067.247
1076.282	1077.876	1120.855
1310.209	1330.788	1384.991
1420.999	1455.298	1465.145
1491.181	1506.385	1531.509
1737.921	2103.776	3043.327
3105.628	3130.94	3143.472
3146.638	3149.816	3155.291
3220.386	3232.531	3236.912

i3 – i2

C	0.060829	1.838201	-0.192079
C	-0.523554	0.588627	-0.791292
C	-1.445108	-0.300621	-0.107956
C	-2.050335	-1.298731	-0.775137
C	-1.688746	-0.083279	1.362792
C	2.773192	-1.181677	0.145242
C	2.062898	0.096957	0.170955
C	1.059019	0.799435	-0.064749
H	0.282736	2.642113	-0.890417
H	-0.382099	2.196937	0.734673
H	-0.420297	0.476114	-1.864073
H	-2.734347	-1.976607	-0.277622
H	-1.879294	-1.454505	-1.835055
H	-2.322336	-0.870322	1.773068
H	-2.183551	0.876837	1.540755
H	-0.745095	-0.075211	1.917102
H	3.629863	-1.136608	-0.532531
H	2.112500	-1.991381	-0.189802
H	3.152749	-1.440843	1.137251

Frequencies

-698.816	55.4511	64.1783
77.7788	164.8181	206.8121
217.9118	297.4839	378.7437
407.6049	436.4949	513.5577
538.9123	694.8245	711.4371
789.3757	840.8337	889.6471
947.6647	1002.365	1026.831
1035.616	1059.455	1072.511
1090.161	1114.119	1170.54
1218.925	1319.106	1384.55
1405.878	1424.201	1451.984

1472.206	1475.737	1477.96
1491.151	1511.092	1651.665
2027.739	3017.872	3045.469
3094.891	3105.567	3107.386
3119.006	3147.705	3156.254
3178.566	3201.336	3246.602

i9 – p39

C	-2.437111	-1.625896	-0.134381
C	-1.358364	-1.212798	0.483000
H	-2.909663	-2.576848	0.115590
H	-2.907856	-1.048847	-0.927283
H	-0.772317	-1.640275	1.286347
C	-0.427006	0.828981	0.073193
C	-0.862439	1.475816	1.195298
C	-1.083324	1.075966	-1.269074
C	3.402170	-0.625409	-0.108357
C	2.039823	-0.112678	-0.034458
C	0.916770	0.311987	0.029738
H	-1.826393	1.971014	1.202969
H	-0.297924	1.438462	2.118255
H	-0.604880	1.932443	-1.752752
H	-2.144427	1.300864	-1.142504
H	-0.977197	0.213624	-1.927777
H	3.490174	-1.384941	-0.889081
H	3.698496	-1.078548	0.840921
H	4.108874	0.177245	-0.334434

Frequencies

-490.664	32.8687	51.3055
90.2675	116.777	179.3437
189.4539	229.5812	252.0917
306.1207	334.1075	367.858
371.7024	484.6617	575.6637
642.7123	657.6315	819.4134
834.5975	906.1744	924.1898
940.9788	1017.517	1048.858
1056.116	1058.533	1088.056
1103.363	1318.329	1390.407
1405.042	1418.452	1421.474
1484.209	1485.501	1488.332
1504.027	1554.945	1664.396
2377.519	3046.202	3051.117
3088.629	3118.3	3120.918
3123.951	3151.52	3159.536
3173.201	3229.279	3261.889

i9 – p38

C	-2.555277	-1.322067	-0.330689
C	-1.421518	-0.694292	-0.620669
C	-0.582243	0.065418	0.350544
C	-1.070792	0.475644	1.568516
C	3.456548	-0.479555	-0.123393
C	2.023065	-0.275532	0.044508
C	0.841632	-0.109440	0.191456
H	-3.109097	-1.848543	-1.099172
H	-2.961304	-1.344607	0.674843
H	-1.029850	-0.738845	-1.632515
H	-0.403105	0.849701	2.333144
H	-2.137655	0.527134	1.748235
H	3.652618	-1.247222	-0.875958
H	3.915936	-0.800420	0.814843
H	3.948362	0.442538	-0.443870
C	-0.668151	1.964630	-0.852784
H	-0.069475	2.616527	-0.228143
H	-1.735152	2.154361	-0.875212

H   -0.210861   1.640547   -1.781133

Frequencies

-578.442	27.7135	70.0477
104.0049	108.9103	150.1505
216.4567	226.1364	285.4122
329.6382	335.1033	437.3237
486.3285	558.7386	565.4085
589.9311	617.5747	674.9921
725.5607	805.232	890.9343
937.4983	955.9603	1040.325
1056.23	1057.93	1065.076
1092.039	1285.62	1333.654
1391.572	1419.563	1420.349
1424.999	1452.415	1484.49
1485.207	1524.569	1719.87
2379.337	3046.671	3091.536
3117.903	3122.043	3155.679
3165.992	3180.444	3246.046
3257.476	3263.275	3268.956

i2 – p22

C	-0.002227	1.874781	-0.100156
C	-0.505348	0.579924	-0.711152
C	-1.501836	-0.302430	-0.029745
C	-2.448013	0.180413	0.768635
C	-1.337084	-1.766759	-0.323804
C	3.055258	-0.596463	0.402574
C	1.960175	0.083052	0.136573
C	0.866473	0.682216	-0.151154
H	0.224815	2.697410	-0.769955
H	-0.384547	2.163026	0.873387
H	-0.546709	0.555165	-1.799117
H	-3.157839	-0.476843	1.259416
H	-2.548031	1.243983	0.955339
H	-2.089682	-2.368024	0.188770
H	-0.342856	-2.105346	-0.014610
H	-1.416997	-1.956199	-1.399601
H	3.902756	-0.574708	-0.273914
H	3.194782	-1.067822	1.369425
H	2.639918	-2.519050	-0.339763

Frequencies

-504.716	56.1049	71.7882
163.6965	181.8591	190.5104
245.8664	281.1267	302.1874
377.3821	405.8086	475.2053
526.0618	591.4257	667.0045
694.1811	727.0016	807.9008
900.3068	935.6801	940.9816
946.3284	977.3398	1026.392
1030.256	1045.197	1069.774
1083.222	1094.497	1118.19
1260.837	1338.209	1398.028
1421.86	1447.176	1462.575
1483.716	1498.171	1533.111
1746.883	2107.314	3035.341
3096.625	3126.141	3131.101

3136.733	3145.735	3152.08
3221.204	3231.57	3238.204

i10 – p41

C	-2.392388	-1.386438	-0.083740
C	-1.457333	-0.655675	-0.674902
H	-2.931033	-2.154925	-0.626083
H	-2.653878	-1.244194	0.960144
H	-1.232023	-0.818031	-1.727388
C	-0.662910	0.430563	-0.029224
C	-0.358359	0.355432	1.459153
C	-0.833160	1.799197	-0.661886
C	3.124137	-0.559635	-0.197418
C	1.903531	-0.235531	0.172894
C	0.697372	0.078338	0.463239
H	-0.300733	1.289988	2.008513
H	-0.736267	-0.488746	2.026134
H	-0.179546	2.533390	-0.185739
H	-1.869700	2.134585	-0.566584
H	-0.580247	1.762037	-1.724977
H	3.896169	0.196130	-0.292806
H	3.425967	-1.599166	-0.265817
H	3.035957	-0.568579	-2.294102

Frequencies

-512.377	65.897	108.9247
118.0951	192.0844	221.2204
259.3807	282.945	306.9342
335.9343	369.292	446.017
481.804	580.2507	652.4302
692.2567	711.1649	750.7347
900.0926	914.039	939.1267
966.7496	980.2972	1011.524
1030.641	1038.604	1065.53
1068.421	1118.27	1215.996
1277.74	1332.256	1382.202
1416.825	1452.793	1462.626
1491.752	1500.773	1534.096
1734.368	2103.139	3042.287
3118.704	3126.202	3131.139
3145.904	3146.016	3158.403
3215.98	3231.835	3240.44

i1 – p14

C	0.786956	1.897250	-0.225479
C	0.416326	0.612204	0.042005
C	-3.583525	-0.286303	0.004081
C	-2.160911	0.028356	0.020231
C	-0.988942	0.291672	0.040395
C	1.392677	-0.520407	-0.013442
C	0.976979	-1.777799	-0.153350
C	2.851896	-0.173140	0.085248
H	0.042212	2.679241	-0.290401
H	1.827567	2.178509	-0.318058
H	0.563296	0.685479	1.900327
H	-4.085094	0.223184	-0.822378
H	-4.059338	0.027155	0.936618
H	-3.741744	-1.361004	-0.113239
H	1.688806	-2.594144	-0.202079
H	-0.075914	-2.023186	-0.222933
H	3.457747	-1.078364	0.135631
H	3.049286	0.425670	0.979986
H	3.184439	0.406458	-0.781605

Frequencies

-1026.14	40.8961	60.8315
94.4746	162.0119	222.8125

285.6213	335.244	344.2247
376.131	409.6603	449.6786
460.4892	485.2043	574.3125
612.2435	661.248	698.1449
773.7923	845.0577	893.6337
948.1353	966.8492	1027.363
1058.704	1064.607	1071.006
1079.439	1223.324	1370.076
1411.435	1414.955	1427.987
1442.791	1483.565	1487.721
1489.586	1500.692	1575.447
1729.228	2386.575	3042.368
3050.97	3104.761	3122.761
3127.155	3142.381	3166.478
3184.176	3258.24	3284.555

i1 – p16

C	-0.672406	2.079782	0.652297
C	-0.261542	1.228584	-0.328568
C	3.336406	-0.717108	-0.155941
C	2.054850	-0.025219	-0.214433
C	0.999457	0.549094	-0.264928
C	-1.598445	-0.603589	-0.098899
C	-2.548913	-0.690548	-0.997624
C	-1.205293	-1.364430	1.098470
H	-0.152557	2.135812	1.601073
H	-1.571998	2.669125	0.525988
H	-0.707970	1.306528	-1.315041
H	3.808715	-0.579818	0.819838
H	4.019544	-0.334906	-0.918753
H	3.208735	-1.789520	-0.324579
H	-3.286194	-1.495024	-0.964580
H	-2.647740	0.023959	-1.810446
H	-1.894636	-2.198586	1.278389
H	-1.207856	-0.715370	1.979297
H	-0.192729	-1.761598	0.986571

Frequencies

-435.94	33.3574	76.5873
129.9863	133.3908	142.8912
172.3298	201.462	260.5091
325.9889	333.8185	349.8603
426.1379	543.4631	565.9799
608.6234	724.3133	843.4183
902.7271	913.1049	942.6011
980.0084	1039.446	1062.204
1062.739	1066.895	1119.624
1190.602	1275.514	1392.56
1423.51	1431.189	1433.801
1462.606	1481.757	1491.38
1492.669	1562.888	1758.578
2379.853	3022.32	3048.013
3092.147	3096.769	3115.826
3120.14	3120.835	3167.623
3173.658	3182.911	3270.067

i1 – p15

C	0.827107	1.900876	-0.578200

```
C    0.467676    0.707034   -0.032556
C   -3.488431   -0.349414    0.181035
C   -2.083807    0.030079    0.105914
C   -0.927215    0.352307    0.054348
C    1.471065   -0.408123    0.077390
C    2.638602   -0.225595    0.686895
C    1.084958   -1.706243   -0.575790
H    0.089258    2.671470   -0.763446
H    1.867541    2.114147   -0.789075
H    0.502022    1.177645    1.762192
H   -4.041586    0.026880   -0.682951
H   -3.950232    0.057166    1.084368
H   -3.594862   -1.436593    0.206510
H    3.385279   -1.011589    0.714313
H    2.873984    0.706355    1.188949
H    1.900035   -2.428843   -0.516067
H    0.827113   -1.550099   -1.627862
H    0.201716   -2.132072   -0.091146
```

Frequencies

-1075.8	31.2903	48.0291
89.8311	150.6231	192.2274
260.3004	301.9252	317.8944
387.3962	408.8642	457.7713
484.1152	513.8881	578.3638
621.3782	671.917	704.0058
764.946	847.9078	903.1758
941.742	968.2118	1032.421
1055.118	1058.521	1070.817
1083.883	1231.687	1332.062
1408.704	1419.63	1425.257
1447.504	1481.204	1483.222
1484.424	1498.317	1577.423
1735.763	2380.994	3044
3047.706	3108.8	3120.683
3122.983	3141.248	3152.908
3164.758	3242.021	3269.844

i10 – p40

```
C    2.465802   -1.333571   -0.055197
C    1.424900   -0.723456   -0.609474
C    0.658636    0.398136   -0.008794
C    0.044822    1.402548   -0.990434
C    1.096085    0.909903    1.344798
C   -3.090220   -0.708872    0.187542
C   -1.948049   -0.117212   -0.089551
C   -0.805020    0.415152   -0.310394
H    2.968221   -2.147635   -0.564083
H    2.852128   -1.050656    0.917974
H    1.071313   -1.053136   -1.584331
H   -0.019844    2.436156   -0.665256
H    0.238154    1.264006   -2.049710
H    0.447716    1.723313    1.675719
H    2.124276    1.281104    1.301837
H    1.045591    0.113766    2.091801
H   -3.747758   -0.315702    0.955157
H   -3.472763   -1.501710   -0.445896
H   -2.588770   -2.205272    1.555806
```

Frequencies

-532.445	73.7158	101.622
151.8368	192.1581	255.0327
270.7402	287.5533	312.1471
365.9901	373.9401	449.39
464.7378	582.1255	619.951
689.51	725.4503	764.6853

901.5466	909.4986	938.9119
948.4242	975.8576	1011.078
1029.236	1037.473	1057.685
1058.389	1107.68	1204.369
1313.763	1337.834	1380.578
1420.377	1451.503	1462.366
1494.28	1508.789	1533.246
1728.288	2102.522	3045.513
3120.406	3121.736	3135.992
3146.857	3151.281	3164.369
3212.332	3233.025	3245.973

i11 – i10
```
C     2.185829   -1.527073   -0.201004
C     1.383935   -0.586928   -0.719228
C     0.750686    0.488743    0.017678
C     0.118101    1.624422   -0.748878
C     1.036178    0.674364    1.480466
C    -2.739349   -1.083292    0.283758
C    -2.004587    0.078609   -0.217943
C    -0.934260    0.697020   -0.397211
H     2.613152   -2.299747   -0.828428
H     2.442649   -1.549895    0.852460
H     1.166946   -0.618833   -1.785452
H     0.104882    2.590421   -0.247976
H     0.366594    1.700273   -1.806087
H     0.398876    1.450845    1.907656
H     2.082735    0.963198    1.635842
H     0.858983   -0.248842    2.038802
H    -3.449130   -0.791232    1.062211
H    -2.055180   -1.831975    0.703561
H    -3.309709   -1.559399   -0.518417
```

Frequencies

-674.989	65.392	94.8079
106.3635	156.0476	189.7353
232.0662	279.8304	306.5326
400.0833	419.4551	448.8706
521.7674	670.7621	722.0728
749.3807	892.2257	942.3724
985.8026	1018.351	1032.043
1034.469	1055.251	1061.569
1077.232	1132.752	1192.534
1270.217	1340.168	1346.38
1409.933	1422.522	1450.634
1475.495	1477.554	1480.704
1486.555	1512.463	1654.901
2022.33	3012.874	3032.961
3091.548	3100.058	3102.421
3117.976	3138.049	3153.356
3165.485	3176.094	3252.337

i11 – i12
```
C    -1.152164    1.729304   -0.655755
C    -1.150738    0.469226    0.146498
C     2.276661   -0.201656    0.103161
C     1.221811    0.022887    0.632336
C    -0.098332    0.302376    1.215881
C     3.564203   -0.476930   -0.525128
H    -0.959444    2.602681   -0.025221
H    -2.105617    1.870131   -1.170710
H    -0.363399    1.709460   -1.424428
```

```
H    -0.034126   1.215182   1.819643
H    -0.375463  -0.514227   1.889783
H     4.261486   0.349621  -0.367110
H     3.448510  -0.620688  -1.602310
H     4.013901  -1.382468  -0.110219
C    -1.733712  -0.750275  -0.443603
C    -2.914176  -1.263450  -0.115388
H    -1.133651  -1.257568  -1.205571
H    -3.544894  -0.794731   0.633930
H    -3.288628  -2.166278  -0.585807
```

Frequencies

-147.058	34.3044	81.6436
95.9098	157.5185	189.9641
203.4845	263.6702	309.9992
356.8782	398.925	439.0489
575.1925	708.1482	739.5433
770.1566	919.7596	970.0317
977.3853	994.7873	1018.245
1059.745	1063.33	1075.173
1159.047	1177.745	1247.552
1308.255	1320.203	1333.595
1405.848	1423.166	1451.167
1465.36	1483.828	1488.602
1491.423	1493.001	1719.525
2387.067	2984.956	3039.476
3051.407	3073.881	3082.41
3091.709	3122.554	3124.537
3124.85	3151.953	3240.859

i4 – i3

```
C     0.040129  -1.462743  -0.208030
C    -1.015420  -0.818195   0.649291
C     3.577539   0.658017  -0.006556
C     2.332781  -0.097903  -0.090050
C     1.311666  -0.726756  -0.160344
H    -0.308210  -1.517357  -1.244730
H     0.216727  -2.491203   0.125823
H    -0.913761  -0.916466   1.727002
H     4.313675   0.128606   0.603530
H     3.407787   1.638858   0.444792
H     4.008813   0.812069  -0.998776
C    -1.880504   0.251152   0.109233
C    -3.118329  -0.000150  -0.311868
C    -1.269839   1.631967   0.050264
H    -3.747927   0.787618  -0.714311
H    -3.540895  -0.997802  -0.261479
H    -1.973223   2.361723  -0.356785
H    -0.366105   1.624265  -0.566801
H    -0.965018   1.957360   1.050098
```

Frequencies

-93.2091	47.5529	101.7009
108.1742	180.9254	212.6218
234.5857	288.5656	303.2885
396.2759	415.1969	459.2143
557.2799	603.078	727.8384
755.8939	793.9416	927.5875
939.4851	998.8341	1028.31
1058.64	1064.915	1077.889
1091.329	1163.033	1218.329
1262.674	1311.145	1387.473

1413.66	1422.621	1443.562
1466.724	1487.12	1489.143
1491.08	1500.609	1725.713
2387.273	3038.665	3043.785
3048.725	3088.091	3105.533
3118.477	3124.09	3128.121
3150.048	3167.927	3238.953

i4 – i6

```
C    -2.438533   -1.163158   -0.330708
C    -1.277325   -0.303569    0.109813
C    -0.141046   -0.997146    0.701947
C     1.645328    0.028528   -0.111499
C     1.152478    1.158086   -0.118441
C    -0.082676    1.925301    0.104008
C    -1.290621    1.026981   -0.083231
C     2.688657   -0.992667   -0.263233
H    -2.880607   -1.700231    0.513793
H    -2.098957   -1.915388   -1.051013
H    -3.219840   -0.567075   -0.806722
H    -0.036490   -2.059430    0.489793
H     0.197024   -0.701812    1.688950
H    -0.060383    2.364497    1.110556
H    -0.150670    2.767289   -0.590898
H    -2.177746    1.496416   -0.497986
H     3.628027   -0.527674   -0.570979
H     2.404210   -1.730956   -1.016732
H     2.857863   -1.519779    0.679304
```

Frequencies

-642.031	77.5611	164.9747
169.1398	189.8538	213.0475
230.2698	345.8609	387.0732
416.3187	455.4259	490.6052
606.7755	681.1735	744.8598
790.1591	841.1022	870.6072
950.3452	981.1273	996.0668
1041.763	1069.888	1071.621
1103.035	1150.079	1210.874
1220.292	1322.806	1366.226
1415.855	1419.413	1472.542
1479.366	1483.936	1487.394
1495.445	1500.138	1672.385
2124.887	3026.299	3037.423
3052.587	3085.653	3099.628
3123.747	3127.278	3132.195
3133.526	3181.937	3220.423

i6 – i8

```
C     2.439616   -1.043501    0.194732
C     1.214445   -0.208181   -0.018955
C    -0.010605   -0.931116   -0.555399
C    -1.282118   -0.218805   -0.136517
C    -1.259102    1.132178   -0.202589
C    -0.046132    1.861784   -0.072356
C     1.183621    1.114008    0.208406
C    -2.435181   -1.030568    0.361705
H     2.715440   -1.561872   -0.730505
H     2.250457   -1.818081    0.946202
H     3.291172   -0.444197    0.521681
H    -0.022784   -1.961175   -0.177024
H     0.080672   -1.026405   -1.648754
H     0.013147    2.884462   -0.435542
H    -1.020719    1.991013    0.802389
H     2.063396    1.636212    0.570901
```

```
H    -3.267058   -0.388401    0.653910
H    -2.138135   -1.636428    1.226939
H    -2.792854   -1.729929   -0.404346
```

Frequencies

-1818.04	93.0292	162.7188
196.0278	224.9553	282.9233
319.5589	379.4166	453.1106
465.6395	511.8668	554.1508
691.4772	746.7065	832.0497
876.5234	885.9863	911.8095
960.5316	1004.201	1034.332
1065.364	1075.386	1154.665
1163.953	1207.255	1224.227
1239.391	1319.03	1368.545
1397.779	1409.911	1416.95
1463.762	1478.208	1483.054
1488.934	1494.367	1578.704
1698.105	2099.084	2983.686
3015.395	3032.202	3048.145
3065.04	3089.997	3133.631
3139.302	3166.261	3191.352

i6 – i7

```
C     2.638230   -0.788217   -0.000004
C     1.262503   -0.183493   -0.000004
C     0.122481   -1.184604    0.000011
C    -1.188455   -0.478037    0.000006
C    -1.337973    0.830560    0.000004
C    -0.257193    1.857130    0.000004
C     1.076904    1.138219   -0.000006
C    -2.628855   -0.887377   -0.000009
H     2.782251   -1.425001   -0.879946
H     2.782288   -1.424908    0.879999
H     3.417451   -0.023916   -0.000058
H     0.212777   -1.845742    0.873306
H     0.212771   -1.845766   -0.873266
H    -0.331394    2.513031   -0.875605
H    -0.331384    2.513023    0.875620
H     1.954219    1.782012   -0.000014
H    -2.717059    0.521359   -0.000010
H    -3.053897   -1.294591    0.918202
H    -3.053876   -1.294589   -0.918232
```

Frequencies

-2256.92	77.4138	119.8993
190.2783	252.8833	306.1788
388.3743	419.8058	443.4742
472.3626	487.2263	552.0982
723.8559	800.6449	839.8882
903.7115	936.4053	956.0645
964.9409	986.5816	1043.791
1067.153	1079.631	1086.132
1086.972	1164.007	1200.931
1225.344	1242.03	1319.626
1356.551	1407.712	1422.292
1446.162	1466.731	1468.538
1484.013	1491.022	1751.232
1804.249	1876.04	3014.227

3036.196	3036.351	3036.391
3062.096	3077.25	3092.675
3136.965	3149.186	3169.979

i10 – i9

```
C   -2.649925  -1.159308  -0.243222
C   -1.490056  -0.892383   0.340822
C   -0.651654   0.332769   0.112192
C   -0.067102   0.920182   1.367987
C   -1.203115   1.337178  -0.887092
C    3.365920  -0.496866  -0.277800
C    1.922572  -0.295794  -0.315213
C    0.773368   0.042202  -0.020204
H   -3.189514  -2.070979  -0.013758
H   -3.103186  -0.490567  -0.966825
H   -1.073034  -1.599538   1.054568
H    0.184018   1.971712   1.392829
H   -0.068939   0.348945   2.286222
H   -0.512351   2.174979  -0.996269
H   -2.166321   1.722077  -0.541218
H   -1.334550   0.873845  -1.867545
H    3.846599  -0.028951  -1.141164
H    3.610459  -1.562236  -0.301540
H    3.806764  -0.067167   0.629873
```

Frequencies

-684.988	78.4559	82.7192
106.872	138.441	262.7133
277.2584	289.3994	308.6293
371.5363	399.4933	436.7246
481.7435	628.3544	644.3966
676.6092	736.7171	825.6045
940.144	957.4773	982.9087
1035.64	1044.768	1047.736
1061.689	1082.037	1171.186
1279.821	1294.187	1353.157
1412.539	1418.761	1441.643
1458.2	1477.746	1483.157
1497.033	1509.516	1736.235
2098.894	3022.514	3051.045
3092.328	3115.922	3130.002
3144.216	3152.199	3166.286
3167.446	3247.57	3288.69

i12 – i17

```
C   -2.852099  -0.046859   0.437088
C   -1.431240   0.068580  -0.027616
C   -0.746561   1.228825   0.001601
C    0.600343   1.412822  -0.487507
C    1.632374  -0.439932   0.092854
C    0.677635  -1.200152  -0.093577
C   -0.753780  -1.234963  -0.431514
C    3.020713  -0.083811   0.412744
H   -3.490562  -0.457395  -0.354097
H   -3.260501   0.923175   0.727169
H   -2.932294  -0.727207   1.292883
H   -1.220597   2.084054   0.481714
H    0.831167   1.147158  -1.513373
H    1.161333   2.263881  -0.109553
H   -1.256848  -2.068055   0.069979
H   -0.871421  -1.416486  -1.508684
H    3.597870  -0.985089   0.632251
H    3.063030   0.575595   1.283020
H    3.494525   0.433311  -0.425753
```

Frequencies

-677.016	74.5539	138.5372

151.4244	193.0927	214.6667
251.8043	347.0251	375.2344
405.7434	434.3718	505.5519
629.0838	636.2828	761.1252
797.0334	815.8054	886.8709
935.9816	981.0006	1036.397
1052.057	1064.275	1071.393
1151.095	1159.711	1202.215
1227.792	1327.41	1362.259
1414.712	1416.409	1472.162
1480.254	1481.486	1485.947
1489.15	1497.196	1659.452
2108.778	3023.868	3028.917
3047.567	3072.203	3081.691
3118.732	3128.414	3128.891
3133.089	3139.015	3217.51

i17 – i18

C	2.861398	-0.129874	-0.000151
C	1.364426	0.007268	-0.000001
C	0.764614	1.199567	0.000000
C	-0.725961	1.445448	0.000129
C	-1.446159	0.141932	0.000111
C	-0.856938	-1.035978	0.000167
C	0.607222	-1.313806	0.000123
C	-2.876541	-0.301790	-0.000220
H	3.200693	-0.687309	0.879917
H	3.356288	0.843214	-0.000022
H	3.200540	-0.687013	-0.880466
H	1.391880	2.088122	-0.000115
H	-1.007827	2.048218	0.873929
H	-1.007981	2.048256	-0.873594
H	0.901344	-1.906452	-0.875405
H	0.901418	-1.906327	0.875713
H	-3.454077	-0.193482	0.918520
H	-2.180927	-1.530647	-0.000269
H	-3.453721	-0.193180	-0.919151

Frequencies

-2281.91	74.5615	149.72
198.2813	257.0886	315.1591
385.0558	406.8803	447.626
458.9099	482.6761	595.1089
735.2443	783.8861	809.0648
915.0014	946.9913	956.343
958.4254	982.9209	1057.642
1063.82	1071.947	1088.774
1093.711	1168.514	1214.887
1220.723	1238.595	1318.702
1372.769	1400.446	1423.243
1435.657	1469.102	1472.558
1479.922	1497.113	1752.891
1805.641	1874.582	3015.856
3024.125	3033.321	3037.748
3050.332	3081.938	3089.316
3135.014	3154.362	3176.26

i17 – i19

```
C    2.850728    0.013891   -0.407270
C    1.401333    0.057919   -0.017249
C    0.674629    1.182100    0.047363
C   -0.786070    1.200918    0.446275
C   -1.440210   -0.123477    0.096524
C   -0.702049   -1.228609    0.342502
C    0.717936   -1.198657    0.345230
C   -2.800408   -0.122809   -0.524238
H    3.447329   -0.483995    0.364201
H    3.256828    1.016276   -0.556040
H    2.987966   -0.551059   -1.334865
H    1.143917    2.137153   -0.176047
H   -0.876528    1.435028    1.518091
H   -1.303639    2.016697   -0.071820
H    0.044190   -1.937943   -0.514284
H    1.276378   -1.979998    0.856981
H   -3.536752    0.357805    0.131802
H   -3.136662   -1.140118   -0.728514
H   -2.798358    0.442496   -1.464335
```

Frequencies

-1851.11	100.1097	151.5409
155.8352	241.1512	256.3712
295.6796	365.2282	438.2125
456.1039	525.4716	575.9572
691.1847	752.6188	789.7945
839.9615	910.353	938.0847
963.5191	998.4452	1044.566
1066.574	1075.759	1155.928
1183.533	1204.881	1213.668
1235.104	1337.243	1347.774
1401.23	1411.854	1423.287
1471.821	1479.967	1485.257
1488.814	1496.573	1583.756
1709.882	2103.192	2991.666
3021.059	3040.922	3051.088
3071.793	3101.535	3132.166
3142.481	3150.177	3170.061

i7 – p3

```
C    2.565629   -0.856711   -0.104207
C    1.234985   -0.175611   -0.023961
C    0.052565   -1.043720    0.328766
C   -1.302945   -0.446338    0.014257
C   -1.375029    1.003905   -0.044421
C   -0.251233    1.758944   -0.088486
C    1.071091    1.141621   -0.178188
C   -2.386265   -1.210065   -0.178147
H    2.573013   -1.600578   -0.908470
H    2.781663   -1.393824    0.826530
H    3.372979   -0.145031   -0.285282
H    0.103087   -1.224079    1.414201
H    0.150324   -2.028226   -0.139381
H   -2.353701    1.469675   -0.089147
H   -0.329575    2.830820   -0.229222
H   -0.185680    2.336998    1.950558
H    1.924519    1.781694   -0.376033
H   -3.361987   -0.766445   -0.344192
H   -2.327432   -2.293153   -0.173239
```

Frequencies

-594.292	77.2221	161.6409
195.7223	220.253	289.1179
297.5619	374.4621	418.1956
481.6659	487.3599	512.1192
576.8434	686.1358	736.8592

821.2468	868.8919	878.9565
904.2307	929.561	953.2568
980.2637	999.304	1010.317
1068.629	1077.473	1180.038
1200.744	1239.379	1321.12
1338.839	1382.23	1419.034
1431.98	1453.843	1470.117
1483.541	1494.48	1590.217
1680.191	1741.303	2992.682
3028.819	3076.374	3085.751
3132.87	3150.194	3182.394
3189.087	3208.5	3239.366

i8 – p1
```
C     2.514641  -1.009682  -0.068819
C     1.227413  -0.234940  -0.047447
C     0.000000  -0.922647  -0.023528
C    -1.227413  -0.234940  -0.047447
C    -1.207883   1.152327   0.002142
C     0.000000   1.841750   0.034607
C     1.207883   1.152327   0.002142
C    -2.514641  -1.009682  -0.068819
H     2.532029  -1.725835  -0.895077
H     2.631402  -1.577964   0.859921
H     3.377226  -0.349139  -0.172769
H     0.000000  -1.432869   1.820580
H     0.000000  -1.997229  -0.186404
H    -2.143603   1.701704   0.007195
H     0.000000   2.925495   0.070311
H     2.143603   1.701704   0.007195
H    -3.377226  -0.349139  -0.172770
H    -2.631403  -1.577963   0.859922
H    -2.532028  -1.725835  -0.895076
```

Frequencies

-723.097	71.8511	78.1466
181.7583	224.6108	275.5878
300.1297	358.9788	416.8444
489.8595	527.2639	543.0044
548.3253	726.9405	744.2945
792.0956	920.5589	927.324
969.7551	996.8228	1003.57
1026.68	1042.196	1063.988
1068.398	1130.236	1186.081
1200.327	1288.249	1324.52
1345.546	1417.023	1419.373
1448.115	1488.994	1489.519
1495.05	1509.196	1545.477
1657.922	1658.373	3038.807
3039.447	3103.54	3103.714
3134.663	3134.888	3165.047
3180.126	3188.257	3206.962

i18 – p6
```
C     2.838128  -0.013347  -0.239588
C     1.349323  -0.081400  -0.061106
C     0.666955  -1.226541   0.010432
C    -0.813904  -1.270202   0.264482
C    -1.536295   0.031071  -0.016068
C    -0.730882   1.241851   0.018942
C     0.619752   1.192096   0.040956
```

```
C    -2.850844    0.079069   -0.265562
H     3.099944    0.544477   -1.144574
H     3.277712   -1.009595   -0.312225
H     3.301090    0.505799    0.606455
H     1.188555   -2.176714   -0.057135
H    -1.277142   -2.086207   -0.297377
H    -0.962330   -1.518431    1.326602
H    -1.243200    2.198062   -0.010225
H     0.981592    1.511031    2.140230
H     1.191340    2.112245   -0.026550
H    -3.360228    1.025997   -0.408396
H    -3.450732   -0.822242   -0.331725
```

Frequencies

-539.124	62.588	171.3562
199.9894	230.9786	267.1546
308.3102	317.9989	408.4914
429.7671	490.1952	573.6736
625.2268	702.3437	744.9249
783.6702	815.6526	834.0671
910.5515	941.724	960.447
983.8524	999.7156	1012.906
1073.695	1088.889	1196.108
1200.508	1232.769	1313.081
1345.462	1371.674	1420.177
1431.168	1457.352	1474.305
1485.571	1499.735	1600.724
1684.304	1753.137	2996.696
3034.343	3082.663	3094.564
3134.171	3149.613	3175.837
3177.032	3196.638	3238.769

i19 – p2
```
C    -2.939346    0.001395   -0.008035
C    -1.433060   -0.005902   -0.023357
C    -0.705809    1.172894   -0.099944
C     0.696810    1.162647   -0.054613
C     1.402249   -0.057093   -0.048138
C     0.665164   -1.230819    0.025643
C    -0.725489   -1.208685    0.048650
C     2.904123   -0.057203   -0.059476
H    -3.346329   -0.780330   -0.654236
H    -3.335035    0.961148   -0.346131
H    -3.317710   -0.176878    1.003283
H    -1.224935    2.123313   -0.168257
H     1.237794    2.083519   -0.248538
H     0.997783    1.606483    1.742231
H     1.183524   -2.184062    0.056456
H    -1.272239   -2.145062    0.103714
H     3.294599    0.518924   -0.903086
H     3.303211   -1.070883   -0.126906
H     3.291489    0.400421    0.857088
```

Frequencies

-830.99	33.7783	83.1182
137.9549	277.255	294.5886
312.7605	379.5933	413.1963
454.7494	467.7179	534.7883
659.3395	723.7633	742.8255
828.2979	844.8143	883.0991
973.3059	993.431	1016.652
1030.38	1046.082	1066.514
1070.623	1140.76	1211.509

1234.738	1248.486	1324.612
1342.391	1418.979	1421.094
1437.138	1489.286	1492.428
1495.407	1506.755	1562.488
1628.713	1675.072	3037.874
3044.138	3101.913	3110.262
3132.555	3133.234	3173.953
3175.546	3190.939	3194.15

i8 – i32

```
C   -2.522478  -1.034962  -0.165265
C   -1.278559  -0.256939   0.143038
C    0.052978  -0.987059   0.139285
C    1.274185  -0.232739   0.009871
C    1.236743   1.123392  -0.029999
C   -0.032500   1.840949  -0.023103
C   -1.210023   1.173461   0.023298
C    2.561043  -1.001382  -0.080927
H   -2.532218  -1.997274   0.355777
H   -2.597786  -1.248742  -1.240042
H   -3.417760  -0.484971   0.135033
H    0.038673  -2.061508   0.002906
H   -0.636474  -0.654347   1.188052
H    2.159822   1.686989  -0.105479
H   -0.024076   2.922645  -0.085349
H   -2.147977   1.718444  -0.030897
H    3.421778  -0.333352  -0.139627
H    2.562833  -1.643736  -0.967633
H    2.684855  -1.652480   0.790076
```

Frequencies

-2570.45	126.8398	140.8083
180.8906	211.5815	265.3566
321.62	385.5976	485.5923
496.7639	516.1098	610.93
685.2722	716.9955	745.1167
830.8386	869.0689	940.5473
967.6035	981.0734	1021.812
1044.363	1061.603	1069.76
1152.375	1185.48	1221.558
1248.968	1298.453	1314.907
1390.063	1415.013	1425.467
1457.38	1482.751	1486.394
1497.16	1503.02	1601.065
1628.462	2206.181	3004.853
3036.822	3075.355	3098.188
3116.738	3136.318	3173.36
3190.34	3203.391	3210.394

i18 – i37

```
C   -2.834240  -0.012514  -0.302781
C   -1.371614   0.056952   0.055761
C   -0.640292   1.230299  -0.031870
C    0.823704   1.250115   0.296084
C    1.532590  -0.059201  -0.023023
C    0.752831  -1.260253   0.104281
C   -0.629146  -1.223136   0.188199
C    2.841870  -0.076515  -0.341912
H   -2.947104  -0.212877  -1.372134
H   -3.339805   0.926818  -0.072012
H   -3.342146  -0.813651   0.240587
H   -1.153993   2.166779  -0.214616
H    1.319524   2.080010  -0.214840
H    0.954601   1.443590   1.375217
```

```
H      1.257931   -2.219142    0.112352
H     -1.164630   -0.501851    1.239606
H     -1.218103   -2.133196    0.187974
H      3.366486   -1.010895   -0.510604
H      3.413016    0.839928   -0.439968
```

Frequencies

-1929.63	84.2207	171.8189
198.8154	283.7729	318.0246
405.5229	427.5348	493.4521
562.6892	606.0233	641.3738
674.3518	746.8996	760.7051
788.6859	860.1443	884.4449
926.3654	944.1152	987.6594
1004.994	1067.663	1085.863
1140.911	1168.949	1205.078
1234.68	1296.735	1333.391
1350.372	1399.933	1425.096
1446.688	1472.502	1488.793
1496.93	1522.588	1562.422
1625.02	1797.361	2946.923
3045.339	3080.837	3114.068
3134.469	3148.613	3191.513
3198.642	3208.894	3238.649

i19 – i38

```
C     -2.940202    0.025189   -0.096683
C     -1.445123   -0.039173   -0.011569
C     -0.755600   -1.205100   -0.014665
C      0.676191   -1.257342    0.097828
C      1.448763    0.046470    0.134189
C      0.655798    1.241606    0.073415
C     -0.698249    1.224338    0.044498
C      2.910865    0.030441   -0.199335
H     -3.362037    0.527889    0.781534
H     -3.382845   -0.970765   -0.162598
H     -3.258113    0.599580   -0.974368
H     -1.290336   -2.146394   -0.101911
H      1.127379   -0.652023    1.163392
H      1.229413   -2.170307   -0.077804
H      1.184306    2.190741    0.049821
H     -1.253204    2.156028    0.026239
H      3.421508   -0.807779    0.284630
H      3.401495    0.951219    0.125858
H      3.067777   -0.076760   -1.280862
```

Frequencies

-2664.31	103.3298	172.0547
189.2124	252.8315	275.3707
348.9925	371.4981	405.3156
434.7162	612.1496	633.5801
675.5163	707.8419	752.2534
787.2885	890.6399	928.6603
966.7737	977.6013	1019.871
1048.345	1063.236	1092.644
1170.053	1186.114	1222.133
1255.104	1295.989	1336.587
1388.784	1418.844	1424.499
1463.189	1480.978	1486.626
1498.419	1503.813	1591.179

1638.505	2199.493	3007.423
3021.793	3074.994	3076.1
3116.689	3125.939	3168.317
3175.017	3195.82	3218.859

i7 – i30

```
C     2.537880   -0.902618    0.148159
C     1.218226   -0.212070    0.039308
C     0.018558   -1.046436   -0.318930
C    -1.326299   -0.400699   -0.013170
C    -1.384735    1.034815   -0.002279
C    -0.236869    1.808916    0.009983
C     1.097400    1.165898    0.071530
C    -2.418057   -1.166936    0.185009
H     2.788583   -1.431736   -0.782036
H     2.521859   -1.659289    0.941525
H     3.347267   -0.202050    0.365820
H     0.082595   -2.021298    0.177010
H     0.054456   -1.267067   -1.400658
H    -2.352900    1.520461    0.031012
H     0.609709    1.668446   -1.060779
H    -0.280572    2.881997    0.149007
H     1.943000    1.796340    0.324503
H    -3.392876   -0.721393    0.351330
H    -2.357738   -2.249635    0.185610
```

Frequencies

-1946.12	82.9745	163.2867
200.4973	277.9997	308.2269
414.0912	462.9222	481.9342
508.5414	573.0457	650.1073
721.4634	732.8031	808.2979
857.9705	866.3154	908.7672
949.0721	963.6323	986.6479
1007.535	1044.859	1060.574
1127.737	1190.356	1202.797
1237.039	1303.96	1324.737
1361.959	1399.151	1419.907
1447.249	1473.845	1478.098
1494.617	1531.46	1574.456
1623.086	1796.102	2948.933
3006.92	3059.264	3062.056
3123.962	3150.931	3192.179
3204.273	3223.985	3241.312

i7 – i31

```
C    -2.549159   -0.871955   -0.131672
C    -1.231548   -0.170797   -0.011536
C    -0.046915   -1.036584    0.342680
C     1.307220   -0.425541    0.025327
C     1.393138    1.009319    0.038893
C     0.162417    1.830206   -0.001657
C    -1.106228    1.170688   -0.111908
C     2.373339   -1.206990   -0.239457
H    -2.788357   -1.418468    0.789287
H    -2.524555   -1.613286   -0.938851
H    -3.362927   -0.172643   -0.333941
H    -0.131036   -2.007541   -0.157215
H    -0.091069   -1.257507    1.422002
H     2.339560    1.501657   -0.148873
H     0.825722    1.571816    1.092455
H     0.268386    2.887272   -0.205728
H    -1.985130    1.785664   -0.276652
H     3.348640   -0.779737   -0.445665
H     2.287181   -2.287304   -0.260840
```

Frequencies

-1886.66	81.306	174.8912
210.5956	291.2886	327.5392
415.9977	461.7037	479.2132
501.8966	548.0304	639.8229
697.0269	726.8551	834.6501
844.6633	863.9994	894.7973
927.0543	948.1691	964.056
1013.85	1049.451	1064.195
1142.533	1188.524	1234.563
1245.739	1301.923	1334.844
1370.014	1398.735	1419.484
1436.326	1466.454	1479.415
1483.986	1498.35	1635.395
1651.666	2123.277	2974.906
3022.246	3063.613	3074.986
3130.181	3154.96	3190.393
3207.2	3229.911	3245.126

i38 – p42

```
C    2.754923   -0.000057    0.515048
C    1.327583    0.000080    0.038736
C    0.646204   -1.201282   -0.196554
C   -0.674774   -1.211378   -0.595674
C   -1.402760    0.000035   -0.692223
C   -0.674846    1.211450   -0.595589
C    0.646162    1.201385   -0.196424
C   -2.494203   -0.000127    1.194593
H    3.292425   -0.882921    0.160710
H    2.803176   -0.003941    1.609393
H    3.290521    0.886431    0.166999
H    1.177397   -2.141440   -0.081221
H   -1.177248   -2.152574   -0.789067
H   -2.355161    0.000024   -1.209794
H   -1.177350    2.152642   -0.788917
H    1.177284    2.141567   -0.080981
H   -3.070009   -0.919127    1.146816
H   -3.070150    0.918786    1.146876
H   -1.660622   -0.000085    1.887710
```

Frequencies

-581.638	52.0435	87.8642
140.0722	169.1611	226.7923
349.7375	422.9284	436.0288
520.2384	566.0435	604.4288
634.9271	689.868	782.3013
797.8959	837.4894	880.9895
957.8567	985.2093	994.9585
1003.975	1026.941	1033.243
1061.953	1108.619	1178.939
1207.456	1248.286	1311.955
1358.011	1420.055	1426.193
1428.706	1479.247	1493.394
1508.13	1514.225	1597.059
1646.535	3036.63	3081.617
3101.49	3127.591	3172.531
3173.385	3184.654	3198.658

| 3206.323 | 3237.479 | 3249.598 |

i38 – p2

C	2.943502	-0.000104	0.008803
C	1.438791	0.000246	0.026316
C	0.718807	-1.197543	0.032387
C	-0.662634	-1.203575	0.008137
C	-1.394807	0.000008	-0.078407
C	-0.662880	1.203612	0.008195
C	0.718691	1.197803	0.032343
C	-2.890463	-0.000186	0.145075
H	3.319229	-0.012015	-1.019587
H	3.346840	-0.879392	0.516274
H	3.347136	0.890297	0.496112
H	1.256220	-2.140300	0.065557
H	-1.200216	-2.146111	0.018619
H	-1.560755	-0.000068	-1.887480
H	-1.200573	2.146081	0.018743
H	1.255909	2.140660	0.065441
H	-3.355968	-0.883877	-0.294868
H	-3.356088	0.883776	-0.294193
H	-3.105775	-0.000615	1.218280

Frequencies

-966.938	51.8738	127.0476
183.6667	286.7652	305.9737
375.9995	410.9792	442.9888
456.9941	514.1546	552.3559
657.4287	719.3778	740.802
821.7594	844.5084	849.4608
973.4791	989.9427	995.684
1030.876	1036.27	1064.517
1068.093	1153.236	1210.38
1238.815	1250.025	1311.156
1343.156	1419.988	1421.179
1454.085	1491.483	1493.977
1495.402	1508.103	1547.183
1615.623	1673.088	3041.327
3046.454	3107.587	3118.628
3131.459	3142.044	3175.738
3175.846	3193.621	3196.784

i37 – p45

C	-2.346637	0.321810	1.303982
C	-1.364434	-0.219122	-0.670525
C	-0.641041	-1.351856	-0.430714
C	0.824651	-1.310408	-0.118942
C	1.396854	0.082788	0.066915
C	0.628371	1.196189	-0.493429
C	-0.658423	1.059338	-0.835431
C	2.555954	0.288102	0.698703
H	-1.453654	0.455619	1.902705
H	-2.946355	-0.556744	1.513006
H	-2.887696	1.224176	1.038820
H	-2.362559	-0.305466	-1.083045
H	-1.123047	-2.323235	-0.455146
H	1.045963	-1.922247	0.762786
H	1.360647	-1.796226	-0.948616
H	1.121852	2.159300	-0.576144
H	-1.219824	1.909288	-1.208176
H	2.976518	1.283827	0.790218
H	3.116382	-0.529331	1.140226

Frequencies

-532.672	39.6114	111.596
127.2961	164.0879	271.1685
383.9728	408.186	487.6466

526.7756	546.6807	560.9126
599.3956	693.9896	709.6288
770.7632	815.4854	851.2677
905.686	929.555	948.1655
954.3233	964.7147	989.2527
1005.327	1033.708	1180.658
1196.417	1219.845	1319.888
1344.583	1397.552	1421.271
1423.256	1434.652	1452.516
1469.845	1543.691	1679.577
1724.005	2994.374	3055.048
3088.789	3147.859	3176.148
3183.033	3196.447	3207.203
3235.435	3249.411	3260.619

i37 – p6
```
C    -2.801517   -0.062501   -0.349783
C    -1.346568    0.038535    0.031997
C    -0.654549    1.200503   -0.046836
C     0.815072    1.260446    0.241022
C     1.543061   -0.042414   -0.012831
C     0.743800   -1.259500    0.131804
C    -0.593366   -1.221963    0.174307
C     2.841850   -0.089929   -0.318551
H    -2.891084   -0.453897   -1.368579
H    -3.289942    0.912525   -0.311786
H    -3.339450   -0.742018    0.315046
H    -1.692636    0.198477    1.940717
H    -1.180472    2.133385   -0.223112
H     1.286489    2.076755   -0.312092
H     0.933227    1.510168    1.308287
H     1.267625   -2.209517    0.166397
H    -1.164340   -2.139911    0.270104
H     3.356455   -1.037740   -0.435344
H     3.427432    0.812722   -0.456408
```

Frequencies

-782.405	74.4434	185.1682
225.5014	275.677	309.5929
382.2872	402.7057	412.4924
479.9787	502.4816	564.9302
623.8035	712.7702	746.6687
780.8415	795.2823	824.903
915.6642	944.3268	952.2038
984.5319	1006.618	1011.612
1061.6	1090.428	1193.619
1200.52	1228.163	1312.453
1345.913	1366.621	1420.262
1430.182	1452.823	1471.965
1488.529	1498.981	1619.853
1689.797	1732.447	2979.136
3042.808	3091.986	3112.353
3140.719	3149.106	3176.074
3184.14	3197.681	3237.213

i32 – p42
```
C     2.133354   -1.279218    0.889838
C     1.125594   -0.298720   -0.773935
C    -0.175710   -0.852309   -0.671862
```

```
C    -1.201506   -0.160924   -0.053226
C    -0.957753    1.144936    0.397984
C     0.277336    1.754343    0.181980
C     1.302310    1.064332   -0.436078
C    -2.562980   -0.780420    0.129223
H     2.022397   -2.333153    0.655094
H     1.529020   -0.910755    1.710877
H     3.144072   -0.887649    0.832446
H     1.838160   -0.769031   -1.442218
H    -0.350043   -1.858689   -1.039371
H    -1.754932    1.698774    0.883661
H     0.426728    2.784464    0.487183
H     2.258451    1.542389   -0.615656
H    -2.777945   -0.941320    1.189968
H    -2.632033   -1.745547   -0.376379
H    -3.347750   -0.131607   -0.269142
```

Frequencies

-577.333	37.9523	108.1316
138.741	145.4494	240.6212
349.5952	402.3133	477.2827
525.0235	571.6423	584.3113
644.5639	676.7589	766.104
807.6077	863.4974	885.9665
901.564	991.589	1000.768
1004.862	1008.644	1052.843
1066.2	1105.994	1180.941
1195.595	1234.774	1324.146
1352.261	1419.54	1425.971
1428.692	1463.105	1491.288
1504.086	1527.272	1612.018
1641.887	3043.443	3082.269
3108.559	3131.186	3174.399
3177.206	3188.245	3193.905
3208.863	3238.727	3251.007

i32 – p1
```
C    -2.497876   -1.017345   -0.145293
C    -1.205184   -0.264028    0.075813
C     0.028434   -0.947898    0.002204
C     1.239171   -0.274261   -0.017012
C     1.226243    1.124519   -0.022216
C     0.023460    1.822341   -0.036597
C    -1.181358    1.143190   -0.015163
C     2.545908   -1.023742   -0.019648
H    -2.460407   -2.010218    0.306243
H    -2.675777   -1.137928   -1.218526
H    -3.346707   -0.480275    0.281380
H    -1.353055   -0.327253    1.882242
H     0.020095   -2.034128    0.001246
H     2.165840    1.667551   -0.038071
H     0.030607    2.906120   -0.072702
H    -2.118959    1.688469   -0.029206
H     3.244405   -0.598490   -0.744626
H     2.399898   -2.077378   -0.265241
H     3.021274   -0.973120    0.964722
```

Frequencies

-981.233	42.6135	171.0109
192.9587	215.6632	275.6231
388.4217	439.4285	461.4139
481.6591	529.8271	554.4428
580.9013	701.1786	741.8312
793.4969	892.1052	915.0551
931.4845	1002.029	1006.167

1014.591	1038.645	1067.446
1067.701	1133.134	1187.259
1199.125	1279.678	1316.693
1347.448	1419.041	1421.877
1453.325	1491.972	1493.895
1496.158	1512.236	1530.313
1635.469	1663.594	3045.144
3047.235	3111.76	3119.727
3133.633	3143.384	3174.271
3179.438	3189.453	3206.769

i30 – i36
```
C   -2.560075  -0.846191   0.020922
C   -1.195104  -0.247470   0.122298
C   -0.007394  -1.065304  -0.288521
C    1.333960  -0.399453  -0.033274
C    1.376492   1.050640  -0.124522
C    0.251212   1.809651  -0.081961
C   -1.044894   1.224254   0.118446
C    2.425013  -1.135869   0.214491
H   -2.606547  -1.829771   0.496853
H   -2.842844  -0.976808  -1.034468
H   -3.317386  -0.207596   0.483935
H   -0.092742  -1.241903  -1.376358
H   -0.035864  -2.053008   0.182166
H    2.350072   1.525306  -0.184088
H    0.321018   2.890751  -0.120069
H   -1.079622   0.616605   1.209367
H   -1.943257   1.824008   0.018864
H    3.394811  -0.671532   0.358109
H    2.377101  -2.217601   0.278416
```

Frequencies

-1882.36	99.984	159.3703
202.992	284.0164	307.4447
411.3166	424.8013	464.0123
497.4767	581.5944	672.9759
717.8158	765.5764	837.6516
855.817	887.7154	912.1342
946.1538	959.7825	970.1662
1006.652	1047.653	1084.807
1167.288	1177.516	1221.329
1253.17	1300.301	1325.777
1354.561	1401.788	1418.124
1456.095	1473.765	1480.883
1489.981	1506.037	1586.053
1686.995	2194.752	2938.827
2995.749	3074.168	3078.997
3121.32	3149.224	3186.144
3193.354	3211.697	3237.566

i30 – p3
```
C   -2.536419  -0.883847  -0.015014
C   -1.209866  -0.199816   0.051250
C   -0.000543  -1.082243   0.199649
C    1.342630  -0.400258   0.025403
C    1.366333   1.057073   0.142046
C    0.239618   1.779048   0.110548
C   -1.072836   1.144098  -0.029004
C    2.457537  -1.097723  -0.209664
H   -2.666303  -1.569292   0.829979
H   -2.609788  -1.487142  -0.927711
```

```
H    -3.360318   -0.168455   -0.012799
H    -0.079825   -1.931842   -0.488128
H    -0.044952   -1.521829    1.207891
H     2.333777    1.544105    0.206116
H     0.280867    2.861368    0.157597
H    -1.955217    1.774534   -0.006900
H    -1.277784    1.381439   -1.995773
H     3.420006   -0.604854   -0.292812
H     2.440807   -2.176026   -0.328745
```

Frequencies

-680.825	39.581	121.2738
182.0176	271.9952	296.7835
312.1466	362.6369	419.0748
491.4592	495.9954	526.1404
573.7447	702.6141	733.448
814.7247	872.8831	887.7767
921.7883	929.0248	966.0124
979.4523	1002.27	1010.437
1059.993	1076.073	1183.681
1205.979	1235.157	1317.734
1341.669	1378.287	1417.203
1431.024	1448.795	1469.069
1482.025	1486.861	1638.111
1686.336	1730.457	3001.464
3030.626	3064.271	3086.852
3142.143	3153.317	3183.119
3190.026	3213.307	3241.02

i30 – i35

```
C    -2.511773   -0.957007    0.084021
C    -1.214750   -0.251029   -0.144964
C     0.044434   -1.050954   -0.130621
C     1.344735   -0.424316   -0.004616
C     1.360585    1.045409   -0.070154
C     0.254846    1.788734   -0.027867
C    -1.130116    1.222436    0.129640
C     2.490119   -1.121799    0.142911
H    -2.696717   -1.092790    1.160727
H    -2.515247   -1.951079   -0.372237
H    -3.354166   -0.394361   -0.328326
H    -0.516043   -0.708774   -1.212614
H    -0.049049   -2.122287    0.012641
H     2.331574    1.524918   -0.146254
H     0.338180    2.870728   -0.065458
H    -1.467195    1.412840    1.165379
H    -1.836563    1.772346   -0.504521
H     3.445684   -0.616037    0.216972
H     2.491061   -2.204338    0.203600
```

Frequencies

-1935.45	106.6649	154.842
218.8728	276.5805	318.9613
350.4168	404.3864	456.9397
508.6659	576.3534	643.6226
696.8945	776.5033	804.2774
852.4817	870.1872	911.9176
926.8199	961.1164	1006.937
1016.835	1036.21	1056.128
1159.8	1211.576	1213.716
1268.118	1299.019	1329.235
1366.257	1397.78	1422.063

1455.169	1469.305	1480.464
1487.602	1502.444	1633.412
1740.305	2197.671	2933.594
2988.236	3040.45	3077.388
3119.543	3159.629	3173.264
3188.57	3196.122	3250.381

i31 – i33

C	-2.578962	-0.849335	-0.101843
C	-1.250206	-0.187746	0.124968
C	-0.033901	-1.035692	0.170917
C	1.282745	-0.471896	0.025864
C	1.412609	1.031637	0.206917
C	0.160132	1.789246	-0.136548
C	-1.060063	1.218560	-0.119053
C	2.362859	-1.233463	-0.234722
H	-2.651147	-1.799606	0.434133
H	-2.722966	-1.062634	-1.168047
H	-3.400639	-0.210907	0.230479
H	-0.174853	-2.108620	0.102530
H	-0.691510	-0.585841	1.232890
H	2.258015	1.397853	-0.382783
H	1.673774	1.233674	1.257916
H	0.256692	2.851744	-0.332278
H	-1.947067	1.818508	-0.297246
H	3.346050	-0.792489	-0.352503
H	2.282377	-2.309547	-0.344082

Frequencies

-1888.36	83.5136	159.9186
219.6904	287.0987	309.8815
414.1763	442.3332	501.0148
528.33	554.5279	660.0897
696.5138	720.9859	796.5233
855.2651	863.2358	933.6855
945.3566	965.3899	974.0469
1022.986	1039.011	1057.474
1165.9	1188.178	1228.345
1257.135	1307.392	1339.048
1344.116	1404.071	1425.495
1450.463	1467.199	1477.624
1494.602	1508.317	1635.003
1641.316	2115.737	2980.217
3027.954	3081.237	3097.034
3129.837	3150.907	3181.181
3199.696	3203.572	3240.564

i31 – p3

C	-2.604639	-0.770752	-0.072005
C	-1.254328	-0.129032	-0.009456
C	-0.093002	-1.024238	0.345774
C	1.265701	-0.464470	-0.003421
C	1.378195	0.996315	0.038383
C	0.274187	1.767138	-0.092390
C	-1.052352	1.184631	-0.186455
C	2.302080	-1.241762	-0.322995
H	-2.830111	-1.285694	0.869029
H	-2.637939	-1.528060	-0.862824
H	-3.391623	-0.038547	-0.260794
H	-0.223511	-2.014841	-0.100785
H	-0.130108	-1.177909	1.436408
H	2.367632	1.438188	-0.004454
H	1.584318	1.151415	2.197972
H	0.373624	2.845449	-0.148700
H	-1.891123	1.840413	-0.397148
H	3.283035	-0.818596	-0.510862

SUPPORTING INFORMATION

H   2.200764   -2.318791   -0.402451

Frequencies

-537.547	100.4084	147.3914
206.8674	236.4631	276.496
300.6162	353.6639	418.338
477.8869	488.332	518.4463
587.6054	701.6079	741.7143
801.3142	876.14	879.781
914.0303	934.4336	957.3403
985.2648	989.1289	1015.58
1067.159	1084.166	1181.979
1202.708	1231.679	1319.957
1343.9	1381.935	1421.702
1434.834	1457.083	1473.385
1482.526	1500.615	1596.324
1707.948	1738.296	2992.513
3033.553	3076.407	3090.623
3135.246	3152.184	3184.478
3195.6	3212.697	3240.611

i19 – p6

C	-2.926548	0.049064	-0.083383
C	-1.429492	-0.037928	0.008019
C	-0.760844	-1.194323	-0.009681
C	0.734041	-1.269162	0.127217
C	1.454571	0.044910	-0.086279
C	0.659838	1.259185	0.068062
C	-0.679268	1.219249	0.115857
C	2.762897	0.100348	-0.373414
H	-3.342816	0.534000	0.805806
H	-3.379966	-0.939371	-0.176469
H	-3.229926	0.647349	-0.948770
H	-1.298628	-2.135410	-0.079984
H	0.961871	-1.621559	1.144826
H	1.139416	-2.032616	-0.543616
H	1.184728	2.208793	0.097775
H	-1.244141	2.142868	0.201669
H	3.699309	-0.084883	1.925712
H	3.273017	1.051096	-0.482516
H	3.345981	-0.798323	-0.542815

Frequencies

-309.493	55.2738	107.0304
137.6063	172.3746	237.659
277.4278	308.8099	407.5865
428.4462	480.3408	575.2893
621.6159	725.6004	746.8121
782.5177	811.6791	829.2351
909.6298	945.1701	959.8392
983.6876	1004.458	1015.302
1076.161	1090.947	1203.184
1206.505	1231.259	1317.291
1346.226	1376.076	1425.151
1435.083	1452.819	1476.534
1488.222	1502.31	1662.66
1684.444	1762.981	3002.328
3037.747	3079.951	3097.976

3133.096	3156.555	3178.324
3180.957	3201.341	3246.438

i30 – p43

C	-2.118465	-1.167348	-0.375152
C	-1.182121	-0.394194	0.185291
C	0.111916	-0.941053	0.722093
C	1.300914	-0.277745	0.057996
C	1.150418	1.154087	-0.218832
C	-0.016209	1.791394	-0.107275
C	-1.304067	1.103385	0.263038
C	2.421211	-0.940599	-0.229237
H	-2.019451	-2.247337	-0.392417
H	-1.498928	-1.188958	-2.424298
H	-3.053489	-0.750846	-0.734455
H	0.160227	-2.025416	0.606414
H	0.163733	-0.719202	1.797674
H	2.038289	1.697477	-0.528251
H	-0.068948	2.857717	-0.304595
H	-1.584556	1.397452	1.285466
H	-2.111995	1.451837	-0.386965
H	3.272494	-0.438330	-0.676606
H	2.521042	-2.001962	-0.029510

Frequencies

-460.676	92.3907	100.2039
189.6793	250.1643	305.3323
358.6606	411.7283	438.3215
470.5255	546.2872	571.1321
688.7834	726.1104	770.6119
813.825	860.5979	920.1302
933.3263	939.2083	947.2796
951.204	998.1782	1009.954
1015.483	1027.211	1173.992
1199.482	1231.239	1298.956
1316.861	1338.696	1353.294
1412.159	1450.352	1460.935
1470.329	1482.558	1697.29
1706.679	1751.249	3009.254
3019.245	3089.269	3117.068
3150.843	3155.354	3173.397
3196.94	3240.639	3242.786

i31 – p43

C	-2.400567	-0.764634	-0.377843
C	-1.228209	-0.201428	-0.057566
C	-0.102112	-0.985289	0.578525
C	1.239204	-0.494452	0.099394
C	1.451918	0.984501	0.293890
C	0.225826	1.777580	-0.073682
C	-0.977651	1.226617	-0.251151
C	2.139337	-1.287285	-0.468409
H	-3.517508	-0.593509	1.684854
H	-2.568198	-1.829345	-0.260604
H	-3.202828	-0.181524	-0.817112
H	-0.221898	-2.054440	0.393564
H	-0.164991	-0.829532	1.665275
H	2.309105	1.327355	-0.292666
H	1.700647	1.185345	1.346547
H	0.352483	2.847449	-0.208291
H	-1.819039	1.845326	-0.548846
H	3.092072	-0.902963	-0.818339
H	1.953689	-2.347816	-0.603322

Frequencies

-284.447	98.2215	119.4481
140.3261	181.5556	314.5786

358.1265	406.5297	439.0338
470.2843	546.8477	574.4974
697.7707	724.8166	744.0813
819.3186	864.1913	917.3324
932.5242	939.2216	945.4289
953.0611	998.9313	1012.758
1019.493	1029.798	1176.561
1206.739	1237.139	1301.485
1320.897	1340.468	1357.384
1414.14	1456.852	1463.935
1472.835	1486.096	1678.2
1725.006	1760.007	3008.467
3017.725	3087.142	3117.252
3147.291	3157.924	3170.925
3194.139	3233.703	3248.26

i8 – p3

C	2.572074	-0.934663	-0.064833
C	1.276412	-0.187397	0.000944
C	0.029602	-1.019943	0.165348
C	-1.277948	-0.297102	-0.079407
C	-1.252989	1.157511	0.029543
C	-0.093058	1.831130	0.057445
C	1.193070	1.147263	-0.020205
C	-2.409792	-0.962176	-0.350838
H	2.601104	-1.585465	-0.945805
H	2.690277	-1.582654	0.811276
H	3.426188	-0.256628	-0.108632
H	0.026610	-1.392612	1.201832
H	0.089625	-1.914691	-0.463212
H	-2.201878	1.683690	0.037232
H	-0.097014	2.914727	0.107132
H	2.094394	1.747189	-0.096508
H	-3.350978	-0.439144	-0.479615
H	-3.083170	-1.543657	1.993049
H	-2.419386	-2.038498	-0.484729

Frequencies

-264.732	53.19	110.6568
132.4853	148.2568	203.7069
292.893	336.5894	416.73
465.7359	491.6159	513.2424
578.8419	706.5367	737.1182
814.2171	874.1593	876.3841
909.5433	927.9238	950.801
979.7606	1001.924	1009.057
1066.721	1081.442	1181.454
1204.687	1234.233	1320.16
1341.339	1379.188	1416.321
1433.361	1445.442	1469.216
1483.31	1487.837	1662.682
1682.121	1751.466	2997.047
3031.529	3070.577	3087.373
3136.632	3156.305	3182.459
3191.888	3211.494	3245.15

i33 – p45

C	2.371065	-1.041157	0.986328

```
C    1.002388   -0.381641   -0.848989
C   -0.195207   -1.001998   -0.623196
C   -1.302885   -0.320356    0.008675
C   -1.034585    1.061124    0.579055
C    0.173222    1.745183    0.001214
C    1.126226    1.063928   -0.633843
C   -2.515566   -0.892065    0.104653
H    2.371136   -2.118361    0.873941
H    1.756211   -0.621564    1.772186
H    3.281678   -0.511373    0.731826
H    1.746391   -0.874072   -1.462920
H   -0.340955   -2.032327   -0.931378
H   -0.876388    0.959013    1.663104
H   -1.921940    1.691191    0.469882
H    0.270884    2.814184    0.158901
H    2.012898    1.565163   -1.006300
H   -3.358302   -0.370627    0.545570
H   -2.689554   -1.899328   -0.258195
```

Frequencies

-438.287	63.7536	73.0236
91.5879	149.4269	280.8033
386.4981	447.441	456.2346
475.0298	490.9479	533.9588
600.5418	660.7498	729.5824
775.4801	781.4026	822.7327
880.266	927.5389	945.6481
950.8801	965.7803	993.026
1010.962	1033.763	1174.535
1201.548	1230.119	1321.105
1338.208	1401.366	1412.256
1415.566	1435.119	1461.71
1470.592	1521.912	1648.287
1722.518	3003.962	3087.41
3103.125	3154.639	3185.269
3190.535	3207.254	3221.035
3243.798	3269.235	3280

i33 – p47

```
C   -2.549406   -0.847759   -0.080177
C   -1.172402   -0.253376    0.046070
C   -0.053626   -1.029039    0.070443
C    1.282595   -0.464829    0.011834
C    1.396964    1.028946    0.226940
C    0.158291    1.790642   -0.146409
C   -1.031063    1.193252   -0.190636
C    2.359043   -1.236272   -0.193109
H   -2.562255   -1.895649    0.223152
H   -2.882581   -0.785930   -1.122194
H   -3.272978   -0.302568    0.529956
H   -1.262732   -0.113673    2.069325
H   -0.149970   -2.110198    0.108175
H    2.273928    1.425081   -0.291340
H    1.574998    1.202155    1.300039
H    0.249270    2.857642   -0.319694
H   -1.931397    1.759362   -0.406918
H    3.353873   -0.812396   -0.276303
H    2.267468   -2.313217   -0.283933
```

Frequencies

-721.294	97.2153	150.2086
183.8703	288.6364	336.9192
362.1559	406.1769	437.9556
455.9379	532.319	545.4822
567.1099	686.7606	708.9024
753.3822	863.8459	873.4212

904.7625	939.9723	957.2309
984.1315	1011.704	1026.167
1047.886	1054.148	1190.19
1205.023	1235.502	1317.897
1350.387	1375.649	1409.741
1439.477	1454.071	1463.455
1482.114	1495.225	1594.297
1678.832	1730.976	2996.817
3043.092	3099.536	3114.053
3144.256	3152.41	3180.752
3181.525	3205.7	3242.025

i35 – p44
```
C   -2.065222  -1.270090   1.045752
C   -0.998447  -0.378634  -0.853794
C    0.244971  -0.917714  -0.736273
C    1.320035  -0.234570  -0.038468
C    1.006146   1.100337   0.488752
C   -0.161183   1.701659   0.259649
C   -1.249493   1.077953  -0.562187
C    2.533540  -0.790625   0.131759
H   -1.533178  -0.677183   1.779821
H   -1.813461  -2.321506   0.985968
H   -3.092832  -0.997350   0.831754
H   -1.738905  -0.889797  -1.459108
H    0.431972  -1.926498  -1.090801
H    1.771287   1.597890   1.076988
H   -0.344819   2.695286   0.656864
H   -2.219076   1.217438  -0.074013
H   -1.327735   1.617147  -1.518350
H    3.324671  -0.268817   0.658561
H    2.759988  -1.776502  -0.258828
```

Frequencies

-465.924	86.8318	94.7276
130.3904	207.3587	328.6946
367.3433	378.2031	477.9442
482.9017	520.2108	572.7417
609.2664	670.541	778.9565
794.2252	803.52	822.2718
891.2311	893.1538	940.0698
954.2695	969.0171	989.6774
1013.081	1032.204	1172.604
1209.375	1225.717	1334.155
1387.317	1388.379	1416.746
1422.435	1441.917	1468.847
1476.803	1566.192	1646.73
1741.845	3006.464	3071.132
3098.11	3155.658	3174.641
3183.154	3197.113	3205.009
3246.773	3262.001	3275.004

i35 – p46
```
C    2.488348  -0.940231  -0.075435
C    1.132176  -0.299943   0.032944
C   -0.009287  -1.024512  -0.018333
C   -1.334778  -0.419998  -0.019008
C   -1.380844   1.045222   0.032916
C   -0.276462   1.789091  -0.000439
C    1.096631   1.201249  -0.109029
C   -2.451642  -1.164266  -0.051922
H    2.889644  -0.793305  -1.084706
```

```
H     2.441312   -2.012283    0.122341
H     3.195426   -0.490323    0.626051
H     1.095259   -0.269303    2.044490
H     0.047734   -2.109418   -0.001464
H    -2.357234    1.514437    0.100982
H    -0.350516    2.871531    0.034871
H     1.529206    1.462300   -1.087309
H     1.764712    1.659557    0.629123
H    -3.434056   -0.705727   -0.048530
H    -2.406334   -2.247138   -0.086016
```

Frequencies

-718.547	112.7264	164.8934
219.5348	289.1501	337.3275
378.3345	410.987	470.0226
484.2458	497.817	546.7634
588.9342	684.1999	710.4336
793.4263	875.3562	882.9482
903.0589	928.5809	950.8266
977.9556	1010.293	1020.868
1045.345	1065.641	1177.748
1206.979	1228.821	1321.027
1366.818	1400.196	1418.526
1436.752	1464.999	1468.692
1489.868	1496.874	1650.384
1669.702	1751.146	3003.295
3039.244	3059.043	3105.321
3143.92	3162.234	3177.279
3178.308	3199.821	3253.284

i36 – p45
```
C     1.669963   -1.593195    1.080392
C     1.196039   -0.110116   -0.826281
C    -0.184437   -0.653080   -1.091357
C    -1.224693   -0.157046   -0.110816
C    -0.997222    1.176915    0.436706
C     0.208024    1.778398    0.344070
C     1.340539    1.113379   -0.257388
C    -2.303931   -0.879373    0.211090
H     1.772757   -2.526370    0.539272
H     0.733111   -1.399337    1.586996
H     2.567188   -1.139825    1.480590
H     2.027817   -0.574604   -1.342956
H    -0.185154   -1.743852   -1.136078
H    -0.477184   -0.301831   -2.093493
H    -1.814187    1.657124    0.965654
H     0.353548    2.761258    0.779501
H     2.318755    1.575678   -0.190439
H    -3.070243   -0.481574    0.868020
H    -2.452098   -1.881964   -0.175561
```

Frequencies

-364.153	88.2349	99.2975
129.4772	185.1686	288.4849
391.6509	426.8055	438.6112
473.9216	499.7098	564.8519
605.1714	672.7329	747.1323
775.9265	782.7131	830.687
898.2904	929.8846	947.3824
962.6319	975.8157	997.7267
1005.875	1038.844	1182.012
1197.956	1218.144	1318.767

1333.575	1401.173	1415.189
1421.873	1442.221	1455.923
1480.409	1514.64	1659.3
1704.287	2997.779	3105.817
3112.141	3152.291	3176.025
3190.305	3198.847	3213.143
3240.467	3275.959	3285.555

i36 – p3

C	-2.555396	-0.800843	0.029782
C	-1.208273	-0.142496	0.009681
C	-0.032592	-1.011926	-0.365289
C	1.318207	-0.406846	-0.059919
C	1.388596	1.051120	-0.104281
C	0.273089	1.800114	-0.053617
C	-1.040164	1.195586	0.073355
C	2.391461	-1.157145	0.209004
H	-2.578913	-1.629615	0.742434
H	-2.782899	-1.216913	-0.958870
H	-3.343273	-0.093807	0.294751
H	-0.790456	-0.349684	2.122959
H	-0.100023	-1.170563	-1.454007
H	-0.123218	-2.000688	0.091679
H	2.368369	1.517075	-0.119832
H	0.345799	2.882162	-0.049961
H	-1.895669	1.839756	0.248997
H	3.364790	-0.705730	0.368439
H	2.325919	-2.237380	0.281108

Frequencies

-537.939	103.6555	164.4699
202.0768	281.8299	308.3085
342.6708	377.206	419.483
482.3875	488.3819	516.0567
589.0871	684.2102	740.1304
799.5513	874.3244	878.3524
911.3496	931.9555	961.7282
986.7704	994.7005	1014.918
1059.161	1085.223	1183.584
1201.872	1234.075	1320.498
1341.268	1380.009	1420.904
1435.018	1461.063	1475.345
1484.244	1496.725	1611.644
1685.007	1724.552	2988.838
3037.633	3093.126	3103.943
3144.4	3150.868	3186.551
3195.82	3213.035	3239.865

i30 – p46

C	-2.501241	-0.924960	-0.096575
C	-1.150374	-0.284159	-0.056902
C	-0.012006	-1.010635	0.024946
C	1.325769	-0.398132	-0.026469
C	1.364714	1.065831	0.007515
C	0.256878	1.804954	0.025268
C	-1.119810	1.215038	-0.000286
C	2.438261	-1.136804	-0.108374
H	-3.063433	-0.687481	0.814608
H	-2.430761	-2.010652	-0.179829
H	-3.088146	-0.548861	-0.941306
H	-0.063715	-2.090161	-0.084095
H	-0.087481	-1.354697	1.955300
H	2.340699	1.540805	0.015696
H	0.328390	2.887856	0.053936
H	-1.681855	1.549240	0.885353

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H   -1.681298   1.621718  -0.853781
H    3.417764  -0.674311  -0.154553
H    2.396690  -2.220253  -0.126072
```

Frequencies

-724.75	93.6802	114.2323
184.5505	267.2623	295.0597
321.6667	374.8245	420.039
485.7444	508.6162	542.6435
593.6542	708.4731	711.7194
795.3319	883.7707	904.4821
912.5915	931.3785	969.2915
973.2737	1008.826	1018.01
1045.246	1062.26	1182.593
1207.129	1228.726	1317.218
1361.647	1403.197	1417.292
1435.661	1455.99	1468.484
1481.718	1490.546	1653.113
1694.186	1762.391	2998.869
3023.621	3030.523	3089.687
3137.215	3161.13	3176.401
3179.363	3203.158	3250.894

i31 – p47
```
C   -2.573575  -0.802882  -0.041143
C   -1.185877  -0.237529  -0.047643
C   -0.084635  -1.014556   0.086133
C    1.266608  -0.454138  -0.006176
C    1.388092   1.024584   0.279217
C    0.155029   1.804401  -0.076026
C   -1.032529   1.207986  -0.207032
C    2.321233  -1.213946  -0.308445
H   -3.154151  -0.382889   0.787168
H   -2.564989  -1.888803   0.064255
H   -3.100602  -0.547680  -0.966419
H   -0.184408  -2.095765   0.099164
H   -0.209297  -1.161031   2.272777
H    2.269460   1.440089  -0.216379
H    1.559395   1.152621   1.359655
H    0.246461   2.880758  -0.177676
H   -1.920478   1.792958  -0.426597
H    3.313620  -0.789641  -0.416425
H    2.218918  -2.284152  -0.452827
```

Frequencies

-456.252	109.9989	137.4999
173.01	209.2957	250.6275
297.0099	337.3102	427.1846
453.0704	527.2979	552.0258
577.5938	701.6832	719.8991
760.7194	875.5035	885.4012
921.9987	944.4212	957.4426
984.5153	1008.891	1023.536
1047.393	1064.51	1197.475
1208.276	1229.032	1317.303
1352.807	1371.219	1413.681
1446.281	1454.073	1464.417
1484.621	1493.437	1619.398
1707.908	1737.704	2996.51

3040.409	3097.703	3100.359
3141.709	3151.307	3175.315
3184.019	3200.057	3239.761

i1 – i69

C	-0.842894	2.064530	-0.150296
C	-0.466359	0.624694	-0.179765
C	3.503308	-0.293696	0.197417
C	2.090127	0.036357	0.062940
C	0.920480	0.303277	-0.043864
C	-1.465077	-0.444844	0.034281
C	-2.695582	-0.189128	0.494661
C	-1.029045	-1.843237	-0.317211
H	-0.064246	2.806795	-0.058672
H	-1.883847	2.348790	-0.155620
H	-0.629719	1.238658	-1.247730
H	3.653519	-1.374505	0.136275
H	3.899056	0.049274	1.156999
H	4.090533	0.172933	-0.597871
H	-3.421041	-0.986814	0.606362
H	-3.008752	0.802930	0.795716
H	-1.849241	-2.550331	-0.185531
H	-0.193685	-2.157656	0.314664
H	-0.682329	-1.897789	-1.353572

Frequencies

-1855.51	24.1153	60.1399
88.8029	155.3513	174.137
269.8574	295.846	320.2414
387.5745	418.8729	434.5443
486.1933	560.737	573.5971
640.7592	653.8766	763.5284
839.0956	900.7009	961.0981
1015.638	1049.032	1054.55
1057.122	1072.534	1170.739
1204.341	1330.69	1357.617
1418.217	1421.042	1425.32
1451.652	1482.445	1483.279
1486.321	1500.56	1685.529
2234.779	2353.066	3043.867
3045.822	3109.902	3114.222
3118.859	3140.668	3162.205
3190.876	3248.726	3317.477

i12 – i13

C	-1.986153	-1.717427	-0.197528
C	-2.197640	-0.275094	-0.494017
C	-1.284360	0.537925	0.037546
C	-0.272140	-0.222371	0.861672
C	-1.192489	2.021725	-0.107959
C	3.618684	-0.143330	-0.404965
C	2.236955	-0.163806	0.058345
C	1.093773	-0.176952	0.441513
H	-2.727121	-2.226691	0.419064
H	-1.598547	-2.341545	-1.003267
H	-3.029675	0.080323	-1.096702
H	-0.395756	-0.107796	1.942270
H	-0.837549	-1.380468	0.586317
H	-0.230495	2.300660	-0.549268
H	-1.252679	2.514122	0.868296
H	-1.992249	2.409435	-0.742560
H	3.791503	-0.924372	-1.150330
H	4.312491	-0.306209	0.423509
H	3.860293	0.818515	-0.864970

Frequencies

-1883.97	64.5446	84.5566

93.167	167.8091	214.2727
228.4182	246.9739	345.1512
373.1434	419.1873	457.3327
549.4892	601.7041	634.3038
771.1781	833.6231	897.1603
923.2052	941.498	1034.678
1051.96	1052.826	1055.213
1074.592	1104.512	1197.929
1210.805	1290.976	1343.373
1391.35	1416.72	1419.876
1449.213	1479.688	1481.967
1490.24	1494.226	1655.268
1754.222	2339.628	3041.059
3047.731	3084.961	3096.445
3103.368	3115.701	3124.27
3135.23	3172.355	3175.784

i12 – p9a
```
C     3.162310   -0.954492    0.039197
C     2.540692    0.219774   -0.069191
C     1.090913    0.434429   -0.084389
C     0.205152   -0.787694    0.047109
C     0.597357    1.676859   -0.187577
C    -3.850239   -0.076754   -0.025836
C    -2.412687   -0.322890   -0.003656
C    -1.230459   -0.528885    0.017612
H     4.244230   -1.012058    0.041160
H     2.627121   -1.893651    0.129239
H     3.140978    1.122448   -0.154479
H     0.458942   -1.492078   -0.754145
H     0.457023   -1.298854    0.984437
H    -0.469385    1.857771   -0.236235
H     1.260071    2.527675   -0.300747
H     0.363596    2.262891    1.984016
H    -4.122489    0.701650    0.691137
H    -4.402275   -0.983353    0.233864
H    -4.176044    0.245470   -1.017855
```

Frequencies

-412.304	30.2132	55.9375
89.3692	136.2742	159.769
213.3686	216.0612	238.803
294.1526	388.0361	417.6251
421.772	517.0392	535.6675
659.4085	802.5731	814.4994
840.2729	944.2629	951.5168
959.6592	974.9938	1037.73
1058.48	1059.218	1066.043
1181.067	1253.677	1280.341
1334.395	1393.888	1420.436
1425.892	1463.544	1477.184
1485.983	1486.518	1664.174
1714.497	2398.687	3033.448
3047.82	3065.244	3121.043
3121.377	3155.98	3160.93
3167.428	3246.949	3256.491

SUPPORTING INFORMATION

i19 – i39

C	-2.819952	-0.156096	-0.156676
C	-1.437048	0.296227	0.145614
C	-0.829368	-1.046197	0.350270
C	0.529646	-1.209283	-0.283511
C	1.363850	0.045554	-0.030102
C	0.765208	1.239138	0.081614
C	-0.694868	1.386070	-0.029373
C	2.850262	-0.135719	0.016219
H	-3.507388	-0.275067	0.680546
H	-2.079229	-1.383192	-0.229532
H	-3.280358	0.137202	-1.097493
H	-0.956871	-1.449875	1.358387
H	1.042966	-2.093647	0.102841
H	0.446315	-1.346836	-1.371714
H	1.369297	2.131857	0.214582
H	-1.120743	2.346948	-0.297917
H	3.141449	-0.783996	0.850171
H	3.369617	0.818470	0.125741
H	3.208567	-0.620026	-0.899945

Frequencies

-2292.89	114.0621	183.3099
206.9802	272.9619	312.3189
338.9974	399.548	452.4148
493.9042	540.2548	579.9488
730.1812	803.2946	819.9181
841.4707	891.6372	924.6973
932.7382	970.1663	981.782
1039.577	1067.29	1081.75
1100.194	1167.013	1206.557
1209.743	1303.025	1315.921
1333.814	1366.402	1385.276
1422.526	1427.373	1474.693
1485.156	1496.496	1692.168
1729.831	1835.051	3005.257
3029.484	3084.256	3085.865
3103.556	3105.073	3130.917
3182.925	3202.603	3204.423

i37 – i39

C	2.861856	-0.026835	0.023243
C	1.366836	-0.049608	-0.155640
C	0.622907	1.228203	-0.142450
C	-0.808839	1.255937	0.294830
C	-1.536141	-0.054546	0.041180
C	-0.742184	-1.269977	0.123792
C	0.614027	-1.258322	0.065156
C	-2.853026	-0.073237	-0.200950
H	3.114523	0.095003	1.082427
H	3.315500	0.806546	-0.520120
H	3.317691	-0.952796	-0.334307
H	1.000805	0.444350	-1.239582
H	1.201292	2.142696	-0.191263
H	-0.832992	1.442925	1.382042
H	-1.348860	2.083867	-0.171708
H	-1.271901	-2.214555	0.190292
H	1.167103	-2.191036	0.111202
H	-3.383065	-1.008495	-0.346794
H	-3.432717	0.841804	-0.257148

Frequencies

-1892.11	86.1115	174.3918
215.0498	274.7716	304.6332
399.5378	431.9519	456.1435
542.8648	615.6037	638.1216
695.5422	730.6423	773.2558

796.3898	896.0891	926.949
943.6204	950.5378	985.1167
1009.789	1051.12	1077.787
1162.46	1178.88	1202.891
1255.023	1304.848	1330.088
1352.513	1418.025	1424.215
1433.94	1473.853	1482.557
1494.978	1509.992	1588.056
1689.102	2207.561	2959.363
3036.019	3085.126	3103.079
3129.417	3152.59	3180.853
3200.443	3209.545	3241.247

i11 – p30

```
C    -3.499070    0.147592    0.282879
C    -2.437754   -0.505891   -0.182995
C    -1.058993    0.012945   -0.190678
C     0.004881   -1.036146    0.072822
C    -0.776270    1.302688   -0.405594
C     3.900254    0.298198    0.049709
C     2.518551   -0.169140    0.053005
C     1.383453   -0.559309    0.058764
H    -4.488740   -0.292940    0.248134
H    -3.406653    1.134173    0.725565
H    -2.568807   -1.517374   -0.565460
H    -0.204164   -1.505524    1.042246
H    -0.108731   -1.834985   -0.671225
H     0.248072    1.656069   -0.407855
H    -0.929487    2.138075    1.716517
H    -1.557455    2.007115   -0.665383
H     4.382042    0.086593   -0.907939
H     4.477277   -0.193287    0.836865
H     3.946329    1.376468    0.221057
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Frequencies

-372.387	44.7061	54.9081
84.8536	119.2166	148.384
184.053	213.2251	255.1998
302.423	356.2786	393.4151
417.5714	468.6694	593.8976
672.9857	787.1198	802.7225
858.5141	943.5478	961.2884
967.5075	973.9108	1028.104
1055.595	1062.518	1100.615
1177.835	1217.113	1254.021
1341.928	1380.663	1421.011
1430.459	1466.527	1473.684
1484.488	1490.424	1686.249
1721.903	2400.38	3030.821
3052.92	3060.415	3124.862
3126.353	3144.692	3158.783
3169.659	3249.241	3263.745

i1 – i68

```
C     0.973676   -1.293755    0.936921
C     0.361497   -0.736916   -0.300122
C    -3.616127    0.285762   -0.119635
C    -2.204297   -0.073643   -0.183002
C    -1.043052   -0.372830   -0.241323
C     1.388884    0.338153   -0.039966
C     1.084909    1.496180    0.631899
```

```
C    2.718373   0.176654  -0.738100
H    0.513843  -1.078644   1.890089
H    1.777250  -2.014259   0.881120
H    0.585901  -1.309452  -1.201057
H   -3.738000   1.363831   0.010835
H   -4.108617  -0.214982   0.717623
H   -4.131289  -0.003665  -1.038876
H    1.854176   2.232179   0.832145
H    0.086984   1.679660   1.011118
H    3.520839   0.659091  -0.176449
H    2.669742   0.641322  -1.728298
H    2.985993  -0.872715  -0.878286
```

Frequencies

-630.056	69.8109	91.2281
96.1745	170.635	224.8719
278.6758	328.0906	351.092
385.837	418.7125	507.3958
546.1565	573.1642	579.3729
686.3105	754.601	759.155
835.39	968.1967	987.4461
1020.995	1059.122	1061.696
1063.861	1115.419	1175.269
1213.881	1273.088	1385.425
1403.562	1426.333	1431.568
1455.584	1485.974	1490.655
1497.796	1500.711	1543.452
2399.699	3047.07	3050.376
3103.446	3116.168	3121.376
3125.283	3138.764	3161.571
3182.253	3260.089	3306.054

i13 – p7b
```
C    3.087804  -0.926614  -0.370014
C    2.471244   0.151585   0.129231
C    1.028536   0.418236   0.070102
C    0.138411  -0.589674   0.132592
C    0.625732   1.861928  -0.033336
C   -3.921498  -0.208207  -0.072792
C   -2.471681  -0.333055  -0.001037
C   -1.273117  -0.433735   0.058506
H    4.162161  -1.042992  -0.291279
H    2.920430  -2.431376   1.323020
H    2.550165  -1.674036  -0.943572
H    3.073760   0.919585   0.611087
H    0.502195  -1.603891   0.271226
H    1.046493   2.432904   0.801128
H   -0.457928   1.977790  -0.022436
H    1.016173   2.304422  -0.955275
H   -4.391345  -1.190878  -0.160083
H   -4.219709   0.389358  -0.938076
H   -4.314978   0.276323   0.824753
```

Frequencies

-411.67	9.0604	81.1692
87.8341	108.7597	131.4124
160.2154	231.6205	242.9554
276.4982	302.6136	398.6258
414.3231	507.3333	517.7363
556.1239	714.8019	820.3912
846.6871	899.5283	960.4289
1008.635	1028.325	1052.354
1054.305	1057.808	1086.189

1206.436	1247.613	1321.695
1367.578	1418.415	1420.841
1458.248	1483.657	1484.108
1486.075	1491.924	1663.078
1705.452	2367.763	3038.618
3045.537	3097.918	3116.409
3121.362	3147.521	3151.255
3159.52	3171.308	3249.213

i13 – p29

C	2.776705	-1.581164	-0.338718
C	2.244313	-0.173787	-0.271151
C	1.117265	0.134762	0.316295
C	0.013738	-0.042852	1.051734
C	0.898363	2.445731	-0.312125
C	-3.727993	-0.463593	-0.518020
C	-2.391458	-0.311527	0.041284
C	-1.281088	-0.193921	0.494323
H	2.896004	-1.895964	-1.379875
H	3.761398	-1.640977	0.135104
H	2.105721	-2.280807	0.160761
H	2.838598	0.600003	-0.747145
H	0.088379	0.048373	2.133126
H	1.790557	2.810630	0.181675
H	-0.059187	2.706914	0.118553
H	0.935518	2.280777	-1.381401
H	-4.074404	0.474295	-0.960575
H	-4.441965	-0.755759	0.256001
H	-3.739682	-1.229371	-1.297952

Frequencies

-468.032	20.3377	32.9219
57.3725	78.4441	135.9341
160.6939	166.3631	185.5148
249.4081	304.8555	385.5872
425.5624	453.3682	462.9273
486.9854	565.0637	735.3659
786.9093	807.14	873.68
907.6135	1052.353	1057.158
1063.965	1089.688	1111.528
1209.872	1320.691	1408.787
1411.546	1415.718	1423.003
1430.576	1482.676	1484.361
1488.138	1498.652	1961.121
2348.26	3040.016	3044.206
3102.936	3103.709	3114.635
3119.832	3142.616	3147.439
3175.567	3276.104	3279.768

i69 – p15

C	0.841569	1.948307	0.200403
C	0.463265	0.671901	0.008714
C	-3.490357	-0.358763	-0.209046
C	-2.083489	0.010405	-0.130517
C	-0.924214	0.326286	-0.066756
C	1.449671	-0.441015	-0.089033
C	2.557092	-0.306401	-0.816983
C	1.119888	-1.701009	0.663682
H	0.869995	2.088195	2.506621
H	0.112749	2.748664	0.230309
H	1.890685	2.207689	0.275503
H	-3.612051	-1.442794	-0.146981
H	-3.925916	-0.021858	-1.153237
H	-4.057300	0.095891	0.607108

```
H    3.291370   -1.102936   -0.871748
H    2.753246    0.592440   -1.390447
H    1.917302   -2.438528    0.562014
H    0.188710   -2.137659    0.291561
H    0.970659   -1.487374    1.726512
```

Frequencies

-374.851	22.8963	55.2585
90.1183	134.8737	149.041
186.3497	211.0292	262.9175
300.1701	328.933	405.4131
410.7096	484.0822	582.2276
639.454	676.4525	764.4912
796.5174	850.1542	944.3777
947.6688	971.0036	1033.715
1053.767	1058.185	1073.779
1085.311	1239.632	1348.388
1412.719	1419.935	1433.615
1448.773	1482.479	1483.13
1483.67	1499.971	1645.583
1727.315	2370.671	3044.684
3047.65	3110.15	3120.308
3123.441	3140.562	3153.353
3166.046	3242.641	3265.198

i68 – p20
```
C    0.997575   -0.728890    1.210967
C    0.226211   -0.689454   -0.129437
C   -3.780689    0.175984   -0.207647
C   -2.356439   -0.135215   -0.178390
C   -1.182519   -0.389444   -0.152113
C    1.200275    0.366754    0.252578
C    1.310936    1.702943    0.205337
H    0.433501   -0.504790    2.109822
H    1.740100   -1.511021    1.312986
H    0.548181   -1.425255   -0.858363
H   -3.946018    1.252423   -0.115438
H   -4.307604   -0.319574    0.611771
H   -4.230138   -0.155118   -1.147263
H    1.877914    2.242867    0.955822
H    0.913351    2.262339   -0.634292
C    3.112830   -0.386636   -0.885563
H    3.879368    0.044131   -0.253849
H    2.950284    0.078040   -1.849816
H    2.971984   -1.460294   -0.825772
```

Frequencies

-484.796	16.8826	63.8288
82.8719	103.2781	174.0393
204.1792	234.2749	303.7351
320.6629	373.8987	482.2717
491.2881	505.3156	541.6033
584.0371	717.9512	766.5874
837.3558	857.7246	914.7833
937.215	1007.792	1032.358
1057.022	1058.745	1071.836
1107.58	1132.953	1217.71
1361.078	1417.724	1420.127
1423.659	1443.008	1477.034
1484.833	1486.679	1699.966

2391.571	3045.615	3096.553
3117.288	3119.013	3139.1
3144.94	3168.686	3230.808
3239.544	3260.212	3273.055

i39 – p6

C	2.821556	0.079135	0.293292
C	1.526798	0.055819	-0.034436
C	0.794483	-1.224943	-0.367262
C	-0.684340	-1.168102	-0.101277
C	-1.352218	-0.005495	-0.040671
C	-0.604280	1.250618	-0.134553
C	0.736455	1.283205	-0.119086
C	-2.838679	0.074839	0.151200
H	3.399126	-0.833446	0.394228
H	3.338781	1.016195	0.470114
H	1.250347	-2.069852	0.154619
H	0.929169	-1.424283	-1.441909
H	-1.223765	-2.109469	-0.061593
H	-0.510215	-1.373998	2.275945
H	-1.168881	2.177734	-0.164358
H	1.265045	2.231255	-0.115309
H	-3.308070	0.616762	-0.676458
H	-3.081760	0.616348	1.071246
H	-3.288427	-0.917696	0.210229

Frequencies

-328.445	72.9869	132.1287
160.6375	195.8294	253.4712
282.3075	311.6722	408.664
426.3041	485.409	568.9321
626.2178	711.6813	746.7967
785.9445	819.0008	832.6634
915.9025	944.7797	960.3596
986.4887	1005.835	1012.978
1070.212	1087.264	1200.851
1202.977	1231.043	1313.851
1346.521	1371.219	1420.219
1435.021	1457.202	1475.802
1485.115	1498.695	1642.947
1702.748	1744.336	2992.442
3035.935	3093.512	3096.384
3135.064	3149.295	3172.373
3180.52	3194.678	3237.747

i39 – p28

C	-2.836178	0.035877	-0.039732
C	-1.506935	0.037768	0.081373
C	-0.701670	-1.213120	0.336042
C	0.618208	-1.192110	-0.441974
C	1.398945	0.067262	-0.160241
C	0.608324	1.290240	-0.048066
C	-0.732414	1.278450	0.017178
C	2.734833	0.080737	-0.043886
H	-3.408315	-0.884314	0.008999
H	-3.389652	0.957175	-0.188985
H	-1.285023	-2.101166	0.082764
H	-0.476263	-1.263981	1.408339
H	1.219689	-2.072941	-0.206356
H	0.395906	-1.225228	-1.515860
H	1.143729	2.234844	-0.036094
H	-1.281963	2.214708	0.042642
H	2.984152	-0.353443	2.249828
H	3.277435	1.007544	0.108960
H	3.321629	-0.823827	-0.158406

Frequencies

-324.854	79.5821	132.0041
165.3741	201.8081	296.2891
359.4363	384.9303	439.391
445.8972	558.8872	621.038
714.5381	749.76	765.6932
779.3586	805.0995	855.6551
929.2756	935.058	938.0897
984.9299	996.2147	1012.943
1035.636	1062.737	1181.396
1202.332	1247.503	1310.236
1346.084	1360.446	1362.437
1428.477	1445.687	1472.275
1486.134	1487.357	1655.66
1693.979	1730.588	3033.973
3042.145	3106.207	3108.148
3148.967	3151.412	3170.92
3192.066	3237.574	3242.15

i13 – i14

```
C     1.884259    1.934709   -0.077382
C     2.048396    0.479374   -0.390342
C     1.276357   -0.512205    0.053050
C     1.508278   -1.952575   -0.328416
H     2.789702    2.339222    0.386860
H     1.711929    2.509123   -0.993500
H     1.043040    2.111320    0.595605
H     2.875134    0.221645   -1.050538
H     0.623285   -2.362152   -0.825740
H     1.688863   -2.566839    0.560042
H     2.364111   -2.053874   -0.999730
C     0.125387   -0.277005    0.965552
C    -3.632796    0.250905   -0.447548
C    -2.287792    0.048069    0.068726
C    -1.156679   -0.107928    0.497665
H     0.290851   -0.304231    2.039624
H    -3.830222    1.315141   -0.610636
H    -4.382762   -0.125808    0.252928
H    -3.766383   -0.263607   -1.402755
```

Frequencies

-95.4265	86.0189	131.82
133.4484	154.9263	178.0093
202.963	247.834	257.6437
323.39	386.5347	429.9505
495.7372	572.4856	624.9553
785.3952	839.3972	864.8171
973.9304	1044.478	1054.141
1061.894	1066.783	1072.198
1106.144	1210.621	1223.175
1349.218	1406.096	1411.394
1419.92	1436.05	1476.351
1484.368	1485.391	1488.963
1490.081	1500.167	1761.501
2175.69	3038.249	3039.872
3040.877	3097.709	3101.506
3105.853	3119.475	3130.618

| 3133.477 | 3153.104 | 3163.56 |

i14 – i16

C	1.089847	2.061862	-0.367348
C	1.197520	0.936312	0.602247
H	1.206766	3.032181	0.119671
H	1.841932	1.980612	-1.161212
H	0.109161	2.050919	-0.866252
H	1.026171	1.110414	1.659841
C	1.327821	-0.453161	0.122874
C	0.254069	-1.189361	-0.200162
C	2.725515	-0.998454	-0.005779
C	-3.603517	0.132795	0.073170
C	-2.226011	-0.333047	-0.023410
C	-1.087576	-0.716773	-0.099446
H	0.387362	-2.206024	-0.561815
H	2.730635	-2.013599	-0.408899
H	3.222963	-1.006410	0.969507
H	3.326456	-0.359886	-0.661759
H	-3.998206	-0.020201	1.081232
H	-4.246451	-0.407987	-0.625867
H	-3.672796	1.198950	-0.157331

Frequencies

-168.751	62.1589	76.2303
103.3731	155.2806	185.1444
205.8686	232.6339	278.6325
299.8659	369.654	434.596
479.0948	547.5119	598.3171
806.4729	835.4686	855.7607
983.5014	1013.55	1040.034
1052.301	1058.47	1077.344
1122.153	1199.432	1211.731
1327.021	1408.792	1414.749
1416.022	1419.903	1476.591
1482.377	1482.864	1490.13
1494.321	1494.885	1705.868
2375.387	2994.689	3037.566
3049.483	3054.376	3098.845
3118.176	3120.273	3124.685
3133.102	3165.587	3182.858

i69 – p18

C	0.869749	2.036451	-0.009362
C	0.424055	0.596424	0.021388
C	-3.390066	-0.228827	0.160120
C	-2.102153	0.049923	0.124614
C	-0.869552	0.310501	0.075800
C	1.424232	-0.488907	-0.012225
C	2.733101	-0.223256	-0.078733
C	0.912107	-1.903402	0.033001
H	0.010689	2.705045	0.026703
H	1.434794	2.245314	-0.922723
H	1.520323	2.258133	0.841877
H	-4.001614	-0.371922	-2.170034
H	-4.133371	0.559536	0.205229
H	-3.738978	-1.254752	0.207361
H	3.461896	-1.025522	-0.103467
H	3.123089	0.786795	-0.110986
H	1.734850	-2.617968	-0.013583
H	0.231842	-2.097424	-0.800799
H	0.347646	-2.080674	0.952803

Frequencies

-393.204	57.2647	90.3309
125.1276	136.9201	165.9269
187.2305	214.0356	275.4042

319.9633	345.6483	411.3223
427.6859	514.4664	562.5947
589.7419	599.1527	659.8905
740.8948	875.4713	896.0877
936.3125	976.1891	1020.721
1034.027	1046.811	1073.18
1150.749	1161.358	1350.245
1405.573	1417.722	1438.898
1445.949	1481.659	1489.003
1493.828	1503.015	1683.799
1713.985	2163.426	3048.325
3055.642	3112.187	3120.149
3148.449	3152.493	3158.656
3171.224	3239.516	3256.143

i69 – p19
```
C    0.807807   1.934368  -0.293077
C    0.341838   0.516038  -0.075403
C   -3.464825  -0.236904   0.338925
C   -2.178454   0.018700   0.205334
C   -0.948748   0.256800   0.062109
H   -0.039202   2.617606  -0.339099
H    1.372617   2.013721  -1.227611
H    1.469854   2.257595   0.516021
H   -4.181287  -0.703072  -1.926482
H   -4.201611   0.558044   0.302014
H   -3.816297  -1.241207   0.549065
C    1.354466  -0.569082  -0.023208
C    1.041553  -1.826387  -0.343868
C    2.751261  -0.184809   0.392718
H    1.781834  -2.617066  -0.294064
H    0.041614  -2.093345  -0.666703
H    3.399207  -1.061466   0.426357
H    2.752811   0.281405   1.383030
H    3.191073   0.535442  -0.303702
```

Frequencies

-377.428	38.7858	89.4124
122.5935	132.9334	187.3475
226.7857	247.1079	285.1837
323.0576	326.1671	407.1581
452.4615	512.8955	571.2748
583.6145	622.5085	662.4084
737.1735	878.3858	902.085
941.5695	976.6564	1024.615
1032.826	1051.379	1074.52
1140.923	1172.125	1324.415
1407.821	1418.056	1443.513
1446.292	1482.995	1492.022
1500.125	1512.841	1690.204
1717.887	2169.603	3044.009
3047.704	3106.288	3108.36
3141.464	3154.334	3160.229
3162.427	3240.916	3254.22

i13 – p33
```
C    3.144918  -1.035684  -0.056386
C    2.386041   0.253951  -0.041259
C    1.058045   0.448153   0.007049
```

```
C    0.108091   -0.662260    0.052762
C    0.476894    1.836959    0.014700
C   -3.766873   -0.211935    0.142317
C   -2.457828   -0.364556    0.123043
C   -1.205845   -0.510867    0.090559
H    3.707888   -1.133399   -0.990664
H    3.877701   -1.052937    0.756459
H    2.514147   -1.918727    0.045401
H    3.009309    1.145406   -0.078975
H    0.495747   -1.676405    0.051986
H   -0.107549    2.006257    0.924041
H   -0.202576    1.978214   -0.830952
H    1.261539    2.593011   -0.038897
H   -4.215062    0.775389    0.168026
H   -4.430072   -1.068655    0.194013
H   -4.371741   -0.170720   -2.197156
```

Frequencies

-401.606	51.537	85.2664
91.0652	128.7273	153.5568
162.004	241.1535	251.4597
268.6275	288.7985	387.8779
409.322	517.7112	542.606
557.7938	640.4488	801.275
843.5016	875.4688	882.7209
930.0815	1001.767	1033.678
1064.699	1072.324	1073.767
1119.161	1264.187	1304.596
1393.726	1422.131	1428.998
1450.584	1481.973	1483.849
1493.179	1502.87	1680.726
1728.989	2158.844	3046.937
3051.222	3100.437	3114.03
3141.16	3144.926	3152.197
3158.273	3188.24	3239.368

i4 – p5b

```
C    0.114433    1.480716    0.037097
C   -1.172680    1.046226    0.013162
C    3.517310   -0.761394   -0.235599
C    2.300434    0.032116   -0.134763
C    1.284757    0.670169   -0.042415
C   -1.686875   -0.320733    0.076986
C   -1.013679   -1.337864    0.626779
C   -3.072268   -0.506179   -0.491563
H    0.275511    1.909551    2.020581
H    0.283192    2.546398   -0.084813
H   -1.930831    1.822864   -0.054856
H    4.398933   -0.151133   -0.025417
H    3.625112   -1.180163   -1.239454
H    3.499356   -1.590637    0.476323
H   -1.448110   -2.331271    0.662451
H   -0.033577   -1.206249    1.066173
H   -3.409692   -1.538484   -0.387808
H   -3.097816   -0.240730   -1.553010
H   -3.790675    0.141519    0.021725
```

Frequencies

-756.175	39.5674	49.7655
81.4298	157.5055	164.4846
212.3795	239.1073	318.5285
332.9594	366.581	412.9996
446.1801	470.4122	591.3496
669.3507	708.3376	755.6425
823.5233	908.0939	949.3104

988.1412	1004.669	1033.184
1054.859	1057.396	1070.421
1164.028	1272.948	1284.732
1409.779	1418.398	1454.141
1464.218	1482.565	1485.384
1486.623	1500.789	1605.485
1707.425	2374.766	3042.473
3049.958	3103.203	3121.532
3125.356	3143.629	3161.231
3165.299	3183.965	3260.459

i3 – p23'

```
C   -0.046929    1.717913   -0.072977
C   -1.336820    1.122737    0.437827
C   -1.569527   -0.185292    0.537194
C   -1.763535   -1.323858    1.155220
C   -1.553521   -0.823587   -1.689026
C    3.159944   -0.862595    0.068184
C    2.030176    0.057908    0.012209
C    1.098661    0.813243   -0.027742
H    0.178136    2.620743    0.506011
H   -0.194852    2.058675   -1.107527
H   -2.170807    1.809684    0.556523
H   -2.069428   -2.227823    0.644827
H   -1.598654   -1.381151    2.227113
H   -2.298291   -1.609500   -1.648914
H   -0.511241   -1.116373   -1.721516
H   -1.827067    0.073044   -2.232489
H    3.890936   -0.631927   -0.710677
H    2.826145   -1.893373   -0.074261
H    3.664431   -0.800812    1.035579
```

Frequencies

-564.302	39.4364	62.0575
79.4002	94.9008	106.118
174.4178	202.4188	247.654
312.1528	335.6772	393.2596
438.2237	498.5712	517.4568
525.6553	657.3135	768.026
801.4616	832.4908	906.8059
918.4048	942.7155	1016.89
1050.72	1064.555	1115.345
1186.288	1240.111	1325.488
1379.7	1414.76	1417.64
1426.096	1458.879	1480.827
1486.943	1491.444	1943.917
2402.432	3016.9	3052.622
3063.364	3099.529	3124.362
3126.617	3152.981	3171.007
3244.962	3262.984	3273.786

i3 – p5a

```
C    0.029224    1.483310   -0.032363
C   -1.259216    1.053858   -0.104919
C   -1.801114   -0.296347   -0.024419
C   -3.128899   -0.453133   -0.136345
C   -0.896302   -1.478669    0.195093
C    3.504247   -0.663654   -0.083884
C    2.260515    0.093887   -0.060944
C    1.218363    0.693994   -0.033693
H    0.097061    1.994083    1.935320
H    0.197507    2.547092   -0.173021
```

```
H   -2.007271   1.836530   -0.196728
H   -3.590016   -1.432823   -0.080109
H   -3.789009   0.394592   -0.287450
H   -1.480915   -2.396688   0.274513
H   -0.311264   -1.355642   1.110027
H   -0.182926   -1.587277   -0.624643
H   4.358462   -0.016306   0.128379
H   3.661372   -1.123896   -1.062896
H   3.486088   -1.459147   0.665447
```

Frequencies

-745.574	44.6253	82.0669
100.9767	174.3934	221.3587
250.9043	305.3135	309.5852
339.0506	384.7454	435.0099
453.4153	456.4103	589.3276
685.1452	706.0071	761.4641
839.7231	868.5364	927.8735
991.4238	1009.04	1048.834
1056.901	1060.954	1071.436
1156.126	1269.244	1351.386
1411.647	1419.543	1438.74
1469.648	1485.999	1488.635
1494.927	1509.288	1604.124
1678.977	2373.607	3049.086
3061.276	3119.442	3126.265
3133.467	3145.244	3158.656
3165.57	3183.259	3248.359

i11 – p37
```
C   0.892748   2.281323   0.107387
C   1.151601   1.015536   -0.071210
C   1.391385   -0.276650   0.049194
C   0.298744   -1.316567   -0.102398
C   2.790993   -0.811579   0.176036
C   -3.538364   0.162149   0.069534
C   -2.183484   -0.373218   0.008390
C   -1.065352   -0.804595   -0.042343
H   0.846021   2.981950   -0.717123
H   0.709101   2.658777   1.108894
H   1.376060   0.977340   -2.057536
H   0.454230   -1.836488   -1.057487
H   0.440830   -2.075740   0.676727
H   3.044769   -1.429234   -0.693167
H   2.875632   -1.446138   1.064443
H   3.520743   -0.006027   0.250697
H   -3.725524   0.635056   1.036721
H   -4.278394   -0.629867   -0.069541
H   -3.693100   0.911977   -0.710168
```

Frequencies

-697.083	55.4768	72.2706
103.4942	109.1337	115.2179
182.5388	210.1651	260.5431
286.5209	333.0107	398.7954
457.3839	478.0704	531.3598
616.0399	659.7414	772.1178
796.4537	912.8962	927.1544
992.5518	1018.785	1056.055
1061.426	1065.949	1178.452
1189.777	1249.962	1302.553
1373.676	1412.237	1424.711

1466.298	1473.206	1485.958
1486.285	1495.213	1503.459
2027.579	2405.175	3023.304
3032.735	3048.655	3055.844
3092.759	3120.998	3121.974
3150.999	3155.627	3241.397

i12 – p8b

C	0.495283	2.037051	0.253925
C	1.427212	1.199998	-0.205830
C	1.452386	-0.257879	-0.083388
C	0.362026	-1.054829	0.084537
C	2.820562	-0.880348	-0.123144
C	-3.583660	-0.028329	-0.141643
C	-2.173298	-0.382412	-0.058093
C	-1.003882	-0.656278	0.015171
H	0.605620	3.106718	0.116244
H	-0.382634	1.689337	0.783468
H	2.303667	1.626358	-0.691146
H	0.524290	-2.128968	0.100052
H	0.503395	-1.260262	2.137343
H	3.329554	-0.628701	-1.059613
H	2.775256	-1.966820	-0.037171
H	3.441325	-0.496530	0.693295
H	-3.708035	1.053078	-0.239103
H	-4.118384	-0.353667	0.754451
H	-4.053819	-0.502387	-1.007032

Frequencies

-635.517	64.3515	78.7894
88.1144	114.1054	152.0892
218.9314	253.3678	278.1416
311.5427	337.3315	368.6109
428.3721	478.0219	514.7441
574.0147	721.8244	814.1211
848.2001	883.1104	976.3075
1019.854	1041.406	1055.247
1058.309	1063.037	1105.988
1189.64	1223.544	1354.222
1377.495	1415.387	1423.768
1467.627	1482.951	1483.317
1487.966	1494.999	1618.512
1707.297	2373.891	3041.568
3048.798	3101.755	3121.577
3122.082	3142.542	3151.074
3172.846	3174.388	3269.076

i12 – p9b

C	0.962088	2.088339	-0.224032
C	1.625548	1.076118	0.333183
C	1.385479	-0.346915	0.083741
C	0.310168	-0.755287	-0.904051
C	2.134638	-1.277093	0.695160
C	-3.502422	0.013843	0.463634
C	-2.158583	-0.255862	-0.034702
C	-1.047927	-0.477666	-0.431720
H	1.212993	3.115487	0.013265
H	0.142347	1.931895	-0.916590
H	2.425721	1.294181	1.036679
H	0.476207	-0.235711	-1.855146
H	0.407011	-1.823969	-1.112672
H	1.955228	-2.336341	0.551053
H	2.896199	-0.998990	1.415626
H	3.810552	-1.596170	-0.814640
H	-3.459773	0.541457	1.419699
H	-4.054786	-0.916818	0.615132

H   -4.065638   0.632125   -0.239686

Frequencies

-428.088	57.7697	85.989
99.7673	143.5785	161.8
203.5726	214.2236	250.3895
320.5064	402.7124	419.3461
423.9033	492.658	575.9963
676.6878	811.0397	823.4281
826.2534	957.2223	961.6923
963.2576	982.2476	1037.679
1055.992	1061.57	1076.804
1174.537	1229.088	1332.018
1334.227	1363.924	1418.152
1439.9	1470.419	1488.725
1489.32	1500.262	1665.972
1717.565	2399.034	3049.772
3053.763	3101.645	3126.437
3126.79	3159.328	3162.132
3172.894	3251.989	3252.631

i14 – p8b

```
C    -0.466502    1.982702    -0.291274
C    -1.438178    1.156371    0.119842
C    -1.478297    -0.304656    0.012327
C    -0.403391    -1.115109    -0.063175
C    -2.862576    -0.900299    0.029646
C    3.550463    -0.114408    0.038478
C    2.138962    -0.469517    -0.006026
C    0.964148    -0.734284    -0.034479
H    -0.584342    3.055174    -0.188282
H    0.950119    2.093604    1.462703
H    0.413589    1.624020    -0.809226
H    -2.325554    1.600051    0.568159
H    -0.580358    -2.185486    -0.131278
H    -3.378885    -0.642206    0.960459
H    -2.836417    -1.987537    -0.056207
H    -3.465979    -0.504012    -0.793056
H    4.059104    -0.421225    -0.879168
H    4.047738    -0.602753    0.880541
H    3.673210    0.965569    0.153318
```

Frequencies

-406.59	67.0101	83.0797
89.2378	113.6344	168.6228
216.0342	248.8785	265.4978
282.1235	331.4095	366.453
419.5625	477.8241	507.3717
572.5355	743.8027	817.6996
848.9221	858.8719	980.8665
1021.459	1038.353	1056.934
1061.55	1065.503	1113.982
1185.839	1228.41	1352.709
1382.595	1415.749	1423.786
1469.886	1482.011	1484.827
1488.028	1497.676	1653.98
1709.449	2365.089	3043.014
3047.225	3103.941	3118.781

| 3122.063 | 3141.978 | 3151.038 |
| 3167.118 | 3174.118 | 3269.973 |

i14 – p35

C	0.320184	2.040224	-0.093107
C	1.487044	1.123475	0.099998
C	1.508131	-0.213416	-0.012897
C	0.338002	-1.037684	-0.334174
C	2.791129	-0.989254	0.157519
C	-3.420788	-0.242304	0.340367
C	-2.151647	-0.514864	0.113369
C	-0.932837	-0.748391	-0.110274
H	-0.242352	2.167519	0.838686
H	0.661003	3.029126	-0.407904
H	-0.381866	1.657781	-0.837331
H	2.431167	1.604757	0.345940
H	0.549034	-2.011990	-0.774264
H	3.033924	-1.542987	-0.755908
H	2.703799	-1.722045	0.965830
H	3.628031	-0.327374	0.385404
H	-4.200942	-0.950821	0.083931
H	-4.102934	0.917748	-1.655225
H	-3.714170	0.671572	0.846043

Frequencies

-398.826	48.3701	76.5851
124.0974	152.7983	171.5098
186.0049	245.7614	256.9894
291.7921	329.0109	350.6944
427.2224	463.9307	553.4497
586.5323	652.5722	819.3566
847.6733	887.1529	902.4193
922.6952	1018.492	1035.264
1055.632	1075.748	1087.16
1106.535	1214.262	1336.761
1389.82	1417.831	1424.468
1457.647	1484.864	1486.802
1503.751	1506.056	1688.09
1726.685	2168.159	3038.864
3043.009	3098.584	3105.507
3133.536	3136.722	3140.089
3152.244	3165.114	3239.897

i15 – p29

C	3.443759	0.221582	-0.175161
C	2.335157	-0.562080	0.460809
C	1.068789	-0.561599	0.077175
C	-0.068481	-1.144469	-0.281582
C	0.542736	1.736248	-0.048447
C	-3.864791	0.300757	0.122385
C	-2.508193	-0.212210	-0.016050
C	-1.380996	-0.620300	-0.123024
H	3.805053	1.008222	0.496804
H	4.293656	-0.432716	-0.390878
H	3.119625	0.685475	-1.107282
H	2.577852	-1.126419	1.360233
H	0.009004	-2.111320	-0.775446
H	-0.147643	1.733597	0.784987
H	0.113868	1.761488	-1.042489
H	1.502075	2.216505	0.099205
H	-4.261807	0.093925	1.119767
H	-4.533058	-0.159067	-0.609945
H	-3.886507	1.382736	-0.031590

Frequencies

| -502.062 | 30.2114 | 64.1477 |
| 81.913 | 139.7837 | 156.4596 |

163.8765	221.8099	240.1055
285.7509	307.1884	345.2683
449.3541	461.6253	480.6333
537.7699	598.9215	704.7846
784.0257	844.6902	868.9398
905.3268	1046.35	1048.902
1055.987	1080.684	1130.125
1216.055	1304.734	1404.571
1412.082	1419.882	1430.114
1450.293	1482.636	1488.145
1491.676	1503.065	1923.814
2371.859	3038.047	3049.456
3099.042	3108.873	3119.839
3123.465	3134.293	3144.56
3151.558	3277.004	3284.645

i15 – p32

```
C    3.564792   0.085116  -0.064216
C    2.239175  -0.605083  -0.040673
C    1.015823  -0.053846   0.012091
C   -0.142616  -0.948453   0.023619
C    0.729896   1.421003   0.060006
C   -3.863759   0.218251   0.143424
C   -2.605555  -0.172960   0.112808
C   -1.403370  -0.551923   0.070107
H    4.194024  -0.270391   0.758238
H    4.099125  -0.147095  -0.991704
H    3.487175   1.169147   0.016942
H    2.289796  -1.692222  -0.074743
H    0.058739  -2.017415  -0.010182
H    0.183934   1.671177   0.974399
H    0.090163   1.708730  -0.779268
H    1.634610   2.025762   0.024164
H   -4.672554  -0.503731   0.171776
H   -4.450252   0.433245  -2.195273
H   -4.121076   1.270168   0.202650
```

Frequencies

-375.118	51.7943	78.5457
82.7276	94.9954	127.0598
151.5534	227.3574	262.1139
295.8058	311.4377	383.6992
438.6469	445.0633	533.9484
608.5839	620.7687	812.6267
838.3165	876.3026	902.3287
923.1837	1002.295	1034.874
1054.378	1059.675	1067.104
1128.372	1252.785	1326.614
1384.376	1425.102	1435.834
1453.118	1481.931	1487.603
1488.807	1501.637	1686.662
1729.378	2163.703	3043.284
3054.801	3096.5	3112.451
3141.231	3152.426	3154.233
3157.694	3165.701	3240.568

i15 – p7a

```
C    3.460589   0.026670  -0.120983
```

```
C    2.310244   -0.659354   -0.071531
C    0.973869   -0.072863   -0.057390
C   -0.090889   -0.900467   -0.012719
C    0.837303    1.420602   -0.085174
C   -4.014696    0.221120    0.047411
C   -2.611587   -0.169824    0.025096
C   -1.450361   -0.488915    0.006769
H    3.911675    0.436437    2.094618
H    4.413971   -0.486576   -0.151785
H    3.485152    1.107334   -0.205027
H    2.352651   -1.744964   -0.022440
H    0.082170   -1.973433    0.011002
H   -0.210203    1.719836   -0.066017
H    1.300793    1.834655   -0.985942
H    1.343441    1.866485    0.776889
H   -4.655147   -0.641496    0.246270
H   -4.313524    0.652746   -0.911474
H   -4.197818    0.967166    0.825027
```

Frequencies

-390.84	63.079	79.5525
84.0907	122.0673	159.5834
194.5073	236.6589	256.0114
299.1745	309.0101	397.6892
429.4008	453.1052	506.2951
597.6534	710.3573	823.5243
837.4068	884.9899	946.379
994.5094	1020.957	1049.521
1052.05	1067.343	1088.905
1215.363	1247.07	1328.525
1386.438	1410.839	1436.86
1453.076	1480.171	1487.235
1492.895	1497.814	1661.889
1688.625	2368.452	3048.313
3049.152	3109.068	3119.076
3125.781	3154.959	3162.87
3170.834	3173.719	3259.286

i11 – p31

```
C    1.920550    1.894204    0.065312
C    1.360315    0.895434   -0.612007
C    1.270997   -0.498138   -0.147833
C    0.059502   -1.280193   -0.617392
C    2.200996   -1.067241    0.630298
C   -3.479662    0.578640    0.386588
C   -2.234155   -0.087778    0.024639
C   -1.207141   -0.635956   -0.267172
H    1.959512    2.896717   -0.344507
H    2.340492    1.744927    1.054911
H    0.891384    1.105464   -1.571366
H    0.112921   -1.387003   -1.708716
H    0.089369   -2.291026   -0.202235
H    2.106739   -2.096605    0.957744
H    1.468845   -0.486991    2.700444
H    3.116547   -0.547369    0.887257
H   -4.205159   -0.139301    0.777180
H   -3.925147    1.072273   -0.480642
H   -3.303915    1.335079    1.155325
```

Frequencies

-424.981	47.3842	64.9605
122.648	125.4452	154.193
187.0536	208.5398	248.8293
305.7778	386.5986	398.9868
413.2165	509.0314	549.6286
695.2318	784.6172	814.5219

822.7035	931.9068	949.9219
965.2055	976.848	1036.219
1058.955	1066.325	1102.529
1174.496	1209.477	1282.642
1332.252	1347.907	1422.99
1444.898	1464.556	1476.166
1489.036	1492.788	1681.079
1721.501	2398.516	3032.986
3048.581	3100.412	3120.041
3123.648	3152.114	3161.906
3164.5	3247.963	3253.826

i11 – p8a
```
C     2.260370   1.814603   0.049692
C     1.171140   1.041311   0.037994
C     1.178121  -0.411766  -0.055689
C     0.013797  -1.119770  -0.031357
C     2.490092  -1.135024  -0.130395
C    -3.748742   0.472368  -0.041321
C    -2.402333  -0.083864  -0.036015
C    -1.290013  -0.542549  -0.025608
H     2.175988   2.892603   0.119861
H     3.263883   1.406951  -0.009864
H     0.191424   1.505883   0.101120
H     0.054224  -2.193679  -0.187119
H     0.096440  -1.732419   1.941195
H     2.343790  -2.213540  -0.200382
H     3.094673  -0.929958   0.759089
H     3.068463  -0.808360  -1.000044
H    -3.744542   1.503738   0.319552
H    -4.410881  -0.110718   0.603578
H    -4.168053   0.467643  -1.050788
```

Frequencies

-648.571	40.6092	84.2021
97.1791	140.7485	200.3645
232.9338	245.5581	299.9234
312.6088	322.9685	389.3695
432.6001	463.9336	513.408
600.7753	728.6628	797.5363
845.7104	903.9538	952.309
1005.517	1042.353	1054.609
1058.464	1063.278	1073.886
1211.319	1260.486	1329.862
1376.831	1418.702	1423.075
1456.809	1483.252	1484.217
1486.071	1502.752	1612.337
1685.801	2373.21	3040.251
3046.502	3101.721	3118.462
3122.626	3140.287	3158.553
3173.283	3182.255	3247.459

i13 – i15
```
C     3.305431  -0.465398   0.660494
C     2.394324  -0.258437  -0.501379
H     4.255370  -0.908564   0.354943
H     3.535927   0.483068   1.170940
H     2.842557  -1.115485   1.411388
H     2.817177  -0.159867  -1.497574
C     0.989044   0.145237  -0.293283
C     0.002755  -0.764022  -0.326705
C     0.747016   1.609224  -0.032437
```

```
C    -3.968290   0.013464   0.251995
C    -2.551483  -0.257430   0.042995
C    -1.379660  -0.475680  -0.125813
H     0.254217  -1.803106  -0.520199
H     1.306848   1.935805   0.850243
H    -0.311298   1.820007   0.126704
H     1.104174   2.207644  -0.877006
H    -4.252347  -0.178712   1.290107
H    -4.585662  -0.619454  -0.390421
H    -4.201784   1.056912   0.025676
```

Frequencies

-172.21	75.1523	94.2005
99.0473	132.7184	159.7283
208.4581	216.7049	283.4779
314.905	406.0382	443.8161
502.3959	518.4936	577.2569
817.4933	827.6698	900.3914
978.6211	987.4556	1036.667
1058.159	1067.015	1078.018
1114.491	1197.101	1229.704
1339.631	1375.716	1405.583
1411.318	1423.459	1474.419
1485.995	1488.266	1489.38
1491.681	1493.126	1713.485
2373.388	2984.796	3038.838
3045.375	3061.779	3098.019
3117.166	3118.67	3127.007
3147.512	3166.333	3170.789

i15 – i16
```
C    -3.085505  -1.071947  -0.384500
C    -1.797496  -0.759337   0.315847
C    -1.065464   0.352296   0.232116
C    -1.389625   1.560101  -0.609864
H    -2.984063  -1.987459  -0.976064
H    -3.883228  -1.252870   0.343511
H    -3.415933  -0.277061  -1.053718
H    -1.424332  -1.546859   0.967709
H    -0.596282   1.724664  -1.346050
H    -1.434729   2.458044   0.015039
H    -2.337630   1.467354  -1.140419
C     0.192959   0.471359   1.019794
C     3.799421  -0.498262  -0.545896
C     2.505556  -0.152904   0.022557
C     1.421040   0.144995   0.495051
H     0.147799   0.901859   2.016931
H     4.479809  -0.869202   0.225394
H     4.266786   0.375315  -1.011356
H     3.696485  -1.271590  -1.311611
```

Frequencies

-96.6971	75.2794	86.8434
128.697	152.717	177.513
210.7692	264.6599	285.134
338.5288	387.8739	429.3017
468.5411	599.0674	631.8916
771.4755	825.2176	890.8933
982.777	1026.686	1040.741
1057.428	1062.861	1069.739
1115.59	1212.976	1227.195
1364.284	1396.53	1413.799

1424.078	1427.231	1483.98
1484.945	1487.136	1488.101
1491.584	1504.254	1763.911
2175.991	3039.115	3040.235
3044.157	3096.866	3097.582
3105.106	3117.559	3139.869
3151.592	3162.287	3163.462

i69 – p17

```
C    0.644363    2.043756   -0.292689
C    0.340991    0.657828    0.222461
C   -3.531575   -0.615359   -0.017440
C   -2.148197   -0.166677    0.066349
C   -1.000437    0.191101    0.148127
C    1.324633   -0.175700    0.582483
C    2.170085   -0.790408    1.365799
C    1.952800   -1.059665   -1.562068
H    0.455100    2.102418   -1.369782
H    1.686434    2.305891   -0.106561
H   -0.001577    2.777356    0.196625
H   -3.593675   -1.589562   -0.509302
H   -4.136743    0.092467   -0.589180
H   -3.971895   -0.711554    0.978634
H    2.885893   -1.517189    1.001683
H    2.163524   -0.578932    2.431951
H    2.984038   -0.729113   -1.564328
H    1.266176   -0.569480   -2.240288
H    1.746749   -2.091561   -1.307584
```

Frequencies

-495.749	28.2622	33.5519
52.9681	87.9156	110.8667
132.6408	180.2129	199.6453
263.5331	306.1579	369.0908
409.0225	471.787	501.7121
532.974	572.8917	646.6407
698.2093	769.7813	911.6214
921.9857	1009.656	1048.509
1053.243	1057.926	1060.975
1239.757	1321.1	1406.912
1413.271	1419.247	1420.69
1466.206	1482.069	1483.083
1484.513	1498.885	1952.414
2348.299	3038.074	3044.697
3102.754	3106.523	3115.493
3120.463	3136.928	3146.877
3228.431	3273.892	3276.036

i69 – p14

```
C    0.644363    2.043756   -0.292689
C    0.340991    0.657828    0.222461
C   -3.531575   -0.615359   -0.017440
C   -2.148197   -0.166677    0.066349
C   -1.000437    0.191101    0.148127
C    1.324633   -0.175700    0.582483
C    2.170085   -0.790408    1.365799
C    1.952800   -1.059665   -1.562068
H    0.455100    2.102418   -1.369782
H    1.686434    2.305891   -0.106561
H   -0.001577    2.777356    0.196625
H   -3.593675   -1.589562   -0.509302
H   -4.136743    0.092467   -0.589180
H   -3.971895   -0.711554    0.978634
H    2.885893   -1.517189    1.001683
H    2.163524   -0.578932    2.431951
```

```
H    2.984038   -0.729113   -1.564328
H    1.266176   -0.569480   -2.240288
H    1.746749   -2.091561   -1.307584
```

Frequencies

-352.344	34.3911	58.4444
94.5091	126.3455	142.1766
196.1442	244.8158	290.8112
338.4445	350.5564	396.8789
429.7247	463.6666	578.1918
622.5813	686.9342	744.2897
800.2293	847.1382	938.592
955.2626	974.98	1032.402
1054.687	1058.733	1073.918
1080.729	1231.064	1385.41
1417.721	1422.717	1434.476
1450.821	1483.673	1483.817
1490.389	1509.711	1643.754
1720.048	2377.063	3042.271
3047.512	3104.363	3120.079
3123.105	3141.328	3160.683
3178.064	3252.299	3271.942

i16 – p8a

```
C    2.271334    1.682786    0.185735
C    1.153195    0.947116    0.108292
C    1.113274   -0.509084    0.026629
C   -0.062895   -1.167568   -0.038572
C    2.410360   -1.267200    0.012278
C   -3.790207    0.497685   -0.002251
C   -2.455250   -0.085343   -0.017946
C   -1.349646   -0.562669   -0.027798
H    2.220739    2.761905    0.267308
H    3.257148    1.235075    0.245678
H    2.825158    2.005239   -2.011607
H    0.190712    1.449657    0.087882
H   -0.051818   -2.252311   -0.103198
H    2.239732   -2.340660   -0.077841
H    2.976898   -1.086558    0.931270
H    3.038415   -0.947342   -0.825194
H   -3.987936    0.988425    0.954353
H   -4.551573   -0.271432   -0.153046
H   -3.898466    1.243670   -0.793810
```

Frequencies

-393.891	81.6012	87.2631
114.3355	121.1197	157.342
198.2583	241.5556	260.9406
283.1101	326.1677	390.2982
426.9714	466.7278	489.7388
601.431	749.8818	798.6578
847.5634	868.6083	952.2244
1010.646	1032.345	1056.316
1065.568	1069.788	1080.949
1214.472	1258.518	1340.48
1378.087	1423.726	1426.836
1458.411	1483.919	1487.188
1492.729	1505.243	1657.656
1689.668	2369.041	3044.683

3047.021	3105.254	3119.024
3121.471	3144.131	3164.727
3172.653	3192.589	3254.868

i16 – p34

```
C     2.408559    1.763490    0.017501
C     1.196898    0.889149   -0.014034
C     1.139967   -0.450080   -0.024054
C    -0.155816   -1.149580   -0.051268
C     2.336541   -1.366091   -0.013459
C    -3.682362    0.496960    0.205660
C    -2.489761   -0.059168    0.126618
C    -1.351895   -0.594456    0.038490
H     2.412654    2.439506   -0.844018
H     2.395663    2.397316    0.910876
H     3.347112    1.209023    0.014600
H     0.246614    1.419477   -0.031185
H    -0.115473   -2.232981   -0.153324
H     2.316114   -2.031025   -0.882963
H     2.323803   -2.001540    0.878061
H     3.283437   -0.828774   -0.026963
H    -4.583505   -0.106582    0.192266
H    -4.245407    0.987553   -2.114947
H    -3.793792    1.566676    0.344875
```

Frequencies

-362.131	33.1985	64.8757
80.972	91.5545	124.3256
152.2642	228.3815	253.798
263.251	329.2657	361.6108
430.6926	449.7084	541.8731
623.2233	631.1131	799.3933
855.2598	885.2276	907.0056
923.5147	1006.161	1033.594
1043.442	1062.325	1067.511
1137.688	1231.063	1315.956
1387.177	1422.256	1428.818
1457.793	1484.383	1485.557
1492.375	1502.041	1685.383
1734.839	2154.861	3038.433
3043.307	3090.073	3097.835
3144.21	3146.708	3148.548
3162.808	3168.89	3235.058

i4 – i5

```
C     0.168223   -0.449052    0.928543
C    -0.914209    0.563628    0.686744
C     3.894204    0.326510   -0.579729
C     2.571037    0.049927   -0.034830
C     1.477163   -0.169775    0.421521
C    -1.913690    0.101874   -0.065352
C    -1.695218   -1.304681   -0.519192
C    -3.149847    0.854256   -0.450159
H    -0.450874   -1.350353    0.204327
H     0.180969   -0.877859    1.934124
H    -0.864529    1.567962    1.095411
H     4.659664   -0.258559   -0.063802
H     4.145497    1.384780   -0.468933
H     3.938941    0.080361   -1.643990
H    -2.389086   -2.062657   -0.153780
H    -1.416277   -1.448013   -1.563672
H    -3.234660    0.932961   -1.538796
H    -3.149783    1.862104   -0.029197
H    -4.045833    0.333146   -0.096962
```

Frequencies

| -1901.24 | 44.8137 | 60.9985 |

86.1953	169.5854	201.7154
213.1315	293.55	349.9623
362.1435	423.5023	476.8498
502.4726	575.5678	653.6126
790.5876	841.3827	892.9856
946.1784	953.5497	996.3507
1033.588	1049.566	1054.13
1068.443	1109.119	1184.369
1220.671	1304.757	1334.775
1387.123	1414.837	1417.199
1452.94	1481.899	1483.084
1485.272	1490.503	1647.862
1744.227	2343.568	3038.521
3047.991	3091.912	3093.201
3098.787	3117.359	3122.498
3132.277	3172.664	3194.058

i5 – p24

```
C    -0.368059   -0.625406   -0.035465
C     0.691907    0.366182   -0.033324
C    -4.159787    0.290790   -0.152466
C    -2.878641   -0.018052   -0.120563
C    -1.654649   -0.316562   -0.079306
C     2.012547    0.125500    0.011120
C     2.636568   -1.239399    0.067269
C     2.995953    1.261564    0.007635
H    -0.104964   -1.679092    0.000845
H     0.358435    1.399718   -0.071379
H    -4.768850    0.491722    2.201154
H    -4.921104   -0.481325   -0.175778
H    -4.485090    1.323548   -0.213910
H     1.913751   -2.054050    0.069776
H     3.304216   -1.382534   -0.789229
H     3.254218   -1.332974    0.967029
H     3.621833    1.232405    0.906650
H     2.499420    2.232161   -0.034251
H     3.673100    1.182720   -0.850308
```

Frequencies

-404.838	58.2303	80.9419
91.9362	116.3491	147.5156
171.9574	243.3039	245.6396
265.8322	309.0061	379.6578
453.4878	497.1219	530.0516
540.911	604.7678	846.9694
875.0406	885.7975	897.2015
940.6227	971.6067	1015.074
1034.477	1069.797	1103.84
1170.475	1232.623	1306.564
1387.769	1421.557	1428.568
1453.202	1472.797	1489.409
1494.53	1499.878	1680.136
1727.752	2157.318	3028.939
3038.289	3085.356	3091.601
3135.501	3147.286	3154.04
3166.756	3174.29	3234.629

111

i5 – p4b

C	-0.284044	-0.516398	0.166881
C	0.676811	0.343759	-0.197888
C	-4.288260	0.251882	-0.043843
C	-2.858537	-0.017355	0.029071
C	-1.675672	-0.232540	0.086199
C	2.118067	0.066327	-0.134454
C	2.621066	-1.156602	-0.351718
C	2.996114	1.244998	0.189213
H	-0.007776	-1.488948	0.566932
H	0.385296	1.336791	-0.532886
H	-4.557226	1.094565	0.598384
H	-4.864691	-0.618423	0.278851
H	-4.586071	0.497834	-1.066368
H	1.990567	-1.983325	-0.658052
H	3.687828	-1.342293	-0.295131
H	2.476144	-2.074253	1.829947
H	2.737032	1.662066	1.167483
H	2.854120	2.042398	-0.547768
H	4.051507	0.969162	0.197841

Frequencies

-337.77	15.3051	74.2156
84.9323	119.7791	141.808
161.4519	180.2917	223.3525
264.3401	309.2458	379.9751
427.2901	518.6893	529.4336
552.7244	740.771	810.7205
892.7718	914.3055	936.2111
990.0729	1006.657	1031.387
1054.112	1058.038	1072.751
1204.916	1255.072	1331.17
1356.887	1416.291	1419.914
1443.737	1483.485	1483.727
1485.001	1499.104	1679.299
1714.007	2372.878	3038.129
3046.181	3099.802	3117.646
3122.149	3139.318	3156.271
3160.72	3166.069	3246.903

i5 – p4a

C	0.282465	-0.535653	0.011650
C	-0.673795	0.401182	-0.089346
C	4.287142	0.256025	0.019150
C	2.857396	-0.022699	0.015753
C	1.674203	-0.244534	0.012338
C	-2.109853	0.137768	-0.093928
C	-2.592218	-1.280544	0.032436
C	-2.970012	1.164644	-0.193669
H	0.012701	-1.584518	0.099291
H	-0.373308	1.441952	-0.174243
H	4.606558	0.658955	-0.945532
H	4.860277	-0.653601	0.213994
H	4.538069	0.988336	0.790830
H	-2.249627	-1.725189	0.972086
H	-3.681527	-1.326289	0.010735
H	-2.205991	-1.900275	-0.782624
H	-4.041556	1.005078	-0.230637
H	-2.618609	2.185169	-0.300961
H	-3.378953	1.653244	2.060768

Frequencies

-344.089	31.6694	80.4911
83.0481	134.4071	146.5207
200.7522	216.0021	225.6391
259.61	308.3182	414.0873
428.6891	500.6836	538.1523

549.8838	749.3082	818.9204
873.0556	889.0685	937.3679
998.4254	1000.663	1048.17
1053.392	1057.655	1070.484
1211.516	1295.634	1333.487
1351.412	1416.663	1420.838
1449.101	1483.139	1483.624
1489.021	1505.812	1669.326
1699.891	2371.134	3042.216
3046.041	3104.553	3117.341
3122.293	3141.988	3154.497
3171.327	3177.495	3245.58

i5 – p25

C	0.194566	1.491540	-0.070745
C	-1.194364	1.081496	0.047863
C	3.464077	-0.641665	-0.088640
C	2.357741	0.075376	-0.095913
C	1.283854	0.735221	-0.090150
C	-1.700429	-0.164181	0.003875
C	-0.862455	-1.393953	-0.199034
C	-3.175575	-0.392509	0.163494
H	0.358882	2.565587	-0.138733
H	-1.893237	1.902742	0.179894
H	4.436373	-0.174720	-0.201772
H	3.428478	-1.724105	-0.024693
H	4.048381	-0.771173	2.285546
H	-0.261553	-1.607845	0.691237
H	-1.488592	-2.264887	-0.403867
H	-0.157556	-1.264525	-1.024418
H	-3.585172	-0.886105	-0.724931
H	-3.722569	0.537638	0.326621
H	-3.367917	-1.060556	1.010608

Frequencies

-385.708	31.7799	81.615
115.0081	143.3804	171.0927
195.7875	236.6084	255.5113
274.181	313.0435	394.9125
436.1191	479.8644	533.6239
618.4825	718.8307	780.77
848.0722	871.5828	898.3468
925.7072	989.301	1003.761
1034.518	1051.176	1100.208
1157.842	1230.861	1340.347
1392.203	1419.082	1423.551
1456.217	1481.609	1487.283
1490.532	1502.329	1681.935
1704.288	2157.238	3028.288
3040.169	3085.698	3104.88
3129.915	3134.019	3140.937
3145.066	3171.323	3231.595

i5 – p5a

C	0.100960	1.516877	-0.002428
C	-1.180873	1.114075	-0.047845
C	3.565733	-0.639724	0.044896
C	2.324311	0.121372	0.026961
C	1.281460	0.722668	0.011520
C	-1.738527	-0.237373	-0.095632
C	-0.839891	-1.442151	-0.085013

```
C    -3.075331   -0.372570   -0.134007
H     0.280561    2.588292    0.027950
H    -1.925537    1.905696   -0.048885
H     4.184268   -0.395326   -0.822553
H     3.363151   -1.713610    0.026668
H     4.144662   -0.417942    0.945117
H    -0.221906   -1.458563    0.816299
H    -1.429907   -2.359308   -0.122571
H    -0.155002   -1.427894   -0.936314
H    -3.543144   -1.348282   -0.199085
H    -3.731488    0.490851   -0.158396
H    -3.592711   -0.562951    2.161051
```

Frequencies

-348.851	36.8007	48.2015
82.3623	137.5611	159.9541
192.5699	240.2311	247.6496
308.5583	328.4242	426.6652
434.4207	454.4391	599.7155
685.7578	741.4403	760.6418
822.2722	866.0554	935.8729
993.2518	1013.362	1047.604
1053.201	1057.956	1071.501
1164.063	1271.797	1350.714
1409.382	1418.21	1439.064
1464.91	1482.832	1483.409
1484.541	1503.626	1661.421
1695.882	2367.163	3045.148
3052.786	3118.001	3119.606
3122.552	3139.896	3153.178
3157.408	3178.206	3244.113

i5 – p5b
```
C     0.097827    1.544957   -0.077534
C    -1.172146    1.108454   -0.127729
C     3.516860   -0.669603    0.154517
C     2.298824    0.122738    0.065356
C     1.274250    0.751584   -0.004331
C    -1.679587   -0.267916   -0.129908
C    -0.981905   -1.316373   -0.590909
C    -3.072339   -0.431967    0.421567
H     0.262531    2.618833   -0.072580
H    -1.940678    1.878321   -0.129969
H     4.213878   -0.402607   -0.643951
H     3.291029   -1.735598    0.071078
H     4.018541   -0.502503    1.111109
H     0.185583   -2.003031    1.324431
H    -1.418620   -2.309112   -0.596142
H     0.000075   -1.201457   -1.030343
H    -3.785794    0.182095   -0.138179
H    -3.115392   -0.105416    1.465607
H    -3.401851   -1.470775    0.372761
```

Frequencies

-296.073	11.2643	42.0389
81.5018	159.8758	163.6243
184.0722	193.4651	245.8747
294.1937	347.4534	405.6785
428.0248	470.015	598.6124
672.6579	733.6652	757.7566
807.5473	908.6058	947.2095
987.0333	1007.978	1036.783
1052.953	1057.37	1072.729

1172.019	1276.573	1282.087
1415.378	1417.157	1449.645
1460.715	1481.029	1483.139
1486.581	1501.812	1665.202
1708.047	2367.114	3036.488
3045.72	3097.53	3118.95
3121.064	3138.429	3153.19
3162.418	3175.641	3260.84

i5 – p26

```
C     0.370066    0.011812    1.001146
C    -0.764793    0.002131    0.336802
C     4.151876   -0.005579   -0.541749
C     2.802648    0.001055    0.007319
C     1.677873    0.005799    0.432666
C    -2.036840   -0.000015   -0.010045
C    -2.766838    1.282007   -0.306836
C    -2.767505   -1.286273   -0.285944
H     0.311903    0.025313    2.088451
H    -0.053742   -0.053016   -1.557679
H     4.759899   -0.783954   -0.073765
H     4.645057    0.955672   -0.375678
H     4.127371   -0.193184   -1.617976
H    -2.176377    2.155974   -0.032281
H    -3.000999    1.343547   -1.375672
H    -3.716377    1.309880    0.237321
H    -3.717691   -1.304525    0.257433
H    -2.177797   -2.155875    0.003643
H    -3.000167   -1.365454   -1.353955
```

Frequencies

-705.004	14.6744	76.1111
80.5266	84.3299	154.7635
171.9587	174.0041	240.4973
298.0321	299.5321	357.1565
414.241	476.5283	502.215
522.0511	588.1559	794.3487
806.5334	833.5955	969.3938
988.5186	1023.819	1051.955
1059.664	1096.399	1190.854
1233.916	1248.514	1402.278
1413.899	1415.462	1445.859
1477.003	1482.939	1484.116
1488.09	1495.791	1517.2
2014.753	2383.573	3035.346
3038.1	3050.684	3098.517
3100.19	3120.912	3127.194
3142.982	3147.257	3148.835

i38 – p27

```
C     2.769055    0.000000    0.116240
C     1.436236    0.000000   -0.057615
C     0.666334   -1.241635   -0.154368
C    -0.657122   -1.246071   -0.315565
C    -1.491582    0.000000   -0.393551
C    -0.657122    1.246071   -0.315565
C     0.666334    1.241635   -0.154368
C    -2.580542    0.000000    0.695201
H     3.330904   -0.925810    0.166085
H     2.947030    0.000000    2.550399
H     3.330904    0.925810    0.166086
H     1.213741   -2.177104   -0.091176
H    -1.189692   -2.191100   -0.381894
H    -2.010405    0.000000   -1.364243
```

H	-1.189692	2.191100	-0.381894
H	1.213741	2.177104	-0.091175
H	-3.216744	-0.884967	0.608964
H	-3.216743	0.884967	0.608964
H	-2.122592	0.000000	1.687427

Frequencies

-326.86	66.6779	123.7714
149.8823	236.4692	240.2884
274.3902	378.7948	423.4366
444.7331	501.2654	607.7049
677.662	712.6425	790.7084
802.2148	817.9588	834.5726
914.2111	939.9541	960.3912
992.1833	1015.846	1017.535
1048.165	1098.097	1130.461
1191.674	1225.828	1307.1
1335.459	1381.046	1391.815
1411.877	1446.811	1474.529
1500.388	1505.437	1661.061
1701.448	1760.725	2997.178
3041.899	3121.498	3127.861
3156.328	3162.907	3164.102
3187.212	3190.368	3247.666

i37 – p27

C	-2.598396	-0.037380	-0.625134
C	-1.441489	0.031468	0.388177
C	-0.599045	1.249395	0.160074
C	0.744596	1.214978	0.030229
C	1.475808	-0.059665	-0.087825
C	0.681623	-1.270441	0.134470
C	-0.630533	-1.233286	0.364141
C	2.777634	-0.103406	-0.390452
H	-2.207662	-0.132803	-1.641292
H	-3.213802	0.864899	-0.575124
H	-3.241244	-0.897885	-0.421579
H	-1.896608	0.122895	1.387198
H	-1.113008	2.206327	0.150726
H	1.285930	2.124105	-0.211284
H	1.242218	1.587908	1.865790
H	1.204681	-2.221425	0.106890
H	-1.175591	-2.159157	0.527229
H	3.301513	-1.047889	-0.485957
H	3.352386	0.803040	-0.544676

Frequencies

-807.569	66.6585	203.6201
236.9221	262.917	313.0557
372.1346	387.8923	440.9654
469.9253	506.702	609.5075
682.5927	715.9644	785.5409
797.0691	813.6826	834.2148
922.3836	937.3999	957.6245
990.5626	1016.718	1023.603
1045.558	1097.308	1125.812
1190.098	1220.212	1305.829
1330.272	1377.513	1393.827
1412.621	1441.094	1473.459
1500.507	1505.756	1623.728

1692.634	1758.899	2986.427
3041.825	3121.201	3127.471
3154.813	3164.59	3169.549
3188.345	3191.374	3244.6

i34 – p1

```
C     2.571276   -0.988934    0.057746
C     1.251869   -0.267261   -0.006475
C     0.047639   -0.973064   -0.019363
C    -1.182711   -0.331769   -0.054609
C    -1.206299    1.076774   -0.031085
C    -0.001768    1.794717   -0.090875
C     1.208427    1.129110   -0.056436
C    -2.472451   -1.101413   -0.046174
H     2.450437   -2.057262   -0.131526
H     3.028190   -0.874488    1.045703
H     3.276482   -0.590467   -0.676473
H     0.074782   -2.059372   -0.010249
H    -1.651154    1.278065    1.781992
H    -2.146099    1.593434   -0.195778
H    -0.027712    2.877331   -0.139435
H     2.136630    1.691430   -0.079720
H    -2.303894   -2.168385   -0.202153
H    -2.980732   -0.973949    0.915751
H    -3.152826   -0.745295   -0.824489
```

Frequencies

-813.404	130.2682	146.1397
192.1847	210.2601	281.8157
339.1612	375.3894	417.5071
459.0084	523.5133	544.3855
563.8394	723.1647	740.1261
810.679	896.5279	932.4744
961.7882	1005.676	1018.746
1027.746	1038.664	1071.678
1073.983	1122.841	1188.085
1199.543	1286.895	1313.801
1348.486	1425.873	1427.933
1463.881	1495.778	1498.296
1498.994	1520.146	1530.435
1631.7	1669.819	3042.011
3043.34	3106.603	3106.818
3135.89	3138.341	3178.488
3183.47	3189.62	3213.181

i34 – i32

```
C     2.554331   -1.023593   -0.022257
C     1.229715   -0.322594    0.012474
C     0.051566   -0.987909    0.076594
C    -1.231111   -0.333792    0.144937
C    -1.209876    1.180504    0.071905
C     0.056966    1.833636   -0.066084
C     1.222548    1.144571   -0.060067
C    -2.510978   -1.053462   -0.154580
H     2.436936   -2.108498    0.013996
H     3.180873   -0.719836    0.824492
H     3.106856   -0.768442   -0.933763
H     0.051573   -2.075480    0.074332
H    -1.292408    0.498095    1.153870
H    -2.142588    1.695437   -0.117411
H     0.064742    2.913466   -0.174335
H     2.169241    1.665883   -0.147544
H    -2.485000   -2.079817    0.220424
H    -3.369053   -0.553240    0.304724
H    -2.700135   -1.091736   -1.236315
```

Frequencies

-2649.02	135.388	139.0415
180.0321	193.1311	265.5705
373.0116	389.6796	418.454
472.5566	537.1573	609.9229
687.2009	703.8616	764.8061
839.5881	875.3774	961.7865
972.493	977.6797	1031.792
1052.018	1061.235	1072.368
1137.486	1183.212	1210.635
1268.646	1295.083	1333.81
1398.886	1420.017	1426.279
1456.139	1477.724	1484.802
1497.176	1501.538	1592.285
1642.022	2200.072	3005.927
3024.949	3078.188	3078.497
3119.904	3130.043	3169.692
3184.537	3205.102	3221.885

i34 – p47

```
C     2.580437   -0.932217   -0.000739
C     1.221315   -0.297129   -0.014546
C     0.089982   -1.008290   -0.160159
C    -1.232480   -0.393495   -0.134161
C    -1.294781    1.116003   -0.244546
C    -0.009805    1.814178    0.092471
C     1.146343    1.156801    0.176980
C    -2.345851   -1.134222   -0.030850
H     2.520739   -2.011307   -0.151367
H     3.084172   -0.744924    0.953545
H     3.214765   -0.509019   -0.786690
H     0.136937   -2.089741   -0.252854
H    -2.112086    1.504569    0.370345
H    -1.554660    1.379088   -1.280852
H    -0.044235    2.890442    0.227168
H     2.067756    1.689765    0.391330
H    -2.615419   -1.141448    2.437501
H    -3.330146   -0.679699   -0.003505
H    -2.298772   -2.217504   -0.011331
```

Frequencies

-285.166	55.5996	95.5616
131.1956	171.9012	209.3735
294.0776	305.719	424.7324
458.3531	526.7927	547.3947
555.6475	700.6811	711.5805
763.4032	866.4372	884.6174
895.9389	941.2144	955.851
975.5056	1013.077	1026.281
1051.983	1072.072	1194.169
1206.672	1230.22	1318.415
1349.019	1373.51	1418.757
1446.219	1446.598	1457.528
1489.135	1498.158	1672.73
1679.165	1752.193	3002.854
3039.746	3086.233	3098.748
3140.4	3157.851	3176.172

3177.563	3201.572	3247.522

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C	2.439600	-1.011851	0.176390
C	1.284075	-0.328040	0.110320
C	-0.014306	-1.001846	0.084340
C	-1.177297	-0.347736	0.007889
C	-1.226806	1.154310	-0.055406
C	0.115367	1.816683	-0.024655
C	1.257586	1.134851	0.049906
C	-2.500402	-1.052466	-0.025136
H	2.923395	-1.366514	-2.224589
H	2.451525	-2.094119	0.240251
H	3.395397	-0.501584	0.211146
H	-0.009283	-2.087858	0.127918
H	-1.844026	1.530367	0.773726
H	-1.768210	1.459685	-0.962901
H	0.132601	2.901429	-0.068542
H	2.209556	1.656192	0.067077
H	-2.381730	-2.134921	0.046011
H	-3.139056	-0.720881	0.800998
H	-3.037066	-0.825225	-0.952987

Frequencies

-289.866	94.8668	113.8081
129.308	149.949	208.9093
294.1842	341.5081	420.3231
443.5712	487.6937	538.146
589.8688	710.6859	716.0306
801.0208	882.3129	885.405
905.4548	931.1049	952.4072
974.445	1010.542	1017.781
1051.433	1070.194	1179.569
1203.263	1231.298	1319.134
1361.649	1402.113	1423.045
1441.017	1457.92	1465.898
1483.318	1495.794	1664.855
1716.76	1771.165	3007.258
3025.629	3034.867	3091.908
3136.477	3162.004	3175.011
3178.985	3202.096	3252.451

Products

p1 + H

C	2.514963	-1.033952	0.006534
C	1.218549	-0.265606	-0.006499
C	0.000002	-0.941214	-0.011637
C	-1.218547	-0.265611	-0.006540
C	-1.204417	1.127834	-0.000270
C	-0.000003	1.818600	0.002619
C	1.204416	1.127837	-0.000223
C	-2.514961	-1.033956	0.006561
H	2.510011	-1.829121	-0.743379
H	2.680066	-1.502609	0.981512
H	3.365844	-0.381223	-0.198287
H	0.000005	-2.028761	-0.022633
H	-2.142370	1.673914	-0.001767
H	-0.000004	2.903220	0.002943
H	2.142366	1.673921	-0.001681
H	-3.365733	-0.381447	-0.199415
H	-2.680609	-1.501586	0.981945
H	-2.509586	-1.829902	-0.742511

Frequencies

101.1151	101.8826	197.0954
229.1919	276.9222	409.5253
442.0371	525.766	539.3609

549.2396	717.6343	744.0453
787.8462	902.4466	918.2242
927.3635	996.9835	1003.002
1027.264	1040.423	1072.154
1074.803	1136.274	1182.911
1203.896	1291.103	1321.434
1349.55	1420.062	1422.737
1467.381	1494.587	1495.267
1500.325	1519.841	1541.364
1666.199	1686.82	3047.079
3047.695	3113.249	3113.402
3136.376	3136.643	3169.041
3183.593	3191.635	3211.684

p2 + H

C	2.920815	-0.006989	0.006846
C	1.414238	0.005973	-0.002812
C	0.692766	-1.189501	-0.003647
C	-0.692787	-1.189487	-0.003623
C	-1.414238	0.006001	-0.002766
C	-0.695777	1.196480	-0.003557
C	0.695799	1.196467	-0.003582
C	-2.920815	-0.006977	0.006829
H	3.328831	0.996234	-0.131266
H	3.314313	-0.643560	-0.790400
H	3.303991	-0.396264	0.955075
H	1.227326	-2.134906	-0.007382
H	-1.227366	-2.134882	-0.007339
H	-1.228284	2.142624	-0.007012
H	1.228324	2.142600	-0.007058
H	-3.314271	-0.642424	-0.791339
H	-3.328844	0.996431	-0.129871
H	-3.304026	-0.397654	0.954468

Frequencies

50.8421	53.1237	140.081
289.6258	314.3234	391.1122
419.1591	468.4956	500.9141
662.1979	729.5334	739.929
818.2806	848.6467	859.5028
966.3482	989.679	994.8395
1027.397	1047.969	1069.818
1073.135	1152.311	1222.46
1244.155	1251.368	1329.244
1350.768	1421.531	1421.855
1452.633	1493.772	1494.917
1495.476	1510.328	1570.401
1652.298	1698.392	3044.964
3045.256	3109.626	3109.793
3133.108	3133.153	3176.223
3180.226	3194.424	3199.459

p3 + H

C	2.564604	-0.812764	-0.108497
C	1.231008	-0.140155	-0.005522
C	0.048116	-1.028167	0.294126
C	-1.307938	-0.407521	0.031775
C	-1.371903	1.052817	0.084945
C	-0.256682	1.794766	0.024932
C	1.063596	1.183393	-0.097202
C	-2.390865	-1.149356	-0.216954

```
H    2.578131   -1.526363   -0.939572
H    2.780795   -1.383484    0.802267
H    3.369022   -0.090732   -0.259857
H    0.108286   -1.287484    1.363040
H    0.140318   -1.977270   -0.243421
H   -2.350311    1.520954    0.115929
H   -0.324608    2.877414    0.027976
H    1.918811    1.830187   -0.266337
H   -3.365427   -0.691494   -0.348355
H   -2.334628   -2.229809   -0.297297
```

Frequencies

82.2211	162.4214	205.9829
295.7255	340.1813	419.2479
466.0654	490.25	513.3584
581.8149	691.4093	737.8093
804.0696	873.9876	876.123
911.138	931.8734	955.9367
983.1314	997.4677	1013.343
1068.066	1082.527	1182.964
1205.094	1235.625	1319.217
1343.136	1380.113	1420.412
1434.82	1455.162	1472.642
1483.017	1496.219	1669.455
1710.937	1755.922	2993.247
3031.747	3079.574	3088.759
3134.631	3148.666	3183.174
3192.637	3210.643	3236.482

p4a + H

```
C   -0.216585   -0.503344    0.000029
C    0.728450    0.448130    0.000503
C    2.171702    0.201094    0.000075
C    3.018269    1.235576   -0.000325
C    2.660932   -1.221921    0.000019
C   -4.236277    0.213919   -0.000253
C   -2.800384   -0.032611   -0.000104
C   -1.613264   -0.231833    0.000083
H    0.065258   -1.552832   -0.000671
H    0.417377    1.489444    0.001164
H    4.092890    1.090074   -0.000784
H    2.657175    2.258796   -0.000230
H    3.750880   -1.261003   -0.000355
H    2.298293   -1.759366   -0.881628
H    2.298903   -1.759181    0.882034
H   -4.788760   -0.716527   -0.151870
H   -4.512280    0.908068   -0.798107
H   -4.556798    0.648466    0.950280
```

Frequencies

65.9854	77.3066	81.2838
141.3035	175.3228	221.1408
251.5718	307.171	413.2139
420.7097	496.7486	537.3885
539.7464	707.3196	819.1777
872.6332	879.9678	927.1592
990.6811	999.1626	1040.813
1051.3	1059.804	1069.613
1211.086	1291.477	1333.861
1347.231	1413.458	1418.804
1452.218	1479.356	1483.298
1487.104	1501.337	1693.088

1732.885	2374.058	3047.791
3051.658	3109.621	3121.385
3128.303	3146.17	3156.42
3169.859	3175.743	3245.486

p4b + H

```
C    0.250828    0.512567    0.277268
C   -0.725260   -0.270541   -0.199264
C    4.242830   -0.261261   -0.098650
C    2.817596    0.010496    0.032582
C    1.638471    0.228209    0.136373
C   -2.165359    0.013461   -0.078925
C   -2.655467    1.251331   -0.165757
C   -3.048789   -1.189647    0.124319
H   -0.008009    1.419039    0.818937
H   -0.451293   -1.204258   -0.685964
H    4.536745   -0.298201   -1.150840
H    4.498325   -1.221311    0.357346
H    4.833641    0.515671    0.392506
H   -3.717124    1.444518   -0.055821
H   -2.014336    2.102275   -0.367200
H   -4.100730   -0.907584    0.189491
H   -2.773483   -1.723053    1.039405
H   -2.932833   -1.894785   -0.705542
```

Frequencies

22.5545	74.5228	87.4451
118.5984	177.917	218.2704
258.1108	306.5348	378.9001
423.4704	518.9214	528.919
546.763	718.2159	809.42
893.3671	913.6025	938.6573
992.3557	1006.501	1032.24
1054.013	1057.934	1075.906
1204.178	1254.339	1332.261
1353.877	1416.89	1419.657
1447.086	1483.524	1483.937
1485.361	1499.914	1708.673
1728.108	2374.258	3037.782
3045.729	3099.512	3116.919
3121.764	3137.429	3152.411
3158.819	3165.23	3241.195

p5a + H

```
C   -0.028044    1.505802    0.000160
C    1.250328    1.093384    0.000158
C    1.805266   -0.264290    0.000020
C    3.135871   -0.404380   -0.000522
C    0.897546   -1.464063    0.000488
C   -3.515878   -0.616074   -0.000115
C   -2.266160    0.132214   -0.000067
C   -1.216813    0.722157   -0.000070
H   -0.199636    2.579071    0.000471
H    2.000291    1.880080    0.000388
H    3.602522   -1.383233   -0.000583
H    3.796960    0.456133   -0.000969
H    1.482563   -2.385418    0.000904
H    0.245520   -1.462681   -0.876334
H    0.245537   -1.461918    0.877394
H   -4.363779    0.039986    0.211082
H   -3.497252   -1.402474    0.758875
H   -3.685424   -1.088048   -0.971541
```

Frequencies

56.8869	84.3274	106.0189
177.8097	256.5123	309.5893

312.3303	321.342	424.2233
438.8249	455.3279	595.3162
685.7925	719.8847	760.1073
809.7163	866.3833	937.4719
992.3916	1013.248	1055.321
1057.842	1060.398	1074.219
1164.727	1276.95	1356.106
1415.38	1419.256	1439.364
1471.992	1485.751	1489.784
1498.06	1510.932	1684.203
1729.513	2372.504	3048.711
3055.167	3118.743	3125.025
3126.162	3139.967	3155.614
3163.434	3185.512	3244.967

p5b + H

```
C    -0.103363    1.504008   -0.142918
C     1.166705    1.071987   -0.179625
C    -3.518733   -0.699872    0.233266
C    -2.296466    0.080755    0.100180
C    -1.274396    0.706891   -0.011847
C     1.676354   -0.306088   -0.101348
C     1.010709   -1.363417   -0.570307
C     3.041426   -0.440183    0.525136
H    -0.276651    2.574707   -0.205828
H     1.933416    1.841665   -0.238862
H    -4.264967   -0.379547   -0.498215
H    -3.950778   -0.579066    1.230112
H    -3.320778   -1.763092    0.075814
H     1.432437   -2.360245   -0.494755
H     0.043840   -1.264073   -1.046671
H     3.367543   -1.481055    0.552554
H     3.039557   -0.050950    1.548159
H     3.782958    0.137173   -0.037527
```

Frequencies

43.1526	81.0124	132.825
154.5102	167.7401	226.2714
288.5302	341.9421	398.2488
419.9239	466.6237	592.5487
663.9805	719.832	756.2731
803.048	904.7755	954.0289
982.9897	1008.813	1031.18
1060.797	1065.498	1071.164
1171.418	1274.89	1286.972
1407.319	1426.201	1446.485
1464.269	1481.125	1489.457
1491.051	1498.797	1697.986
1730.214	2372.438	3041.208
3048.241	3102.853	3118.355
3124.218	3138.658	3155.998
3160.217	3180.974	3256.354

p6 + H

```
C    -2.854163   -0.052880   -0.176806
C    -1.363694    0.037518   -0.011545
C    -0.697346    1.195062    0.001782
C     0.789030    1.270410    0.216973
C     1.520696   -0.039400    0.006619
C     0.721270   -1.257433    0.139250
```

```
C    -0.617686   -1.219345    0.135692
C     2.827592   -0.091460   -0.265674
H    -3.113490   -0.649778   -1.057417
H    -3.305226    0.934668   -0.289325
H    -3.311953   -0.541294    0.689898
H    -1.232644    2.135045   -0.097026
H     1.226818    2.049739   -0.413579
H     0.961566    1.597219    1.253695
H     1.246182   -2.206099    0.192482
H    -1.185375   -2.142709    0.204518
H     3.343202   -1.041144   -0.360454
H     3.416726    0.809511   -0.400541
```

Frequencies

57.5427	175.8774	240.0451
270.2503	308.9423	406.9
426.3477	477.8578	568.0475
621.2447	713.6911	746.0771
782.342	812.6579	826.612
911.9203	945.032	959.6387
983.7758	1004.455	1015.828
1076.497	1090.838	1202.884
1205.566	1232.444	1315.943
1346.159	1375.936	1425.196
1435.351	1452.172	1475.461
1490.45	1501.708	1670.828
1713.944	1766.61	3001.556
3035.741	3085.903	3095.917
3130.987	3154.874	3175.906
3180.969	3199.122	3243.01

p7a + H

```
C     3.528339    0.050147    0.000281
C     2.386690   -0.637703    0.000246
C     1.040957   -0.058491   -0.000044
C    -0.017867   -0.891393   -0.000253
C     0.895894    1.434424   -0.000234
C    -3.950551    0.205185    0.000429
C    -2.544478   -0.176451   -0.000402
C    -1.381255   -0.487948   -0.000422
H     4.485393   -0.457910    0.000491
H     3.550656    1.134627    0.000104
H     2.430653   -1.724742    0.000407
H     0.160566   -1.963783   -0.000248
H    -0.153601    1.727371    0.000838
H     1.377661    1.867348   -0.882424
H     1.379546    1.867854    0.880661
H    -4.235590    0.638276    0.962871
H    -4.588598   -0.662512   -0.183754
H    -4.153064    0.946854   -0.776554
```

Frequencies

59.0465	76.7708	84.8544
148.0809	191.3318	254.2638
280.9913	303.1753	396.7325
407.4392	451.9849	507.6309
597.0344	688.1567	823.5212
835.2667	885.1556	941.1339
995.2856	1026.165	1049.502
1052.068	1067.524	1090.256
1214.685	1247.414	1334.924
1386.284	1410.817	1436.577

1456.378	1480.214	1487.349
1492.852	1498.206	1687.807
1727.313	2371.848	3049.509
3050.07	3110.267	3119.812
3126.105	3154.207	3160.214
3169.766	3173.015	3255.41

p7b + H

C	-3.121069	-1.047264	0.275050
C	-2.523825	0.042204	-0.201755
C	-1.086033	0.346702	-0.095201
C	-0.164697	-0.624379	-0.219347
C	-0.734511	1.788491	0.135315
C	3.879807	-0.151100	0.093737
C	2.435083	-0.307069	-0.014354
C	1.241122	-0.434553	-0.104169
H	-4.185857	-1.205149	0.147977
H	-2.567344	-1.807303	0.817139
H	-3.131412	0.805593	-0.685627
H	-0.495282	-1.635299	-0.440152
H	0.344178	1.937383	0.183260
H	-1.180747	2.147080	1.068331
H	-1.137121	2.409773	-0.671991
H	4.292967	0.293807	-0.815469
H	4.363525	-1.119203	0.245493
H	4.141835	0.495127	0.935387

Frequencies

72.8756	86.2873	93.0803
123.028	136.5801	224.0548
272.3293	288.9565	387.5662
409.4164	509.4569	517.6362
556.7462	698.448	821.484
846.86	903.2439	966.3233
1011.33	1034.317	1048.776
1058.618	1064.782	1087.79
1200.67	1245.107	1320.78
1361.5	1417.185	1426.412
1463.468	1485.091	1486.966
1489.737	1490.972	1704.893
1723.956	2374.031	3043.233
3047.871	3101.425	3118.742
3121.638	3148.153	3155.455
3160.278	3179.711	3247.005

p8a + H

C	-2.274858	1.778068	-0.000114
C	-1.180708	1.016477	-0.000716
C	-1.172971	-0.448124	-0.000236
C	-0.014156	-1.135673	-0.001492
C	-2.487344	-1.175979	0.001953
C	3.752890	0.441106	0.002004
C	2.404533	-0.110925	-0.001738
C	1.287781	-0.561217	-0.002277
H	-2.199365	2.859196	-0.000655
H	-3.275323	1.358511	0.000890
H	-0.204137	1.492047	-0.001709
H	-0.050361	-2.221840	-0.001268
H	-2.340172	-2.256772	0.002111
H	-3.081144	-0.910452	-0.878409
H	-3.078285	-0.909873	0.884075
H	3.870932	1.185982	-0.789229
H	4.495374	-0.344602	-0.157506
H	3.971475	0.925395	0.957403

Frequencies

84.5758	86.2251	109.5891
131.9927	174.3852	251.7982
279.4159	325.5029	390.0131
390.4953	466.9336	484.8079
600.8026	730.4574	796.1693
846.6078	864.0493	943.618
1012.831	1037.925	1055.365
1063.541	1067.933	1083.226
1214.071	1258.119	1358.376
1382.68	1422.07	1425.965
1464.553	1480.734	1483.409
1492.316	1502.553	1681.122
1730.795	2370.889	3040.075
3047.439	3099.501	3118.814
3121.877	3143.254	3163.637
3173.29	3191.658	3251.628

p8b + H
```
C    -0.518382   2.025720   -0.211580
C    -1.434045   1.163538    0.225688
C    -1.453546  -0.294577    0.026926
C    -0.366614  -1.079512   -0.088157
C    -2.829673  -0.905517   -0.014350
C     3.576595  -0.038148    0.077245
C     2.166264  -0.398522    0.019136
C     0.995493  -0.676133   -0.026498
H    -0.625192   3.086773   -0.015548
H     0.347518   1.707283   -0.778774
H    -2.298917   1.557618    0.757604
H    -0.523555  -2.146103   -0.227953
H    -3.365721  -0.704937    0.919666
H    -2.788956  -1.985979   -0.160222
H    -3.422576  -0.468816   -0.824317
H     3.698496   1.044468    0.164883
H     4.099574  -0.367686   -0.824357
H     4.062779  -0.503710    0.938553
```

Frequencies

51.8472	60.9173	87.1805
107.2721	183.6165	245.2369
281.2084	322.0044	355.9538
396.1122	479.8417	499.5393
571.1055	725.3763	813.7486
847.2429	874.2208	972.8254
1022.161	1037.859	1055.913
1062.15	1066.254	1109.132
1186.118	1225.712	1352.18
1383.193	1416.618	1423.851
1468.182	1482.622	1488.008
1488.076	1496.637	1699.352
1728.51	2371.839	3040.675
3047.747	3100.454	3119.338
3120.9	3141.871	3147.641
3163.373	3167.539	3257.491

p9a + H
```
C    -3.166799  -0.915433   -0.001091
C    -2.548784   0.264461   -0.001075
```

```
C   -1.095680   0.484515   0.000416
C   -0.212873  -0.748845   0.001746
C   -0.605587   1.724296   0.000695
C    3.845975  -0.051026  -0.001397
C    2.406774  -0.289559   0.000335
C    1.223658  -0.492237   0.001108
H   -4.248628  -0.977315  -0.002264
H   -2.628531  -1.857271   0.000049
H   -3.150764   1.170265  -0.002206
H   -0.466931  -1.358855   0.877009
H   -0.467138  -1.360865  -0.872041
H    0.461625   1.910735   0.002048
H   -1.269737   2.582044  -0.000180
H    4.125311   0.644413  -0.796677
H    4.391847  -0.984135  -0.160981
H    4.172847   0.373944   0.950827
```

Frequencies

55.9247	71.0647	93.2754
148.6809	209.1581	234.8571
296.7431	378.1557	406.8432
433.4429	517.2859	535.4846
636.3899	791.3547	802.8485
843.4381	939.3904	946.8885
964.8739	973.32	1040.576
1056.841	1061.479	1068.442
1181.211	1253.751	1283.651
1331.187	1394.941	1420.765
1439.298	1462.431	1479.71
1486.167	1490.059	1694.373
1746.703	2399.192	3034.058
3053.44	3065.466	3124.604
3127.828	3155.9	3161.76
3168.979	3249.825	3256.526

p9b + H
```
C   -1.098374   2.025545   0.203516
C   -1.728853   0.976906  -0.320833
C   -1.439816  -0.434934  -0.036455
C   -0.333549  -0.775343   0.944827
C   -2.152934  -1.399479  -0.620375
C    3.424500   0.105477  -0.504410
C    2.100777  -0.203149   0.024332
C    1.005600  -0.456830   0.444666
H   -1.387446   3.036453  -0.059325
H   -0.268552   1.917655   0.893465
H   -2.540244   1.148179  -1.024693
H   -0.504474  -0.239346   1.885777
H   -0.383453  -1.841787   1.180251
H   -1.962031  -2.448883  -0.424909
H   -2.948436  -1.164034  -1.319672
H    3.344368   0.634204  -1.457482
H    3.999074  -0.808834  -0.672392
H    3.987095   0.737238   0.187372
```

Frequencies

59.4297	88.1105	99.0838
155.4482	202.3211	242.911
311.1718	400.5742	409.8812
419.0822	486.9932	572.1413
658.964	797.559	813.7252
822.5602	949.0736	956.4969
962.9132	978.6077	1037.848
1057.65	1058.704	1073.364

1174.178	1228.725	1327.419
1333.715	1360.577	1417.724
1439.662	1468.33	1488.459
1489.384	1492.995	1692.639
1746.328	2398.526	3050.369
3052.548	3099.227	3125.077
3125.289	3156.125	3159.358
3172.06	3244.173	3252.486

p14 + H

C	0.799880	1.908412	0.001468
C	0.423576	0.621545	0.001277
C	-3.573106	-0.276302	-0.002088
C	-2.149889	0.036943	0.000546
C	-0.977168	0.301789	0.001433
C	1.397151	-0.502076	0.000269
C	0.984284	-1.770185	0.002558
C	2.861805	-0.156243	-0.003386
H	0.061137	2.699644	0.002177
H	1.842846	2.198760	0.000903
H	-4.079113	0.228060	-0.829196
H	-4.043482	0.045644	0.930394
H	-3.734776	-1.351413	-0.111025
H	1.696924	-2.587448	0.001870
H	-0.069547	-2.022167	0.005448
H	3.469264	-1.061930	-0.004339
H	3.130932	0.434242	0.877890
H	3.126620	0.433320	-0.886584

Frequencies

35.5981	56.9775	94.6777
157.5253	223.675	285.0508
331.5119	340.7095	394.6484
419.568	450.8558	576.3708
617.1909	684.7818	723.5422
794.7004	843.347	939.74
950.6723	967.1968	1027.096
1058.547	1064.292	1071.472
1077.286	1227.941	1380.031
1417.963	1427.011	1432.262
1443.31	1483.584	1487.691
1489.335	1502.407	1673.194
1730.466	2383.278	3040.227
3049.844	3101.884	3120.807
3125.929	3138.869	3164.174
3179.685	3255.054	3272.4

p15 + H

C	0.825364	1.960581	-0.430338
C	0.468402	0.707183	-0.126616
C	-3.471768	-0.348276	0.234660
C	-2.069448	0.025720	0.106528
C	-0.915836	0.349043	-0.000751
C	1.471856	-0.379956	0.069207
C	2.567065	-0.170808	0.797270
C	1.171200	-1.699450	-0.587504
H	0.082747	2.739110	-0.555468
H	1.868453	2.218162	-0.570945
H	-4.031566	-0.069286	-0.661649
H	-3.929385	0.154557	1.090445
H	-3.576629	-1.426086	0.379947
H	3.314752	-0.947102	0.920881
H	2.739729	0.773854	1.300328
H	1.978272	-2.414596	-0.421594
H	1.029626	-1.571098	-1.664989

H   0.242991   -2.121738   -0.191695

Frequencies

64.7445	86.4102	93.0905
157.5743	205.9942	263.6055
286.1635	330.9649	400.8138
411.6426	488.9813	583.062
643.6396	678.5894	751.7362
792.9912	854.1053	953.5436
956.6991	979.8697	1037.007
1057.847	1062.525	1078.287
1089.974	1242.265	1347.943
1418.839	1424.489	1443.165
1458.232	1484.536	1485.654
1489.64	1504.816	1690.274
1733.271	2379.153	3046.603
3049.623	3110.393	3121.292
3124.935	3143.215	3152.988
3166.839	3243.514	3264.631

p16 + C₃H₅

C	-2.399426	0.473677	0.000001
C	-1.471392	-0.482327	-0.000012
C	2.564241	0.161451	0.000016
C	1.124440	-0.061610	0.000040
C	-0.065584	-0.237953	-0.000009
H	-2.129897	1.523631	-0.000017
H	-3.453698	0.223627	0.000029
H	-1.774515	-1.526164	0.000006
H	2.792614	1.229603	0.025236
H	3.022491	-0.263392	-0.896744
H	3.029335	-0.306731	0.871280

Frequencies

24.4431	140.0762	188.5809
332.0014	390.8488	545.7793
709.4461	726.7034	964.8887
1023.757	1054.747	1055.003
1058.66	1201.186	1328.813
1418.595	1451.104	1483.735
1484.151	1707.08	2378.718
3046.618	3118.232	3122.656
3157.391	3168.863	3255.855

p17 + CH₃

C	-1.079423	1.883732	0.000004
C	-0.726736	0.411732	0.000045
C	3.268172	-0.474577	0.000007
C	1.843085	-0.170383	0.000001
C	0.663775	0.064856	0.000027
C	-1.647793	-0.522189	0.000041
C	-2.574777	-1.432743	-0.000029
H	-0.657100	2.370616	0.882969
H	-2.160694	2.023703	0.000220
H	-0.657503	2.370504	-0.883218
H	3.575773	-0.899508	0.958928
H	3.856930	0.428995	-0.175812
H	3.511356	-1.196610	-0.783527
H	-2.973345	-1.830171	0.928670
H	-2.973241	-1.830095	-0.928808

Frequencies

59.5215	89.7159	136.5545

161.5731	198.5896	269.2183
303.8111	384.5862	492.9915
539.6843	561.1188	657.4269
674.8394	901.8971	935.5956
1020.834	1051.873	1054.786
1066.792	1067.044	1245.572
1331.852	1414.122	1417.196
1476.084	1480.393	1481.656
1487.752	1510.304	2083.361
2380.708	3052.028	3055.521
3123.017	3125.16	3127.226
3132.608	3156.875	3212.3

p18 + H
```
C    0.778109   2.038737  -0.000040
C    0.346432   0.593645  -0.000057
C   -3.455595  -0.272500   0.000080
C   -2.175802   0.018240   0.000005
C   -0.942149   0.293244  -0.000062
C    1.361932  -0.480226  -0.000008
C    2.668660  -0.199098   0.000127
C    0.865657  -1.900984  -0.000080
H   -0.089146   2.697767  -0.000361
H    1.384428   2.260804  -0.883310
H    1.383882   2.260940   0.883574
H   -4.208699   0.508219   0.000090
H   -3.795994  -1.302701   0.000125
H    3.407360  -0.992666   0.000212
H    3.047557   0.815729   0.000171
H    1.698728  -2.605104   0.000654
H    0.244814  -2.094848  -0.879211
H    0.243607  -2.094492   0.878267
```

Frequencies

54.0572	94.2991	150.0438
161.1429	226.1024	275.3264
319.9107	339.8626	411.5171
426.7535	503.8303	543.3212
588.7604	589.0535	660.1854
742.3754	879.1765	897.3839
935.4284	977.6106	1020.997
1033.705	1048.071	1071.909
1155.932	1161.502	1349.555
1405.524	1417.585	1437.519
1446.924	1483.88	1489.234
1496.151	1501.697	1697.506
1726.832	2230.436	3045.862
3054.163	3109.956	3118.132
3148.224	3150.448	3155.94
3170.916	3235.862	3255.291

p19 + H
```
C    0.708131   1.939638  -0.295317
C    0.260494   0.510748  -0.107184
C   -3.532262  -0.324453   0.213823
C   -2.255110  -0.044301   0.099027
C   -1.024494   0.221986  -0.012005
C    1.295473  -0.553633  -0.028508
C    1.044653  -1.796424  -0.442797
C    2.639493  -0.158337   0.526957
H   -0.149278   2.605656  -0.383555
H    1.321064   2.034551  -1.197457
```

```
H     1.318416    2.271895    0.550203
H    -4.286524    0.451793    0.140188
H    -3.868985   -1.341063    0.387525
H     1.798011   -2.573217   -0.371706
H     0.083799   -2.065534   -0.866514
H     3.302830   -1.022086    0.586880
H     2.538797    0.269282    1.529540
H     3.123600    0.597380   -0.099070
```

Frequencies

43.0416	94.7542	143.393
189.4657	211.8256	274.1318
311.1965	315.0394	404.6385
455.0491	503.1262	553.199
581.3144	617.5746	662.2658
745.2989	884.4459	901.5332
947.8422	974.8706	1021.164
1033.009	1050.142	1074.992
1143.296	1170.733	1325.051
1406.605	1415.947	1443.49
1447.453	1478.658	1485.782
1495.486	1505.499	1707.11
1730.46	2231.403	3043.268
3045.79	3105.096	3106.359
3143.418	3148.882	3160.005
3161.367	3233.737	3253.186

p20 + CH₃

```
C    -1.522330   -1.182822   -0.479668
C    -0.617278   -0.573390    0.618189
C     3.286192    0.349878   -0.233449
C     1.899090    0.020283    0.072239
C     0.755498   -0.250480    0.320579
C    -1.717212    0.185779   -0.011520
C    -2.356035    1.331208   -0.088634
H    -1.071357   -1.335081   -1.454506
H    -2.219125   -1.952920   -0.165029
H    -0.798436   -0.943919    1.623599
H     3.410968    1.425667   -0.380294
H     3.615271   -0.156862   -1.144200
H     3.946408    0.040602    0.580713
H    -3.182430    1.466524   -0.778352
H    -2.068852    2.173257    0.531655
```

Frequencies

86.7949	99.6173	128.7915
229.5196	306.7407	325.7515
379.5933	489.0371	545.0918
630.3792	719.6131	795.177
911.1892	937.684	945.278
1019.788	1055.674	1062.729
1065.061	1080.983	1110.476
1138.738	1212.947	1366.043
1420.348	1443.291	1475.944
1487.767	1492.436	1870.954
2395.701	3051.067	3121.84
3124.499	3130.902	3150.424
3153.576	3221.496	3240.016

p21 + H

```
C     0.258005    1.622261    0.614002
```

```
C   -0.424064   0.770397  -0.460985
C   -1.507570  -0.201404  -0.139607
C   -2.473556  -0.434996  -1.025377
C   -1.457659  -0.896364   1.192742
C    3.099750  -0.942414  -0.274877
C    2.032430  -0.202140  -0.153139
C    0.978482   0.522678  -0.041527
H    0.518262   2.641048   0.346818
H   -0.039606   1.482653   1.648066
H   -0.534581   1.259161  -1.425193
H   -3.266350  -1.146360  -0.821032
H   -2.501050   0.073736  -1.983257
H   -2.234685  -1.658166   1.263122
H   -1.607460  -0.185501   2.011730
H   -0.485605  -1.373193   1.348682
H    3.875047  -0.693205  -0.991728
H    3.241118  -1.828279   0.335399
```

Frequencies

48.9564	83.5858	179.6182
211.8396	249.5325	286.7081
390.6299	407.2218	458.149
521.1271	563.4521	621.4303
664.9352	749.3689	789.6617
869.0079	929.741	933.2745
954.8096	983.2389	1010.147
1022.361	1050.753	1066.036
1076.426	1081.56	1126.984
1316.733	1333.773	1389.336
1421.676	1453.043	1463.023
1494.742	1506.543	1551.283
1736.881	2140.854	3046.664
3108.105	3133.466	3145.015
3151.612	3152.726	3155.855
3222.078	3234.83	3241.768

p22 + H

```
C   -0.177482   1.810640   0.089735
C    0.425915   0.559963   0.708374
C    1.485831  -0.246086   0.027575
C    2.382444   0.298104  -0.788342
C    1.447111  -1.714534   0.345145
C   -3.087384  -0.799954  -0.382311
C   -2.011914  -0.111624  -0.111454
C   -0.950540   0.556524   0.160736
H   -0.456704   2.620450   0.755636
H    0.178467   2.118820  -0.887801
H    0.483297   0.551648   1.796127
H    3.137774  -0.307997  -1.277278
H    2.394925   1.363154  -0.992035
H    2.241352  -2.259206  -0.168142
H    0.481326  -2.139316   0.053271
H    1.556242  -1.879350   1.422469
H   -3.906902  -0.860392   0.326308
H   -3.193657  -1.326004  -1.325301
```

Frequencies

55.3009	78.0065	180.8473
188.2714	253.4139	259.7344
379.1371	404.2789	471.8754
513.4879	567.0165	619.9947
691.0513	726.782	803.2713
875.7959	933.1652	939.022
948.7068	987.377	1025.692
1029.231	1043.937	1064.729

1081.835	1094.973	1114.625
1258.09	1344.435	1398.15
1423.701	1442.731	1457.454
1483.996	1497.514	1552.921
1745.817	2142.246	3039.484
3101.926	3128.646	3135.281
3135.739	3147.379	3157.672
3225.261	3230.608	3243.412

p23 + CH₃

```
C     0.223102    1.027096   -0.273212
C     1.224256    0.324030    0.620808
C    -3.534846   -0.640265    0.032220
C    -2.208075   -0.044920   -0.080360
C    -1.115246    0.442356   -0.175639
C     2.330900   -0.206030    0.187246
C     3.433625   -0.736574   -0.256734
H     0.570649    0.991102   -1.309025
H     0.169897    2.085294    0.007862
H     0.984250    0.263397    1.679086
H    -4.277203    0.109656    0.316184
H    -3.542540   -1.427846    0.789674
H    -3.845200   -1.082323   -0.917761
H     4.352516   -0.161737   -0.310694
H     3.465337   -1.771699   -0.581293
```

Frequencies

43.058	84.3034	112.3313
184.7114	215.1688	298.9736
341.9197	400.1309	474.3404
537.5249	594.488	784.6543
881.9182	886.7723	927.9771
1019.675	1030.867	1060.432
1064.852	1148.9	1173.967
1220.704	1309.845	1381.135
1423.208	1468.648	1484.29
1486.719	1492.793	2092.82
2398.835	3044.514	3053.996
3100.652	3125.793	3127.17
3144.286	3171.71	3226.508

p23' + CH₃

```
C     0.437172   -1.596888   -0.000807
C     1.729375   -0.805849    0.002011
C     1.819882    0.492416    0.000552
C     1.912504    1.789967   -0.000866
C    -2.959256    0.730104    0.001083
C    -1.761518   -0.101712   -0.001247
C    -0.773834   -0.782577   -0.001602
H     0.430358   -2.258901    0.873130
H     0.433008   -2.257258   -0.876008
H     2.645498   -1.391726    0.005486
H     1.952507    2.346979   -0.931239
H     1.946654    2.349459    0.928252
H    -3.662431    0.405315   -0.769826
H    -2.703900    1.774982   -0.191610
H    -3.467649    0.678386    0.967068
```

Frequencies

71.6104	88.7133	110.1597
184.8851	210.7739	318.0281
337.6056	395.8066	468.8656
526.5252	652.7826	773.6593

133

887.3851	887.7944	930.1956
959.4239	1025.016	1058.052
1068.366	1135.493	1189.547
1250.182	1335.02	1384.702
1422.67	1468.012	1490.295
1490.306	1491.658	2096.603
2404.425	3037.853	3051.625
3067.017	3123.973	3124.382
3146.194	3159.054	3229.608

p24 + H

```
C    -0.455833   -0.613099   -0.011046
C     0.613309    0.371962   -0.009905
C    -4.237955    0.326994    0.008792
C    -2.963618    0.012447    0.000724
C    -1.738142   -0.295975   -0.006231
C     1.931705    0.121179   -0.002885
C     2.544740   -1.250099    0.008046
C     2.923770    1.249696    0.003400
H    -0.199091   -1.669201   -0.013500
H     0.286249    1.408360   -0.011984
H    -5.004771   -0.440348    0.010023
H    -4.559411    1.363176    0.014703
H     1.815460   -2.055996   -0.062198
H     3.247792   -1.355680   -0.824899
H     3.121378   -1.395765    0.928130
H     3.581357    1.181398    0.877384
H     2.433649    2.224338    0.017672
H     3.569542    1.201092   -0.880701
```

Frequencies

44.8856	80.0853	85.6518
131.61	221.8703	230.4226
245.0255	308.2353	379.4959
445.8739	496.9654	529.453
534.2236	587.3641	847.247
877.9541	879.8921	890.1731
947.045	975.01	1011.11
1034.926	1072.241	1100.325
1175.269	1230.956	1311.25
1385.271	1420.11	1427.326
1455.034	1471.88	1487.845
1494.067	1499.343	1698.07
1745.217	2230.562	3031.817
3043.923	3086.76	3097.824
3142.377	3149.394	3153.785
3167.038	3174.462	3235.194

p25 + H

```
C    -0.292299    1.471106    0.098778
C     1.106224    1.084431   -0.022648
C    -3.518779   -0.706335   -0.118363
C    -2.430731    0.023975   -0.038177
C    -1.367871    0.703220    0.035834
C     1.632579   -0.151700    0.008621
C     0.818518   -1.399500    0.200012
C     3.111760   -0.353815   -0.153576
H    -0.470406    2.535614    0.242314
H     1.791767    1.919293   -0.139911
H    -4.502879   -0.262200   -0.012533
H    -3.463888   -1.775906   -0.293518
H     0.277879   -1.656805   -0.717141
H     1.457979   -2.245190    0.462898
H     0.064670   -1.271367    0.980520
```

```
H    3.531439   -0.843976    0.732046
H    3.642086    0.586547   -0.313436
H    3.314945   -1.014288   -1.004113
```

Frequencies

39.0281	84.5816	173.3833
187.042	222.7033	242.9259
274.4343	314.6049	400.4052
435.0179	468.7129	532.1255
606.9621	718.4841	783.2355
849.4929	878.0656	901.7263
926.9149	989.2975	1006.281
1033.675	1053.824	1101.295
1160.669	1231.253	1342.673
1391.854	1419.331	1424.023
1457.684	1481.426	1487.799
1493.104	1512.381	1702.892
1718.018	2226.452	3027.969
3040.506	3085.239	3105.798
3131.033	3133.681	3139.188
3142.402	3169.393	3226.93

p26 + H

```
C    0.357974   -0.015585    1.168886
C   -0.799934   -0.007526    0.552637
C    3.994937    0.009830   -0.699203
C    2.696926   -0.001775   -0.036669
C    1.618722   -0.008651    0.495835
C   -1.952851    0.001053   -0.052809
C   -2.650635    1.290800   -0.408502
C   -2.655952   -1.278023   -0.435463
H    0.379092   -0.027559    2.256890
H    4.649192   -0.765181   -0.291751
H    4.491320    0.974881   -0.567711
H    3.882607   -0.170048   -1.771173
H   -2.072157    2.161086   -0.098627
H   -2.812665    1.346592   -1.489932
H   -3.633739    1.334331    0.071690
H   -3.639049   -1.327542    0.044198
H   -2.081076   -2.157063   -0.144110
H   -2.818647   -1.310240   -1.517747
```

Frequencies

68.0243	74.6353	116.5686
160.8069	188.1876	196.4468
224.7073	287.7146	317.5154
361.9682	449.5224	472.7236
546.3714	597.3688	777.9002
806.2839	826.5165	970.716
998.7571	1026.988	1060.4
1063.614	1104.344	1190.571
1226.038	1252.53	1401.892
1415.386	1422.172	1455.261
1477.973	1490.079	1490.496
1492.295	1496.113	1524.027
2088.66	2384.124	3039.258
3041.683	3049.356	3101.947
3103.108	3119.052	3125.001

3146.94   3148.313   3149.218

p27 + H

```
C     0.188301    2.816832    0.000000
C     0.192882    1.477786    0.000000
C     0.196793    0.697847    1.242030
C     0.196793   -0.634782    1.246087
C     0.172470   -1.473719    0.000000
C     0.196793   -0.634782   -1.246087
C     0.196793    0.697847   -1.242030
C    -1.041959   -2.419961    0.000000
H     0.186020    3.380447    0.926512
H     0.186020    3.380447   -0.926512
H     0.202542    1.247472    2.178536
H     0.199298   -1.171096    2.191463
H     1.072254   -2.107561    0.000000
H     0.199298   -1.171096   -2.191463
H     0.202542    1.247472   -2.178536
H    -1.035303   -3.062432    0.884835
H    -1.035303   -3.062432   -0.884835
H    -1.970560   -1.843634    0.000000
```

Frequencies

73.3071	226.4699	233.939
272.6162	373.977	419.6608
444.6773	502.2021	606.1491
676.5457	696.5052	790.2085
802.3195	811.1181	832.3678
918.0574	939.2962	959.4121
991.5642	1013.471	1015.457
1047.438	1100.262	1132.271
1196.309	1230.237	1303.532
1337.151	1383.823	1396.846
1413.663	1447.69	1475.831
1494.304	1506.08	1686.973
1709.194	1776.826	2998.067
3041.053	3118.227	3128.293
3156.359	3168.833	3169.991
3192.273	3195.638	3246.343

p28 + H

```
C    -2.782753    0.052398   -0.103982
C    -1.458656    0.045343    0.063694
C    -0.673847   -1.208425    0.364615
C     0.673863   -1.208436   -0.364644
C     1.458656    0.045343   -0.063704
C     0.670463    1.278838   -0.008144
C    -0.670473    1.278844    0.008111
C     2.782744    0.052413    0.104041
H    -3.363912   -0.862541   -0.062154
H    -3.321832    0.976433   -0.285663
H    -1.255422   -2.095000    0.101374
H    -0.489406   -1.247792    1.445274
H     1.255447   -2.095002   -0.101388
H     0.489434   -1.247830   -1.445302
H     1.212376    2.219936    0.003350
H    -1.212386    2.219939   -0.003432
H     3.321783    0.976461    0.285777
H     3.363928   -0.862511    0.062231
```

Frequencies

86.2168	184.0432	284.2885
359.9289	381.1289	434.4878
445.1158	555.7232	618.5696
707.8007	751.4053	755.203
779.0441	804.7479	851.562

930.6002	936.6126	937.2538
984.3023	995.2872	1011.836
1034.922	1060.428	1183.993
1204.621	1249.047	1309.7
1347.408	1362.899	1365.483
1428.434	1447.078	1473.123
1486.217	1486.268	1668.811
1729.002	1740.976	3039.801
3046.224	3103.34	3106.415
3152.029	3152.077	3175.983
3197.504	3240.684	3240.754

p29 + CH₃

```
C    -3.216735   -0.836561   -0.325832
C    -2.335746    0.019707    0.544274
C    -1.210825    0.548145    0.163604
C    -0.084631    1.089406   -0.234015
C     3.593454   -0.666461    0.074816
C     2.279278   -0.046442   -0.034956
C     1.189999    0.456087   -0.116356
H    -3.361494   -1.820832    0.128623
H    -4.203826   -0.378972   -0.440053
H    -2.779548   -0.972147   -1.315602
H    -2.666956    0.202250    1.565261
H    -0.108276    2.080737   -0.681487
H     3.825809   -0.900500    1.116908
H     4.370186    0.002226   -0.304180
H     3.635344   -1.596045   -0.498680
```

Frequencies

74.659	90.2196	143.3601
184.7718	209.3476	253.0677
302.6356	399.7172	466.6928
529.4842	590.7925	768.2329
808.6158	902.282	913.1845
1055.451	1062.549	1075.088
1095.22	1131.529	1205.637
1303.773	1417.663	1421.32
1462.578	1485.373	1487.523
1496.144	1514.671	2086.649
2385.329	3042.51	3048.134
3107.061	3118.255	3124.55
3138.994	3154.59	3155.552

p30 + H

```
C    -3.515467    0.149903    0.355039
C    -2.457390   -0.428064   -0.205656
C    -1.074026    0.085843   -0.146653
C    -0.018404   -0.997481   -0.007343
C    -0.786899    1.382978   -0.222023
C     3.890226    0.294957    0.092178
C     2.504290   -0.158717    0.056656
C     1.364963   -0.535394    0.026647
H    -4.506254   -0.279277    0.259518
H    -3.421182    1.064712    0.931421
H    -2.592368   -1.372310   -0.731961
H    -0.229764   -1.572122    0.902810
H    -0.139944   -1.706118   -0.836601
H     0.236077    1.735100   -0.156288
H    -1.570234    2.118606   -0.364768
H     4.066944    1.064173   -0.663694
H     4.575663   -0.533444   -0.103069
H     4.137305    0.716523    1.069559
```

Frequencies

43.6038	70.8398	86.7988
120.4208	205.6644	251.2283
300.1845	347.1902	390.0596
414.7141	467.5733	589.9641
662.1289	777.8916	800.3572
859.0144	940.692	962.323
967.1976	971.8318	1043.921
1054.904	1057.801	1101.212
1177.217	1215.866	1253.324
1340.877	1378.685	1416.489
1438.261	1467.642	1469.186
1482.695	1491.074	1720.202
1736.024	2400.47	3033.697
3051.709	3063.345	3121.946
3127.127	3144.08	3158.978
3161.67	3246.12	3253.89

p31 + H
```
C    -1.919154   1.891682  -0.108476
C    -1.418861   0.864335   0.570808
C    -1.302874  -0.515154   0.059918
C    -0.094762  -1.298700   0.539749
C    -2.213566  -1.068516  -0.739259
C     3.460972   0.584441  -0.355718
C     2.208281  -0.088971  -0.033152
C     1.176025  -0.643273   0.227088
H    -1.988213   2.878523   0.334280
H    -2.261852   1.779872  -1.132252
H    -1.027525   1.033127   1.572521
H    -0.168698  -1.425557   1.627592
H    -0.110938  -2.302160   0.106150
H    -2.091856  -2.076491  -1.121102
H    -3.112334  -0.533644  -1.025067
H     4.198003  -0.127378  -0.735925
H     3.883381   1.069054   0.527991
H     3.303670   1.349583  -1.119929
```

Frequencies

48.5138	58.6864	112.179
125.7026	205.9813	242.0672
290.2486	381.1581	402.4237
406.9544	507.9583	544.3462
683.3404	774.0893	814.5131
822.123	936.0971	952.933
956.7725	977.4911	1028.594
1059.856	1066.441	1103.785
1174.123	1211.071	1282.453
1335.238	1346.863	1423.725
1447.435	1467.186	1479.198
1489.402	1493.334	1720.047
1735.117	2398.296	3033.644
3048.7	3099.794	3119.296
3123.985	3150.099	3156.488
3162.796	3244.537	3248.153

p32 + H
```
C     3.490332   0.070109  -0.000006
C     2.159506  -0.611053  -0.000013
```

```
C    0.939580   -0.052107    0.000013
C   -0.227023   -0.939824    0.000026
C    0.661223    1.424845    0.000014
C   -3.937182    0.249945   -0.000024
C   -2.686618   -0.147654    0.000000
C   -1.483250   -0.535574    0.000017
H    4.072128   -0.230002    0.877926
H    4.071257   -0.228222   -0.879133
H    3.417482    1.157573    0.001146
H    2.204047   -1.699052   -0.000100
H   -0.030729   -2.010406    0.000052
H    0.068980    1.697741    0.878385
H    0.068642    1.697644   -0.878158
H    1.570438    2.023973   -0.000214
H   -4.751932   -0.466375   -0.000007
H   -4.189729    1.305007   -0.000056
```

Frequencies

40.5547	58.1485	73.2778
82.5733	206.9016	261.5787
270.4307	310.6258	382.5801
416.286	444.3345	534.9553
604.4239	608.5161	812.0539
837.6545	878.0452	903.3753
926.8533	1004.909	1033.293
1054.922	1057.815	1066.01
1128.48	1253.654	1328.967
1383.757	1423.33	1435.468
1453.401	1479.358	1485.924
1486.436	1500.21	1705.982
1741.263	2231.271	3037.707
3049.715	3089.606	3106.7
3142.183	3148.138	3153.376
3156.398	3164.964	3234.326

p33 + H
```
C   -3.074403   -1.029020    0.000230
C   -2.310538    0.258021    0.000092
C   -0.982052    0.447891   -0.000146
C   -0.031816   -0.666314   -0.000402
C   -0.396757    1.834853   -0.000065
C    3.839653   -0.225236    0.000287
C    2.536043   -0.374547    0.000005
C    1.280131   -0.518552   -0.000236
H   -3.724111   -1.083745    0.879890
H   -3.727315   -1.082068   -0.877136
H   -2.441468   -1.916401   -0.001743
H   -2.932112    1.151553    0.000399
H   -0.422893   -1.679258   -0.000685
H    0.236354    1.988363   -0.879038
H    0.236729    1.988105    0.878683
H   -1.180799    2.593445    0.000209
H    4.291104    0.761290    0.000671
H    4.502944   -1.083856    0.000166
```

Frequencies

27.364	67.4647	88.9763
134.6486	221.376	249.899
257.7249	289.067	378.5048
387.1729	517.622	545.6986
557.3991	630.2206	800.2343
845.8638	884.7314	887.4078
933.1619	1005.257	1033.259
1062.35	1071.909	1072.692

1119.205	1264.095	1306.287
1395.657	1419.089	1427.22
1452.219	1481.619	1485.255
1486.736	1498.414	1700.391
1742.794	2231.663	3041.117
3051.542	3094.584	3113.516
3136.051	3145.678	3149.49
3153.69	3186.599	3234.66

p34 + H
```
C     2.381404   1.726735   0.006219
C     1.151688   0.881349  -0.082274
C     1.057751  -0.453526  -0.026159
C    -0.253327  -1.122821  -0.123776
C     2.222145  -1.397681   0.126520
C    -3.745201   0.589788   0.085433
C    -2.567518   0.014841   0.013696
C    -1.436302  -0.544302  -0.056526
H     2.522306   2.293512  -0.920449
H     2.278202   2.462960   0.810242
H     3.290823   1.154973   0.192231
H     0.221913   1.431467  -0.214246
H    -0.232109  -2.203519  -0.257493
H     2.229367  -2.127530  -0.689376
H     2.138858  -1.960878   1.061698
H     3.184592  -0.888270   0.125624
H    -4.658559   0.011543  -0.006898
H    -3.839221   1.659443   0.239867
```

Frequencies

34.3247	82.6795	120.5346
126.7234	207.2199	234.7318
255.3662	330.6531	359.3658
416.6827	448.122	542.2675
617.8992	623.985	798.7482
862.761	888.9006	915.6421
928.9259	1009.099	1032.455
1047.678	1064.416	1070.6
1138.973	1231.813	1316.845
1386.381	1424.197	1431.861
1458.79	1484.963	1491.011
1493.763	1511.586	1707.271
1745.027	2228.512	3041.915
3048.443	3093.52	3103.44
3143.642	3146.708	3150.183
3163.394	3169.318	3234.553

p35 + H
```
C     0.331444   2.057960  -0.172145
C     1.450010   1.101197   0.098268
C     1.427164  -0.235701   0.002259
C     0.244324  -1.022170  -0.375217
C     2.665562  -1.058627   0.258224
C    -3.498062  -0.141538   0.249227
C    -2.238725  -0.436546   0.030012
C    -1.020238  -0.703639  -0.175206
H    -0.244750   2.260514   0.737794
H     0.725884   3.012545  -0.528609
H    -0.369999   1.669109  -0.913204
H     2.395093   1.551723   0.394303
H     0.443570  -1.990350  -0.834301
H     2.937692  -1.637614  -0.631167
H     2.501023  -1.773858   1.070292
H     3.514665  -0.427308   0.524857
H    -4.293839  -0.810117  -0.062073
```

H   -3.778217   0.779745   0.749581

Frequencies

59.4559	83.4822	173.6614
184.2568	226.997	253.3772
294.087	336.8363	345.1566
410.5585	459.7634	555.3948
588.4428	643.1756	816.4754
848.2153	896.0224	908.1274
926.3828	1020.127	1031.618
1055.914	1073.329	1090.823
1107.337	1215.28	1337.567
1389.994	1415.41	1423.725
1457.159	1486.441	1489.249
1502.094	1515.2	1709.475
1736.995	2233.104	3035.514
3039.577	3096.135	3101.399
3132.378	3133.689	3136.281
3148.97	3162.58	3234.487

p36 + H

```
C   -3.209410  -1.032667  -0.552868
C   -2.173913  -0.333310  -0.184773
C   -1.135395   0.363248   0.183448
C   -0.094504  -0.241787   1.114141
C   -0.909812   1.782738  -0.266849
C    3.657184  -0.307292  -0.595852
C    2.333183  -0.282482   0.015990
C    1.243336  -0.268863   0.519494
H   -4.127968  -1.028349   0.026020
H   -3.185926  -1.639609  -1.452830
H   -0.061258   0.348370   2.038628
H   -0.394183  -1.254964   1.392244
H   -0.875386   2.455036   0.597321
H   -1.701219   2.117320  -0.937421
H    0.050944   1.864846  -0.783467
H    3.719829  -1.088656  -1.357180
H    4.428498  -0.500997   0.153652
H    3.882658   0.649492  -1.073358
```

Frequencies

40.5064	89.787	102.8273
169.6601	186.9955	204.8812
245.5549	293.3931	349.3271
400.1833	448.7222	520.7303
602.3996	627.5838	778.4858
789.3288	890.3496	924.1502
1012.897	1028.361	1060.768
1065.038	1066.003	1168.895
1195.814	1230.135	1309.09
1358.249	1413.921	1424.593
1467.005	1480.302	1485.301
1489.799	1495.48	1514.814
2097.345	2396.94	3036.341
3041.66	3050.969	3105.557
3106.727	3122.734	3124.718
3134.589	3154.028	3215.115

p37 + H

C	0.904026	2.310124	-0.011042
C	1.155977	1.033209	-0.006273
C	1.418133	-0.243517	-0.000959
C	0.329862	-1.304083	-0.032117
C	2.830756	-0.770488	0.032779
C	-3.518895	0.154547	0.021419
C	-2.159973	-0.374046	-0.000642
C	-1.038410	-0.799575	-0.016292
H	0.810884	2.860472	-0.942114
H	0.768421	2.858912	0.915691
H	0.480983	-1.922894	-0.925789
H	0.480594	-1.975501	0.822750
H	3.022538	-1.411931	-0.834133
H	2.992109	-1.377240	0.930308
H	3.558146	0.040931	0.029704
H	-3.735559	0.626763	0.982812
H	-4.251348	-0.640645	-0.138465
H	-3.655625	0.904108	-0.761997

Frequencies

23.4549	72.036	105.5401
132.0712	169.9745	197.2597
244.1894	280.919	331.1108
388.4458	452.4183	474.5709
613.5498	631.442	768.9181
795.1401	893.9701	923.4345
992.9442	1029.21	1059.241
1062.413	1063.864	1175.058
1184.392	1242.708	1309.734
1364.685	1412.411	1422.712
1465.146	1476.714	1484.945
1489.545	1494.76	1511.342
2101.238	2403.915	3029.893
3038.644	3049.211	3059.189
3096.849	3120.305	3123.29
3143.008	3156.222	3224.514

p38 + CH₃

C	-2.723123	-0.942843	0.276836
C	-1.536509	-0.772002	-0.296178
C	-0.677952	0.420811	-0.108047
C	-1.173130	1.661913	-0.029574
C	3.334241	-0.368237	0.093234
C	1.908317	-0.077541	0.022329
C	0.733318	0.173120	-0.032622
H	-3.313237	-1.832121	0.088157
H	-3.132742	-0.208430	0.963004
H	-1.126253	-1.551446	-0.932990
H	-0.524628	2.514849	0.127436
H	-2.236206	1.841020	-0.139807
H	3.506056	-1.438920	0.226998
H	3.794735	0.157021	0.933682
H	3.841302	-0.053295	-0.822350

Frequencies

58.7533	85.6213	109.936
176.3665	281.5663	322.6166
354.924	420.3484	525.8466
567.7099	714.0173	738.4908
769.76	904.0901	946.3704
967.1748	1028.71	1058.913
1062.957	1082.545	1098.454
1296.222	1338.892	1424.372

1438.431	1461.674	1484.918
1487.598	1692.251	1722.055
2380.586	3051.575	3123.809
3126.731	3153.308	3171.644
3179.104	3247.258	3268.839

p39 + C₂H₃

C	1.132268	0.116939	0.000006
C	1.796695	1.274582	-0.000002
C	1.821464	-1.223775	-0.000002
C	-2.958892	-0.044793	-0.000003
C	-1.503105	0.019257	0.000003
C	-0.302028	0.087385	0.000004
H	2.881162	1.292559	-0.000003
H	1.275929	2.224319	-0.000006
H	1.530025	-1.803090	0.880591
H	2.906399	-1.105518	0.000068
H	1.530131	-1.803018	-0.880677
H	-3.303658	-1.081675	0.001438
H	-3.369142	0.448185	-0.885041
H	-3.369253	0.450666	0.883595

Frequencies

40.6061	114.1576	134.1695
169.315	310.0292	360.8824
383.2361	548.8619	579.0869
664.7475	742.5326	933.451
938.2265	1035.907	1056.124
1056.163	1072.148	1097.043
1331.673	1414.291	1420.324
1441.78	1477.039	1483.222
1486.848	1498.116	1717.304
2378.255	3045.836	3052.882
3112.028	3125.709	3125.819
3143.108	3165.867	3260.304

p40 + H

C	-2.495684	-1.243580	-0.167536
C	-1.405222	-0.813660	0.456445
C	-0.596612	0.372097	0.073683
C	0.096112	1.118403	1.223322
C	-1.049190	1.182045	-1.120339
C	3.115420	-0.775718	-0.445136
C	1.985841	-0.251834	-0.055295
C	0.869441	0.262414	0.314814
H	-3.024448	-2.122968	0.180840
H	-2.898214	-0.743283	-1.041624
H	-1.038782	-1.358404	1.324296
H	0.200600	2.194063	1.121202
H	-0.076406	0.766559	2.235857
H	-0.362037	2.010352	-1.302924
H	-2.050208	1.591009	-0.954213
H	-1.073654	0.561291	-2.019878
H	3.742127	-0.275305	-1.175897
H	3.460380	-1.724323	-0.047401

Frequencies

76.2588	107.1339	165.5501
246.8279	274.6057	308.6594
347.71	358.6237	446.7933
465.1407	583.6495	602.4361
626.1708	724.4406	767.3785
868.7148	914.8325	948.686
953.0185	969.5157	1012.198

1021.859	1039.023	1061.205
1062.43	1109.865	1206.161
1318.159	1337.677	1384.735
1416.261	1457.858	1460.966
1488.572	1509.397	1551.572
1730.373	2139.715	3045.952
3118.032	3125.144	3138.784
3147.779	3157.801	3171.247
3215.328	3231.337	3252.272

p41 + H

```
C   -2.376715  -1.349998  -0.080452
C   -1.455621  -0.608429  -0.680169
C   -0.605010   0.425421  -0.019120
C   -0.214913   0.251459   1.443365
C   -0.803531   1.834330  -0.547504
C    3.170003  -0.582967  -0.391003
C    1.963772  -0.270827  -0.001904
C    0.773301   0.033598   0.368266
H   -2.962120  -2.075716  -0.633366
H   -2.578812  -1.257735   0.982094
H   -1.289497  -0.718840  -1.750422
H   -0.118457   1.148530   2.047247
H   -0.572649  -0.624222   1.974724
H   -0.112639   2.531202  -0.067691
H   -1.828196   2.168843  -0.362475
H   -0.621222   1.868347  -1.625297
H    3.931364   0.178206  -0.525925
H    3.444512  -1.614128  -0.587760
```

Frequencies

66.0111	120.641	127.5422
231.8764	271.3518	302.3725
315.4963	351.7065	441.9432
477.5504	574.4598	605.8165
667.2436	712.1242	747.575
876.0646	910.599	953.1672
965.7536	976.7731	1011.122
1030.119	1042.605	1060.187
1069.272	1120.109	1216.383
1278.876	1336.572	1388.595
1410.628	1453.804	1459.849
1488.126	1506.75	1553.919
1735.54	2138.54	3047.023
3122.183	3131.312	3134.597
3142.091	3149.975	3162.91
3220.849	3225.336	3246.68

p42 + CH$_3$

```
C    1.195538   1.199818   0.002023
C   -0.193735   1.196971  -0.009046
C   -0.908973   0.000002  -0.012244
C   -0.193737  -1.196970  -0.009045
C    1.195536  -1.199819   0.002023
C    1.895986  -0.000001   0.008429
C   -2.415550   0.000000   0.009653
H    1.731705   2.142463   0.002303
H   -0.732363   2.139656  -0.017490
H   -0.732367  -2.139654  -0.017490
H    1.731700  -2.142466   0.002302
H    2.980100  -0.000002   0.014617
H   -2.820424  -0.884482  -0.487029
H   -2.820427   0.884525  -0.486952
H   -2.788313  -0.000044   1.038980
```

SUPPORTING INFORMATION

Frequencies

34.8642	207.7988	350.0785
417.0356	478.6255	533.5122
639.4238	717.9088	748.6522
808.5812	866.281	920.6975
995.496	1010.276	1013.52
1024.216	1064.215	1067.412
1121.635	1186.055	1217.239
1245.97	1332.672	1363.76
1419.204	1477.626	1499.92
1511.653	1547.483	1660.972
1684.996	3050.519	3116.919
3140.232	3183.009	3184.436
3198.008	3207.204	3220.419

p43 + H

```
C   -2.097858   -1.232195   -0.516646
C   -1.199512   -0.459379    0.081025
C    0.096804   -0.986202    0.639622
C    1.282905   -0.260390    0.040895
C    1.093620    1.176108   -0.185046
C   -0.095395    1.772278   -0.078891
C   -1.368433    1.030408    0.233720
C    2.433906   -0.873739   -0.235999
H   -1.943747   -2.301257   -0.620366
H   -3.016747   -0.822498   -0.923711
H    0.184823   -2.063313    0.485259
H    0.106811   -0.804887    1.723843
H    1.971424    1.758776   -0.448936
H   -0.176061    2.843715   -0.235638
H   -1.671245    1.262902    1.265410
H   -2.176772    1.389534   -0.409805
H    3.281020   -0.326351   -0.636064
H    2.564274   -1.937956   -0.072071
```

Frequencies

102.8299	121.9869	306.5873
354.9817	406.641	439.2356
469.0592	542.7892	572.2869
688.4891	717.5625	744.8351
813.2412	862.5536	917.9593
933.2465	940.0491	947.2836
955.1106	1000.079	1013.496
1019.165	1030.357	1174
1203.474	1235.402	1299.382
1319.737	1339.006	1355.851
1413.596	1455.653	1463.359
1473.28	1486.64	1699.911
1750.795	1760.651	3009.778
3022.523	3089.852	3116.202
3147.358	3155.64	3167.103
3192.603	3233.452	3242.854

p44 + CH$_3$

```
C   -1.042990    1.251076   -0.000004
C    0.289724    1.243525   -0.000006
C    1.068751    0.000000   -0.000001
C    0.289724   -1.243525   -0.000006
C   -1.042991   -1.251076   -0.000003
C   -1.868365    0.000000    0.000006
```

```
C    2.407902   0.000000   0.000006
H   -1.577451   2.196253  -0.000006
H    0.840985   2.179018  -0.000009
H    0.840984  -2.179020  -0.000011
H   -1.577451  -2.196253  -0.000006
H   -2.540333   0.000000  -0.869782
H   -2.540289   0.000001   0.869833
H    2.971511  -0.926496   0.000008
H    2.971511   0.926496   0.000010
```

Frequencies

116.4393	305.867	372.729
384.6247	510.2396	558.1417
601.2898	686.549	789.3702
802.7072	803.9673	896.1845
914.7541	960.7094	964.237
975.8652	1013.785	1023.656
1027.59	1185.131	1229.457
1230.296	1338.353	1395.328
1399.501	1449.145	1458.141
1475.877	1686.516	1711.33
1778.503	3014.857	3032.297
3156.411	3175.788	3176.547
3197.461	3200.398	3246.299

p45 + CH$_3$

```
C    1.831094   0.043797  -0.133275
C    1.227349  -1.144539  -0.085295
C   -0.243150  -1.272168   0.199734
C   -1.029444   0.013410   0.027950
C   -0.271722   1.262990   0.113557
C    1.066810   1.278335   0.038837
C   -2.350322   0.014089  -0.173146
H    2.899677   0.114201  -0.303620
H    1.796011  -2.060911  -0.204866
H   -0.683634  -2.067411  -0.408592
H   -0.350096  -1.605861   1.243053
H   -0.831321   2.190100   0.187448
H    1.602697   2.220656   0.071158
H   -2.906347   0.943072  -0.240169
H   -2.910672  -0.909329  -0.274580
```

Frequencies

63.8772	260.4228	383.5535
437.1575	482.1043	552.5186
596.8266	674.3314	760.124
775.535	826.3803	906.1617
937.4333	954.0288	966.3779
985.6579	1006.255	1017.25
1036.084	1190.576	1209.371
1229.833	1322.024	1350.695
1403.023	1440.465	1448.149
1474.563	1664.696	1705.32
1747.358	3004.996	3087.622
3154.335	3183.136	3189.162
3205.166	3216.2	3242.72

p46 + H

```
C   -2.502470  -0.950538   0.000011
C   -1.144409  -0.314249   0.000013
C   -0.014848  -1.027508   0.000090
C    1.319293  -0.421252   0.000019
C    1.362279   1.044575   0.000080
```

```
C     0.254372    1.783769    0.000040
C    -1.120699    1.190281   -0.000108
C     2.436827   -1.160190   -0.000093
H    -3.077106   -0.639834    0.879705
H    -2.436399   -2.039938    0.000790
H    -3.076526   -0.641052   -0.880491
H    -0.064925   -2.113388    0.000191
H     2.338819    1.518849    0.000155
H     0.325327    2.867304    0.000088
H    -1.682848    1.560380    0.869818
H    -1.682589    1.560248   -0.870270
H     3.417683   -0.697938   -0.000158
H     2.396497   -2.243956   -0.000141
```

Frequencies

98.0283	127.8892	194.6462
292.8185	335.9744	420.4396
440.1147	487.3031	538.7111
584.0904	694.3638	711.4303
793.4194	878.2767	883.3785
903.435	930.4697	953.1698
974.4961	1006.749	1017.487
1048.384	1066.788	1179.861
1207.216	1230.381	1320.846
1363.617	1403.028	1418.134
1440.274	1461.012	1468.752
1478.865	1493.691	1686.984
1721.792	1782.071	3006.279
3024.211	3030.212	3086.216
3136.578	3161.257	3172.764
3177.463	3201.525	3250.752

p47 + H
```
C    -2.572178   -0.845121    0.039428
C    -1.186035   -0.270945    0.008721
C    -0.082253   -1.031035    0.100009
C     1.265214   -0.465512    0.028874
C     1.382334    1.030102    0.237160
C     0.128732    1.790525   -0.088491
C    -1.054072    1.181689   -0.168467
C     2.336822   -1.234813   -0.183789
H    -2.555456   -1.928554    0.169087
H    -3.105913   -0.617399   -0.889469
H    -3.153612   -0.409490    0.858807
H    -0.170551   -2.111415    0.174058
H     2.232621    1.426812   -0.324408
H     1.613517    1.214566    1.297481
H     0.207078    2.865956   -0.210291
H    -1.955397    1.753608   -0.367828
H     3.332094   -0.811914   -0.270105
H     2.244236   -2.311510   -0.278004
```

Frequencies

86.1886	149.7816	197.4024
293.3714	310.4419	425.0958
452.6088	524.9006	547.7813
564.2832	697.2429	710.6875
762.4669	869.77	885.5038
907.9335	941.9996	958.3021
979.7316	1011.462	1024.802
1050.874	1070.723	1194.574
1206.929	1233.519	1318.658
1353.367	1371.354	1415.437

1444.778	1453.045	1461.583
1487.503	1495.332	1679.042
1708.67	1757.524	3000.718
3039.048	3091.619	3098.039
3139.132	3150.206	3173.828
3175.524	3199.843	3238.053

Fragments
CH₃

```
C   -0.000134   -0.000001    0.000023
H   -1.080503    0.038158   -0.000046
H    0.507588   -0.954443   -0.000046
H    0.573721    0.916289   -0.000046
```

Frequencies

470.9451	1399.8856	1409.5749
3117.6199	3301.0861	3304.8947

C₂H₃

```
C    0.705692   -0.145170    0.000001
C   -0.586151    0.030184    0.000004
H    1.596113    0.468363   -0.000011
H   -1.031552    1.027946   -0.000006
H   -1.281806   -0.806397   -0.000015
```

Frequencies

714.0578	840.5185	933.8993
1052.7836	1393.8374	1668.5191
3080.5313	3173.8401	3244.2107

C₃H₅

```
C    0.126237   -0.386841   -0.000019
C    1.338706    0.100442   -0.000011
C   -1.268068    0.077619    0.000003
H    1.517336    1.179754    0.000009
H    2.219186   -0.536480    0.000075
H   -1.313040    1.176378   -0.000504
H   -1.802178   -0.283061    0.883344
H   -1.802554   -0.283908   -0.882763
```

Frequencies

162.6044	313.5774	482.5915
894.4127	900.2700	939.9177
1051.0870	1105.6621	1389.0212
1418.5574	1456.6454	1477.9920
1768.2413	3001.6799	3066.9166
3090.8621	3119.3826	3174.2916

SUPPORTING INFORMATION

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) for all intermediates, transition states, reactants, and products involved in the *1,3-pentadiene* + 1-propynyl reactions at the ωB97P-D/6-311G(d,p) level.

Intermediates
i20

C	0.819905	2.575899	-0.187733
C	1.058093	1.271061	0.481816
C	-0.773672	-0.210099	-0.146681
C	-1.965023	-0.340969	-0.061859
C	-3.410075	-0.513496	0.035009
C	0.687489	-0.015228	-0.209883
C	2.262828	-1.968326	-0.258800
C	1.408070	-1.197547	0.396726
H	-0.256421	2.764670	-0.322459
H	1.266000	2.596593	-1.189486
H	1.232124	3.407387	0.386870
H	1.209451	1.232243	1.556017
H	-3.841034	0.195919	0.745988
H	-3.887348	-0.353815	-0.935043
H	-3.657769	-1.523381	0.371328
H	0.969822	0.059997	-1.268628
H	2.491769	-1.797229	-1.306565
H	2.761128	-2.800177	0.225988
H	1.186586	-1.389977	1.444416

Frequencies

61.6271	71.6599	74.6454
119.9903	122.8981	154.9042
227.2592	285.7224	290.6561
394.4126	418.3753	447.6265
505.0071	545.3347	676.7701
811.0921	908.9782	968.1059
975.1623	1005.164	1046.474
1058.849	1062.989	1086.817
1141.531	1158.42	1189.721
1261.017	1291.256	1334.415
1382.166	1418.717	1422.583
1464.071	1474.8	1484.639
1490.106	1491.956	1741.437
2384.576	2989.305	3027.686
3048.322	3055.158	3118.582
3124.258	3130.016	3145.962
3164.684	3188.801	3237.561

i21

C	-0.151325	-2.649483	-0.277013
C	-0.240893	-1.330890	0.455270
C	0.716343	-0.255717	0.170449
C	1.890403	0.264354	0.226339
C	2.620191	1.476582	-0.172992
C	-0.719243	-0.082905	-0.287879
C	-2.464559	1.682354	-0.228631
C	-1.566474	0.917861	0.384383
H	0.562814	-3.315274	0.213825
H	0.186833	-2.496894	-1.305033
H	-1.124999	-3.146472	-0.303437
H	-0.574186	-1.399212	1.489492
H	3.410315	1.241008	-0.891311
H	1.939130	2.203175	-0.636541
H	3.089935	1.955072	0.690799
H	-0.888816	-0.209131	-1.355040
H	-2.636335	1.607596	-1.298208
H	-3.058117	2.405085	0.318797
H	-1.413240	1.022109	1.457104

Frequencies

64.2682	113.4174	132.8276

149

141.4772	174.5187	202.3595
237.3665	269.7478	404.4836
423.2737	433.8168	571.4284
626.1119	737.6835	796.6776
868.5238	939.9051	993.0908
1007.669	1013.404	1035.666
1042.215	1050.907	1055.221
1127.467	1138.962	1200.149
1207.945	1297.099	1339.982
1393.81	1404.394	1423.64
1465.725	1469.598	1483.747
1485.983	1506.333	1726.333
1885.786	3008.069	3049.905
3091.037	3116.31	3123.759
3126.903	3138.517	3145.506
3152.283	3161.917	3246.968

i22
```
C    -0.159619   2.329145   0.488600
C    -0.182497   1.104551  -0.450652
C     1.010493   0.276665  -0.253753
C     1.998173  -0.384205  -0.081046
C     3.198209  -1.188332   0.122213
H     0.748028   2.915244   0.331021
H    -0.189248   2.004829   1.530967
H    -1.026005   2.967967   0.298464
H    -0.145251   1.489741  -1.480117
H     3.387555  -1.344135   1.187048
H     3.093593  -2.167998  -0.350624
H     4.073435  -0.696862  -0.309667
C    -1.476120   0.347392  -0.301929
C    -2.819457  -1.631965   0.188055
C    -1.610095  -0.980858   0.049536
H    -2.374774   0.933182  -0.485481
H    -3.758568  -1.114429   0.021942
H    -2.866672  -2.677936   0.463638
H    -0.696610  -1.543962   0.226669
```

Frequencies

68.0504	78.8397	124.116
134.9627	174.0736	205.6695
247.4832	303.3475	344.0547
386.6541	438.7645	533.1055
552.8202	640.3622	705.1532
768.2491	807.5017	904.0048
981.9815	1015.019	1028.329
1062.703	1066.118	1067.806
1098.947	1184.187	1206.767
1291.44	1301.094	1319.526
1368.972	1402.255	1427.639
1488.836	1491.605	1494.782
1499.237	1504.574	1523.112
2395.929	3008.907	3051.384
3052.619	3122.207	3126.687
3134.129	3143.496	3154.513
3160.595	3171.405	3256.527

SUPPORTING INFORMATION

i23

C	0.993000	-1.747945	0.887626
C	0.536868	-1.055223	-0.415427
C	-0.815058	-0.498098	-0.273039
C	-1.927722	-0.063659	-0.150448
C	1.177394	1.772150	0.757071
C	1.823151	1.192466	-0.313153
C	1.559088	-0.044012	-0.886234
C	-3.271513	0.484925	-0.007739
H	0.275650	-2.517752	1.180413
H	1.077195	-1.021572	1.697793
H	1.970702	-2.213575	0.742098
H	0.474991	-1.829727	-1.187797
H	0.338103	1.294991	1.247415
H	1.485765	2.743952	1.122649
H	2.635870	1.757483	-0.764480
H	2.180459	-0.354298	-1.720042
H	-3.776910	0.060257	0.863237
H	-3.235243	1.570162	0.117102
H	-3.877832	0.266453	-0.890332

Frequencies

20.3756	75.5571	93.2448
142.0468	218.114	228.5071
255.8771	304.3161	338.4661
407.1091	469.1385	529.9479
545.4335	657.9969	710.8206
750.6702	823.607	890.6292
975.6092	999.8792	1035.303
1058.022	1058.378	1087.178
1093.856	1168.055	1218.251
1248.228	1323.212	1363.475
1406.951	1419.486	1436.649
1474.353	1485.621	1486.536
1497.447	1501.275	1536.228
2390.056	3046.049	3049.282
3051.494	3118.474	3119.165
3132.229	3144.257	3150.642
3164.465	3187.508	3262.787

i24

C	0.094776	2.222176	0.275448
C	-0.032079	0.862325	-0.352111
C	3.568338	-1.117734	0.111060
C	2.295225	-0.427672	-0.062187
C	1.246047	0.139087	-0.209043
C	-1.165772	0.073158	0.262719
C	-2.236910	-0.341962	-0.400108
C	-3.371107	-1.113478	0.201015
H	0.581521	3.024873	-0.264684
H	-0.071190	2.336285	1.340390
H	-0.230461	0.981921	-1.423958
H	4.242456	-0.536190	0.745025
H	4.060125	-1.274796	-0.852144
H	3.421212	-2.094297	0.579064
H	-1.060672	-0.144578	1.324777
H	-2.315242	-0.117249	-1.463259
H	-4.317875	-0.577632	0.079468
H	-3.212383	-1.290203	1.267140
H	-3.488597	-2.083539	-0.292574

Frequencies

59.3996	115.8803	137.7841
143.8381	145.1109	186.4264
224.6973	238.0275	282.6959
339.8481	405.0146	433.693
496.6389	539.644	583.923

773.6345	853.7216	893.071
971.2131	1012.429	1064.465
1067.375	1074.265	1080.57
1116.978	1159.386	1182.296
1267.341	1304.871	1335.271
1371.436	1427.213	1429.5
1455.423	1492.263	1492.47
1493.813	1504.677	1773.005
2383.219	3040.137	3047.827
3048.056	3099.666	3119.408
3121.271	3127.124	3149.52
3152.919	3154.811	3268.903

i25

C	-0.907226	1.925355	-0.235887
C	-0.059510	0.874868	0.479638
C	-2.606639	-1.743369	0.053153
C	-2.351557	-0.321089	-0.219626
C	-1.447263	0.575150	-0.039744
C	1.097545	0.259027	-0.196923
C	2.188747	-0.184181	0.421374
C	3.357478	-0.827209	-0.259563
H	-1.309411	2.732627	0.368047
H	-0.607841	2.211372	-1.240294
H	0.028816	0.991929	1.556615
H	-3.472346	-1.871389	0.708828
H	-1.736173	-2.206728	0.537243
H	-2.809456	-2.288891	-0.872764
H	1.014503	0.157681	-1.278927
H	2.254925	-0.081391	1.503780
H	4.278939	-0.263576	-0.080505
H	3.203023	-0.893423	-1.339137
H	3.525569	-1.839527	0.122583

Frequencies

56.199	100.8618	114.5029
156.3729	173.0883	208.0209
223.1963	306.9608	398.9201
426.9732	473.2353	514.5843
669.7229	815.9553	835.6638
874.4498	932.7572	962.0659
1003.678	1016.932	1050.525
1051.903	1064.044	1074.057
1088.791	1112.99	1192.101
1202.894	1279.533	1338.513
1388.546	1402.388	1424.84
1461.689	1468.276	1477.393
1482.597	1503.718	1763.779
1890.263	3009.799	3037.926
3091.711	3095.869	3116.593
3123.288	3123.821	3138.855
3146.76	3153.784	3213.089

i26

C	0.783721	1.767006	-0.000096
C	-0.687449	1.453456	-0.000274
C	3.281800	-1.510823	-0.000493
C	2.398059	-0.350095	0.000509
C	1.671722	0.605667	0.000542
H	1.019318	2.391844	-0.872417
H	1.019017	2.392820	0.871597

SUPPORTING INFORMATION

```
H    -1.347509   2.317394   -0.001206
H     3.267437  -2.010642   -0.972180
H     2.974251  -2.234989    0.757899
H     4.312293  -1.216001    0.212529
C    -1.239379   0.189727    0.000535
C    -2.595858  -0.080178    0.000004
C    -3.176246  -1.454783    0.000019
H    -0.551970  -0.655200    0.001369
H    -3.293622   0.754677   -0.001407
H    -3.817324  -1.618096    0.874478
H    -2.395009  -2.218588    0.007301
H    -3.805097  -1.623075   -0.882444
```

Frequencies

14.3533	66.9179	82.6359
94.1157	178.3895	198.5457
205.9781	230.4258	289.6887
398.4999	428.5639	465.4981
617.4967	723.7462	759.522
765.7547	922.8525	944.4333
982.1777	999.5814	1029.348
1054.539	1066.903	1124.495
1170.611	1206.503	1229.251
1290.432	1305.987	1365.759
1414.156	1420.141	1449.944
1461.548	1478.699	1488.541
1491.65	1507.632	1542.479
2398.699	3011.924	3023.599
3033.443	3052.771	3072.78
3122.881	3124.165	3126.282
3154.832	3161.271	3167.718

i27

```
C     0.364919  -0.535112    0.000037
C    -0.431619   0.741973    0.000027
C    -1.817467   0.774725    0.000005
C    -2.655043  -0.321427   -0.000003
C    -4.145119  -0.235343   -0.000031
C     4.437675   0.092250   -0.000031
C     2.996220  -0.132548   -0.000004
C     1.810952  -0.321364    0.000016
H     0.092869  -1.143378    0.873862
H     0.092850  -1.143401   -0.873766
H     0.122267   1.673146    0.000040
H    -2.283681   1.758501   -0.000006
H    -2.223562  -1.319425    0.000011
H    -4.572350  -0.732968   -0.878440
H    -4.486670   0.802536   -0.000040
H    -4.572383  -0.732963    0.878365
H     4.901992  -0.352819   -0.883580
H     4.901519  -0.349530    0.885415
H     4.664042   1.161383   -0.001961
```

Frequencies

24.8633	36.389	76.97
140.8897	167.2414	170.5048
203.3407	294.5801	351.5471
357.468	388.8216	496.8977
625.116	625.5604	748.8879
810.5873	913.8713	922.047
973.3505	1016.223	1032.358
1058.839	1059.281	1141.465
1175.905	1201.759	1227.354

1240.861	1321.737	1354.088
1417.855	1420.628	1460.313
1479.34	1479.656	1486.476
1486.708	1490.044	1540.731
2398.924	3006.04	3020.888
3029.623	3046.576	3072.415
3118.013	3118.768	3119.733
3145.974	3165.996	3206.782

i28
```
C   -0.280515  -0.102275   0.286462
C    0.516895   0.947722  -0.204633
C    1.877279   1.034791  -0.095660
C    2.769526   0.014274   0.544332
C    3.249140  -1.048533  -0.455479
C   -4.322876  -0.219982  -0.121040
C   -2.874991  -0.172900   0.023645
C   -1.669923  -0.135715   0.143949
H    0.184680  -0.939113   0.798355
H    2.255816  -0.477452   1.376276
H   -0.003441   1.752265  -0.717241
H    2.364150   1.892234  -0.551898
H    3.639432   0.518655   0.976300
H    3.787294  -0.588241  -1.288389
H    2.398578  -1.594743  -0.870857
H    3.918560  -1.765841   0.026588
H   -4.701099   0.704254  -0.564616
H   -4.807417  -0.354230   0.850058
H   -4.623764  -1.052071  -0.764029
```

Frequencies

32.8456	73.6851	76.5192
92.4233	193.033	230.4234
250.8673	260.4682	311.9489
438.0762	465.2514	511.5753
570.4458	754.0072	766.7842
797.5528	851.9902	884.4976
991.7406	1024.646	1051.354
1059.584	1081.29	1089.682
1183.461	1205.622	1248.479
1294.74	1341.302	1362.085
1409.602	1424.716	1480.438
1483.291	1486.367	1499.558
1500.504	1510.314	1538.487
2263.173	3043.338	3047.495
3052.649	3090.102	3110.558
3121.304	3124.409	3131.883
3160.972	3177.85	3184.167

i29
```
C   -0.574044  -1.028895   0.001693
C    0.631068  -0.296969   0.000931
C   -4.249695   0.703767  -0.002438
C   -2.933256   0.081969   0.002436
C   -1.835299  -0.431910   0.002331
H   -0.527469  -2.114745   0.001093
H    0.543394   0.786319   0.002030
H   -4.327616   1.459515   0.784010
H   -5.032311  -0.040955   0.162381
H   -4.445481   1.194810  -0.960120
C    1.866860  -0.869849  -0.001353
C    3.178620  -0.146336  -0.002577
C    3.098947   1.376482   0.001524
H    1.926212  -1.957102  -0.002774
```

H	3.756142	-0.479923	-0.875204
H	3.760219	-0.484392	0.865578
H	2.575312	1.744976	0.887786
H	2.572032	1.749663	-0.880821
H	4.100350	1.812280	0.000761

Frequencies

68.2755	70.7396	114.4539
130.8553	178.5903	194.5496
244.3266	295.5154	317.648
349.0081	440.7527	492.6136
607.9911	708.1082	753.6637
813.2417	841.1242	914.515
980.7129	1037.161	1047.255
1064.047	1092.724	1104.976
1179.274	1207.701	1286.338
1291.369	1316.576	1382.353
1417.604	1423.545	1451.835
1475.597	1481.383	1491.919
1502.291	1515.942	1571.204
2259.306	3017.253	3039.61
3042.247	3053.848	3110.219
3118.936	3126.501	3133.69
3152.24	3169.395	3182.933

i40

C	0.344476	2.562043	-0.091431
C	0.313944	1.067097	0.007940
C	-0.877523	0.375327	-0.004197
C	-1.931015	-0.238723	-0.007443
C	-3.182299	-0.981173	-0.031389
C	1.639844	0.352947	0.072231
C	2.043305	-2.089083	-0.307160
C	1.560792	-1.100727	0.432663
H	-0.656527	2.979522	-0.201033
H	0.948290	2.883384	-0.949884
H	0.806907	3.003375	0.800834
H	2.270005	0.874312	0.808450
H	-3.683631	-0.874571	-0.998370
H	-3.003625	-2.045705	0.139889
H	-3.869384	-0.623637	0.741296
H	2.158054	0.468625	-0.891079
H	2.531776	-1.899534	-1.258843
H	1.964246	-3.123558	0.007900
H	1.064749	-1.328469	1.373560

Frequencies

45.0288	66.4954	102.5475
114.1477	126.8054	154.0473
222.4392	283.1353	301.8119
381.2598	415.9285	445.0243
578.7677	611.3687	702.3301
887.4736	931.4344	966.068
977.8544	1013.814	1045.779
1047.672	1054.919	1062.999
1130.317	1203.694	1249.349
1323.835	1342.301	1403.422
1413.047	1430.431	1453.691
1474.583	1485.058	1486.273
1489.148	1503.183	1743.659

2181.894	2997.597	3012.731
3025.715	3037.903	3060.118
3101.123	3118.541	3143.28
3146.393	3168.959	3237.788

i41

```
C    2.269161   -1.135475    0.500105
C    1.306516   -0.436929   -0.473179
C   -0.081518   -0.940228   -0.354895
C   -1.206452   -0.336675   -0.051504
C   -1.168845    1.157041    0.226596
C    0.201794    1.753220    0.080579
C    1.289799    1.062017   -0.238030
C   -2.546621   -1.011896    0.037677
H    2.303162   -2.210217    0.307765
H    1.942971   -0.978484    1.531116
H    3.281207   -0.734781    0.393141
H    1.671363   -0.617936   -1.493535
H   -1.552631    1.347658    1.238609
H   -1.869075    1.668161   -0.448951
H    0.285664    2.823631    0.247440
H    2.248187    1.568440   -0.327832
H   -2.464449   -2.081319   -0.158099
H   -2.983780   -0.872944    1.032395
H   -3.245630   -0.578657   -0.686146
```

Frequencies

89.0066	140.3472	205.6705
236.784	260.7957	319.4656
375.0423	460.7289	472.9061
514.5093	585.0046	709.6539
756.7211	858.4705	909.3967
913.6869	930.5669	995.7788
1009.797	1019.627	1067.356
1086.233	1101.84	1159.734
1190.338	1209.968	1216.857
1319.427	1337.82	1364.246
1404.358	1414.323	1419.372
1473.097	1491.027	1493.082
1496.38	1506.895	1745.633
1795.311	3013.708	3021.111
3031.855	3037.381	3048.587
3088.529	3126.681	3137.906
3147.106	3155.478	3183.907

i42

```
C    2.163141   -1.176475    0.611760
C    1.334113   -0.489470   -0.433043
C   -0.088073   -1.003857   -0.355617
C   -1.148009   -0.263146   -0.041115
C   -1.033164    1.212954    0.230959
C    0.349711    1.759517    0.040005
C    1.398238    1.007395   -0.269215
C   -2.531361   -0.838959    0.058641
H    2.712830   -2.083185    0.387102
H   -0.217463   -2.066970   -0.544018
H    2.052484   -0.878889    1.648623
H    1.741760   -0.751152   -1.418771
H   -1.376901    1.420633    1.254546
H   -1.736940    1.755645   -0.415819
H    0.475811    2.831597    0.162309
H    2.376135    1.463669   -0.392365
H   -2.536971   -1.912536   -0.138843
H   -2.950584   -0.672251    1.057307
H   -3.207736   -0.354317   -0.654319
```

Frequencies

75.1484	87.1535	147.3901
201.9444	265.8765	330.527
367.0088	459.6481	475.5775
511.969	530.3716	586.2863
723.2036	755.6057	857.671
872.8089	918.937	955.7514
977.198	1013.557	1029.688
1055.175	1075.386	1097.373
1121.49	1187.12	1217.191
1237.066	1304.856	1335.611
1350.609	1412.519	1424.049
1434.103	1454.606	1473.15
1485.658	1498.73	1741.602
1781.916	3012.512	3024.807
3031.559	3032.67	3087.376
3134.031	3149.348	3161.792
3164.883	3186.345	3263.799

i43

C	2.275786	-0.980177	0.528621
C	1.260316	-0.356644	-0.447559
C	-0.076138	-1.020382	-0.328735
C	-1.262313	-0.378756	-0.025038
C	-1.277052	1.119996	0.205295
C	0.059596	1.779910	0.047536
C	1.177996	1.131260	-0.249470
C	-2.456834	-1.075926	0.074912
H	2.375645	-2.055297	0.355842
H	1.952535	-0.825460	1.561240
H	3.262342	-0.524128	0.405019
H	-0.100772	-2.096304	-0.486164
H	1.644521	-0.542038	-1.462809
H	-1.667607	1.324655	1.209804
H	-1.993849	1.582090	-0.484671
H	0.087597	2.856960	0.188124
H	2.110366	1.681783	-0.346613
H	-3.386556	-0.570153	0.309672
H	-2.492370	-2.147788	-0.082815

Frequencies

70.0778	132.5585	261.2191
274.4211	343.7674	408.6712
469.8981	481.3361	507.3989
545.5132	575.3951	717.878
752.0301	761.0988	809.9405
861.4819	921.8451	932.5121
974.5356	1014.088	1019.47
1030.787	1057.279	1086.44
1158.529	1203.358	1236.833
1244.765	1311.143	1334.889
1376.46	1408.355	1426.379
1431.08	1471.692	1479.916
1502.55	1508.33	1525.162
1765.876	2988.375	3032.529
3041.537	3058.611	3117.334
3129.72	3156.438	3161.912

| 3165.402 | 3186.702 | 3254.86 |

i43

C	2.565186	-0.759358	0.109206
C	1.211799	-0.349731	-0.361916
C	0.092885	-1.017976	0.483655
C	-1.249553	-0.446376	0.121738
C	-1.360573	1.038803	0.352469
C	-0.097468	1.763472	-0.034388
C	1.034897	1.150193	-0.362808
C	-2.235067	-1.175294	-0.389805
H	2.927738	-1.763490	-0.078805
H	0.301717	-0.816255	1.541596
H	3.134658	-0.125200	0.779511
H	1.082848	-0.711016	-1.393438
H	0.111731	-2.101046	0.340986
H	-1.568783	1.231005	1.414895
H	-2.210873	1.447880	-0.201926
H	-0.141111	2.848995	-0.046982
H	1.899442	1.740863	-0.654402
H	-3.185519	-0.730210	-0.666813
H	-2.124494	-2.243928	-0.543528

Frequencies

103.9618	127.157	169.5772
283.5481	303.7394	401.4039
427.2387	445.0614	507.5187
546.9724	561.3932	691.2014
743.9486	748.6496	844.1054
883.0906	932.2701	942.737
952.9451	976.3863	1010.533
1011.787	1050.804	1100.329
1126.433	1170.175	1226.392
1242.431	1281.153	1304.769
1331.911	1353.686	1361.77
1419.467	1459.249	1462.656
1473.733	1498.726	1746.607
1755.791	3000.942	3015.503
3039.922	3083.814	3112.176
3149.289	3150.397	3157.439
3185.226	3235.324	3260.322

i30

C	-2.487474	-0.952693	-0.209095
C	-1.171384	-0.267632	-0.083352
C	0.015237	-1.041040	0.394640
C	1.336845	-0.401551	0.027613
C	1.352425	1.062609	-0.025456
C	0.242914	1.802209	0.002934
C	-1.140074	1.220078	0.041835
C	2.436455	-1.120902	-0.201901
H	-2.966310	-1.100032	0.773829
H	-2.382910	-1.944017	-0.661054
H	-3.186371	-0.370877	-0.817844
H	-0.021905	-2.069967	0.023384
H	-0.021213	-1.117714	1.498446
H	2.322653	1.545499	-0.098866
H	-1.635960	1.539484	0.978273
H	0.319877	2.885117	-0.027567
H	-1.744746	1.674330	-0.755471
H	3.383979	-0.643094	-0.428319
H	2.423254	-2.205201	-0.168118

Frequencies

79.4057	93.8658	176.1463
248.8528	300.3684	311.4142
412.4887	447.0551	479.0285

550.7268	665.3452	706.5412
792.0506	847.4082	871.1036
894.454	922.8413	936.2658
960.6553	1002.119	1009.902
1021.254	1028.195	1168.008
1187.315	1198.469	1241.474
1302.457	1334.236	1342.396
1401.6	1416.749	1430.599
1450.221	1459.394	1469.511
1487.737	1495.112	1700.63
1750.893	2919.809	2927.767
2962.281	3025.068	3060.466
3078.118	3108.928	3153.85
3168.558	3191.707	3240.987

i44
```
C    2.570450   -1.014346    0.010424
C    1.259348   -0.286741   -0.011609
C    0.026741   -0.985166   -0.008752
C   -1.183887   -0.361273   -0.000416
C   -1.273442    1.138380    0.010120
C    0.055862    1.825036   -0.000581
C    1.221995    1.135573   -0.009302
C   -2.479494   -1.109809   -0.000479
H    2.436884   -2.082559   -0.173900
H    3.070146   -0.905901    0.980812
H    3.257644   -0.624536   -0.747730
H    0.052278   -2.072770   -0.015069
H   -1.860856    1.464059    0.886788
H   -1.880307    1.475017   -0.848612
H    0.062994    2.910037   -0.001648
H    2.163158    1.678907   -0.016144
H   -2.323402   -2.190336   -0.010600
H   -3.077502   -0.858476    0.884247
H   -3.086482   -0.843372   -0.874578
```

Frequencies

102.931	116.0062	130.0723
194.7818	276.2467	301.8438
399.9382	430.1645	486.0878
532.3924	548.824	693.2966
715.9051	871.9445	880.193
929.3859	940.6525	971.4278
994.484	1006.453	1033.661
1045.747	1051.247	1162.291
1191.543	1205.092	1260.657
1282.746	1335.71	1420.465
1425.24	1435.637	1447.421
1455.954	1476.691	1491.096
1493.807	1500.359	1557.749
1650.739	2946.638	2951.201
3015.827	3023.499	3065.289
3079.909	3126.291	3130.617
3164.143	3172.125	3199.686

i45
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C   -2.380457   -1.229975   -0.155197
C   -1.300099   -0.468342    0.026778
C    0.048910   -1.037559    0.032866
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C    1.171614   -0.311141    0.011980
C    1.142499    1.195412   -0.062076
C   -0.220188    1.767171   -0.236230
C   -1.401252    1.021353    0.280194
C    2.534291   -0.937725    0.034823
H   -2.294524   -2.301846   -0.300556
H   -3.378731   -0.805630   -0.164668
H    0.120597   -2.122674    0.046472
H    1.800891    1.523915   -0.877777
H    1.619673    1.594284    0.852893
H   -0.323715    2.810174   -0.512020
H   -1.475804    1.162435    1.374597
H   -2.330289    1.416721   -0.138215
H    2.477967   -2.023566    0.129393
H    3.086750   -0.699130   -0.880976
H    3.125275   -0.549849    0.872030
```

Frequencies

89.7496	137.6758	148.9918
199.0044	296.7488	365.4709
408.9666	425.9451	460.8736
526.88	544.2211	667.879
717.5063	850.1153	866.3741
883.9525	902.1825	919.6709
928.9226	988.4182	1008.732
1046.399	1062.44	1122.612
1178.105	1189.779	1229.615
1313.969	1332.766	1350.812
1399.713	1406.948	1422.114
1453.919	1457.058	1463.511
1484.527	1493.822	1709.469
1758.18	2929.437	2933.343
3030.237	3033.733	3090.081
3090.552	3134.466	3153.451
3164.447	3204.943	3241.532

i31
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C   -2.593336   -0.710666   -0.117123
C   -1.230166   -0.114940    0.014043
C   -0.118872   -1.014692    0.489701
C    1.242375   -0.509800    0.081965
C    1.468574    0.959801    0.335176
C    0.291513    1.781073   -0.107108
C   -0.962258    1.218993   -0.251005
C    2.156511   -1.292155   -0.479182
H   -2.920368   -1.162970    0.827817
H   -2.601559   -1.513057   -0.865526
H   -3.335267    0.034680   -0.410917
H   -0.270732   -2.033292    0.118019
H   -0.167766   -1.080958    1.589352
H    2.383658    1.294374   -0.161595
H    1.632160    1.115801    1.414054
H    0.441271    2.837581   -0.297092
H   -1.781954    1.853862   -0.577921
H    3.126360   -0.905903   -0.776126
H    1.968149   -2.345803   -0.658865
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Frequencies

96.4348	131.4849	180.1724
278.7265	316.9265	384.5447
435.6697	457.2317	477.6432
565.6806	655.0619	688.2445
740.3267	848.5894	888.4527
916.7675	938.4153	941.423
946.8391	991.9668	1010.85

1021.234	1041.957	1159.928
1176.765	1209.453	1239.146
1305.14	1314.646	1352.852
1358.19	1421.729	1453.239
1463.859	1477.486	1481.182
1483.851	1490.352	1527.517
1755.176	2976.726	2981.521
3016.765	3064.256	3076.174
3088.244	3129.688	3148.2
3167.114	3205.381	3233.558

i32

C	2.228030	-1.105781	0.519544
C	1.259958	-0.388108	-0.447879
C	-0.123747	-0.958546	-0.342887
C	-1.223181	-0.223433	-0.029867
C	-1.092062	1.177006	0.193013
C	0.168234	1.803104	0.080226
C	1.285889	1.094575	-0.231066
C	-2.586964	-0.853125	0.086298
H	2.242174	-2.181775	0.324855
H	1.914401	-0.945959	1.554034
H	3.246137	-0.723800	0.403391
H	-0.223366	-2.027762	-0.513165
H	1.639685	-0.593221	-1.464061
H	-1.968973	1.763433	0.444135
H	0.240769	2.873479	0.244518
H	2.246792	1.593424	-0.312977
H	-2.998449	-0.706450	1.089433
H	-2.549813	-1.925873	-0.111986
H	-3.286300	-0.399656	-0.622476

Frequencies

85.9816	114.2778	174.0151
248.4061	288.2139	358.7597
417.4039	469.5766	503.6676
560.7307	615.7196	701.1058
749.3744	787.3221	818.1258
874.4487	955.449	970.7935
982.4908	1004.982	1056.894
1065.063	1077.435	1095.725
1144.149	1189.234	1212.73
1289.56	1329.652	1337.855
1378.729	1401.469	1420.146
1449.491	1488.381	1496.472
1501.277	1503.436	1583.228
1641.794	2944.394	3038.905
3041.423	3105.163	3118.466
3127.024	3132.417	3161.83
3170.182	3186.214	3201.231

i46

C	1.591786	-1.265282	0.954498
C	1.251769	-0.693908	-0.385836
C	-0.221125	-0.902436	-0.771123
C	-1.166588	0.027620	-0.048210
C	-0.739578	1.248949	0.294056
C	0.634382	1.673089	0.024842
C	1.575215	0.790062	-0.324639
C	-2.566128	-0.453853	0.176625
H	2.590418	-1.631837	1.160709
H	-0.499032	-1.945879	-0.591711

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H    0.934505   -1.068317    1.794893
H    1.880724   -1.167186   -1.145343
H   -0.341451   -0.727864   -1.850329
H   -1.417648    1.953303    0.766415
H    0.882155    2.723687    0.135596
H    2.603850    1.096686   -0.481634
H   -2.573674   -1.326427    0.839534
H   -3.022091   -0.772178   -0.768116
H   -3.196158    0.320562    0.618705
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Frequencies

72.0074	113.5476	141.2423
183.6913	272.9584	334.7886
341.2647	442.3473	501.2474
525.3302	562.3106	606.3918
747.004	756.3054	850.708
854.0787	886.2659	948.0129
964.8402	1002.922	1017.98
1044.426	1071.324	1108.918
1125.974	1182.207	1205.035
1256.171	1300.703	1334.326
1350.562	1400.577	1414.871
1426.928	1454.339	1478.35
1483.509	1489.066	1678.561
1744.715	3012.566	3029.397
3076.06	3082.671	3084.686
3133.185	3151.689	3177.712
3189.483	3210.462	3262.951

i35
```
C   -2.457205   -0.960788    0.105921
C   -1.193820   -0.238687   -0.359256
C    0.049324   -1.030566   -0.079215
C    1.307678   -0.424675   -0.014947
C    1.356465    1.047522   -0.122276
C    0.257709    1.791720   -0.003278
C   -1.088735    1.168588    0.244280
C    2.472462   -1.145733    0.145095
H   -2.437213   -1.113060    1.189467
H   -2.549012   -1.940527   -0.370883
H   -3.352344   -0.382517   -0.139219
H   -1.258949   -0.114521   -1.453852
H   -0.023900   -2.112803   -0.015885
H    2.326857    1.511647   -0.267978
H    0.326468    2.874336   -0.042919
H   -1.258229    1.109818    1.329809
H   -1.885397    1.802037   -0.156898
H    3.436644   -0.653350    0.191299
H    2.451802   -2.225341    0.239112
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Frequencies

127.6151	147.4309	270.0247
276.5751	323.4568	396.2373
447.3198	454.8029	532.2385
556.053	596.9184	691.1269
712.68	765.9744	801.267
877.1029	892.9122	934.0126
957.6913	1007.516	1019.353
1028.981	1077.428	1109.683
1182.438	1193.827	1238.738
1274.452	1314.286	1337.99
1361.483	1374.36	1413.272

1450.093	1452.656	1484.685
1503.243	1512.218	1526.815
1726.102	2959.792	3010.96
3040.424	3090.278	3117.557
3118.17	3159.723	3172.25
3173.394	3196.149	3258.09

i8

C	2.549259	-0.989396	-0.000009
C	1.268948	-0.215171	-0.000002
C	0.000001	-1.018373	0.000024
C	-1.268949	-0.215172	0.000009
C	-1.223843	1.145347	0.000009
C	0.000001	1.852482	0.000000
C	1.223844	1.145348	-0.000008
C	-2.549260	-0.989395	-0.000017
H	2.613056	-1.641975	-0.879422
H	2.612986	-1.642107	0.879309
H	3.420073	-0.330862	0.000074
H	0.000006	-1.703959	0.867206
H	0.000002	-1.704027	-0.867101
H	0.000000	2.935517	0.000000
H	-2.155453	1.704163	0.000010
H	2.155454	1.704164	-0.000018
H	-3.420069	-0.330855	0.000160
H	-2.612956	-1.642197	0.879237
H	-2.613099	-1.641882	-0.879495

Frequencies

105.322	121.3122	146.1784
233.321	271.5806	308.6448
395.1505	463.7989	492.2639
514.9125	529.5915	699.5178
730.1448	864.4786	876.2869
910.5745	921.8337	943.6904
997.9289	1011.912	1041.236
1065.802	1078.291	1128.882
1170.816	1221.361	1244.254
1315.34	1337.058	1398.717
1414.088	1417.337	1444.038
1463.725	1481.334	1481.776
1482.105	1489.225	1570.73
1652.126	2940.093	2940.697
3018.134	3019.617	3069.454
3069.581	3127.566	3127.888
3175.596	3177.772	3220.278

i47

C	0.490914	1.557239	0.004289
C	-0.861957	0.899175	-0.001488
C	3.728803	-0.991462	-0.006044
C	2.578188	-0.094738	-0.001669
C	1.635877	0.648932	0.001381
C	-1.091154	-0.457392	0.011263
H	0.566906	2.226367	-0.863393
H	0.563848	2.216832	0.879767
H	-1.702446	1.587586	-0.013943
H	3.423882	-2.015384	-0.236051
H	4.222645	-0.997122	0.968757
H	4.460961	-0.680896	-0.755452
H	-0.221143	-1.109539	0.021995
C	-2.343607	-1.057719	0.009826
C	-3.635333	-0.303426	-0.010285
H	-2.388939	-2.141524	0.010628
H	-3.765029	0.243098	-0.953146
H	-3.681724	0.439662	0.794225

H   -4.489341   -0.972740   0.102984

Frequencies

56.2899	71.1939	83.9522
93.0912	159.3542	192.9491
202.6581	250.1153	358.4737
392.5047	397.8448	536.1504
618.841	664.842	744.1128
762.8033	923.3807	945.8802
978.7234	994.7356	1024.357
1054.034	1066.556	1094.471
1171.716	1204.309	1229.703
1252.643	1322.343	1373.123
1407.346	1420.032	1457.319
1471.079	1487.049	1490.683
1491.411	1498.835	1533.789
2399.249	3016.266	3022.707
3038.282	3052.903	3072.495
3124.179	3126.638	3136.179
3165.551	3182.886	3197.272

i48

C	0.122267	-0.375176	0.269604
C	-0.578717	0.955118	0.158330
C	4.205809	-0.038632	-0.180003
C	2.761023	-0.160811	-0.019280
C	1.572308	-0.266041	0.109294
C	-1.931493	1.171227	-0.043017
C	-2.981158	0.274437	-0.165986
C	-2.927714	-1.220125	-0.077778
H	-0.088267	-0.832041	1.246935
H	-0.265846	-1.076839	-0.475565
H	0.058593	1.827503	0.253034
H	4.719430	-0.193030	0.772192
H	4.472668	0.953951	-0.551243
H	4.582207	-0.777617	-0.891713
H	-2.214111	2.219047	-0.117458
H	-3.958148	0.705477	-0.361625
H	-3.925454	-1.629823	0.091267
H	-2.283996	-1.568053	0.733413
H	-2.551025	-1.668550	-1.006220

Frequencies

24.6732	39.8995	81.1194
105.6415	139.5495	183.003
211.6389	293.7922	331.7931
393.9892	458.1484	502.7424
596.9484	681.6527	706.2627
820.1357	895.69	924.7751
979.8558	1010.098	1020.65
1058.849	1059.362	1095.913
1176.608	1201.511	1231.433
1264.38	1312.1	1403.024
1419.869	1424.391	1461.235
1464.949	1486.245	1486.763
1491.919	1497.234	1525.644
2398.292	3007.257	3019.859
3047.421	3076.12	3093.551

| 3119.877 | 3120.578 | 3128.472 |
| 3148.903 | 3178.571 | 3194.852 |

i49

C	0.599593	1.696066	-0.360796
C	-0.019359	0.684989	0.565663
C	-3.785614	-0.756677	-0.156333
C	-2.446132	-0.241006	0.101616
C	-1.343841	0.185936	0.321148
C	1.130120	0.288936	-0.404566
C	2.444798	-0.046852	0.123823
C	3.034336	-1.402836	-0.049824
H	1.236067	2.451643	0.085920
H	-0.001536	2.035783	-1.194828
H	0.271069	0.749189	1.608632
H	-4.333160	-0.100746	-0.837971
H	-4.356777	-0.828434	0.772759
H	-3.744220	-1.752982	-0.604200
H	0.785266	-0.318272	-1.236146
H	2.894420	0.634212	0.841424
H	2.803373	-1.815579	-1.037430
H	2.641202	-2.117889	0.689917
H	4.120891	-1.388263	0.067537

Frequencies

34.4042	58.6586	82.6037
95.8463	118.7059	225.6906
279.7611	314.4983	329.1903
435.8239	483.4039	509.73
531.5854	720.1706	768.1159
829.0304	919.5921	954.2209
985.4229	1009.887	1056.637
1058.354	1077.978	1090.597
1095.211	1136.789	1194.777
1222.826	1233.171	1304.093
1384.161	1412.771	1421.258
1458.05	1480.588	1484.697
1486.927	1490.692	1496.14
2384.879	2978.594	3044.584
3061.803	3112.256	3115.718
3118.093	3142.183	3159.83
3168.195	3171.716	3238.369

i50

C	-0.316171	2.063560	-0.014528
C	-0.204935	0.585467	-0.245907
C	3.701029	-0.729892	-0.044892
C	2.322179	-0.260930	-0.123842
C	1.185868	0.120359	-0.192808
C	-1.046519	-0.139556	0.796000
C	-2.236286	-0.703889	0.607112
C	-3.024475	-0.793371	-0.664483
H	-1.237637	2.566688	-0.282025
H	0.406826	2.577305	0.606397
H	-0.600163	0.356876	-1.241678
H	4.315291	-0.038805	0.537651
H	4.141739	-0.816841	-1.041107
H	3.750927	-1.711114	0.433681
H	-0.609325	-0.150127	1.790567
H	-2.708408	-1.159641	1.474950
H	-2.520032	-0.335346	-1.516441
H	-3.994837	-0.300416	-0.546765
H	-3.228527	-1.839063	-0.915142

Frequencies

| 31.2331 | 97.632 | 102.1026 |
| 130.5582 | 134.8187 | 179.4816 |

229.5377	239.8022	296.9853
342.0035	442.7446	495.6487
526.5853	549.425	567.7985
738.8394	779.6526	924.022
982.4565	1004.302	1019.317
1056.956	1065.542	1075.753
1101.358	1132.701	1183.391
1254.517	1299.465	1339.457
1411.935	1423.149	1437.64
1450.315	1488.79	1491.768
1492.087	1504.926	1748.177
2396.116	3042.451	3050.717
3062.169	3098.034	3121.969
3123.725	3138.311	3157.365
3162.077	3188.707	3281.551

i51
```
C    -0.719578   1.770636   -0.062627
C     0.779163   1.708469    0.043162
C    -3.111967  -1.494972   -0.014883
C    -2.254795  -0.319638   -0.034751
C    -1.535879   0.665899   -0.052519
C     1.321340   0.355994    0.399367
C     2.206007  -0.318526   -0.324327
C     2.757660  -1.665646    0.028461
H     1.098673   2.442554    0.796834
H    -1.177122   2.748966   -0.173274
H     1.224930   2.049120   -0.901874
H    -3.596036  -1.612357    0.959872
H    -2.534701  -2.401342   -0.214941
H    -3.898587  -1.418917   -0.770865
H     0.939055  -0.084091    1.319306
H     2.570976   0.124315   -1.250811
H     2.549037  -2.393712   -0.762044
H     2.326601  -2.041376    0.959402
H     3.845466  -1.626458    0.147103
```

Frequencies

45.1422	74.6629	113.9629
117.5632	174.8196	194.4465
209.647	270.9545	285.0917
402.643	407.9032	489.6401
580.4343	613.1492	770.4473
790.2599	920.8001	953.8909
988.6483	1016.017	1044.504
1055.096	1073.655	1106.147
1127.379	1214.564	1236.509
1313.766	1345.59	1367.373
1416.871	1417.825	1439.349
1473.691	1482.178	1488.51
1489.842	1498.534	1779.179
2172.144	3003.524	3030.654
3036.911	3037.382	3097.64
3101.316	3117.938	3121.178
3141.792	3150.118	3172.325

i52
```
C     0.714014   1.953719   -0.143547
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```
C    -0.182050    0.731234   -0.340012
C     2.613536   -1.621560    0.023089
C     2.310075   -0.182862    0.011515
C     1.313441    0.616146   -0.133373
C    -1.073786    0.293109    0.751060
C    -2.218514   -0.379403    0.634114
C    -2.878042   -0.845615   -0.628696
H     0.885445    2.587242   -1.007989
H     0.635534    2.482888    0.801995
H    -0.520282    0.564657   -1.357405
H     3.306654   -1.885652   -0.780479
H     1.695562   -2.210917   -0.106689
H     3.075392   -1.918197    0.968897
H    -0.727295    0.547407    1.750949
H    -2.746530   -0.625552    1.552380
H    -3.002256   -1.933346   -0.618220
H    -2.314663   -0.583507   -1.525285
H    -3.879608   -0.413643   -0.723053
```

Frequencies

36.8151	88.5085	114.5561
117.715	169.7113	196.6581
250.9944	321.2789	390.489
459.0069	524.1373	578.0235
660.4868	765.8732	830.0037
857.7593	924.5518	949.1602
1012.195	1020.363	1047.884
1049.331	1057.787	1065.646
1078.46	1085.315	1178.597
1200.678	1295.485	1328.968
1400.274	1413.039	1454.55
1466.58	1467.766	1479.658
1486.991	1496.108	1752.625
1890.069	3004.317	3038.763
3086.455	3093.642	3110.908
3116.487	3131.972	3145.718
3166.993	3172.888	3206.206

i53

```
C     0.167934    2.511006    0.000526
C    -0.060704    1.024839   -0.000256
C     3.247966   -1.351441    0.001208
C     2.058350   -0.510872   -0.002312
C     1.072645    0.190263   -0.001637
C    -1.366133    0.486693    0.000530
C    -1.690731   -0.838439   -0.000425
C    -3.089668   -1.359260    0.000325
H     0.745576    2.818631    0.878520
H    -0.779306    3.054074    0.005292
H     0.737779    2.820815   -0.881823
H     3.748434   -1.314993    0.972986
H     3.962401   -1.019959   -0.757086
H     2.991468   -2.393099   -0.207197
H    -2.180005    1.210463    0.002078
H    -0.885709   -1.569265   -0.001830
H    -3.279215   -1.984764   -0.879544
H    -3.822829   -0.549018    0.003585
H    -3.276549   -1.989616    0.877262
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Frequencies

54.4557	78.0702	91.9737
105.8017	126.9992	193.2825
198.3711	213.2118	299.9285
351.3307	382.3057	452.3688
550.7509	620.5002	684.0299
793.4691	937.2837	964.085

990.4432	1034.564	1039.462
1052.333	1055.718	1060.32
1134.717	1238.48	1265.604
1361.097	1383.009	1414.444
1417.146	1424.817	1477.409
1480.631	1485.936	1487.946
1489.331	1497.388	1573.487
2286.025	3027.612	3031.065
3045.327	3079.614	3087.418
3114.359	3119.806	3123.265
3133.849	3153.795	3177.595

i54
```
C     0.815531    2.438578    0.002468
C     0.657742    0.939709   -0.000070
C    -3.210143   -0.333404   -0.001316
C    -1.826681    0.119793   -0.000750
C    -0.664776    0.457950   -0.000020
C     1.795897    0.108752   -0.003137
H     0.334664    2.883126   -0.874971
H     1.868895    2.725464   -0.000197
H     0.340369    2.879366    0.884933
H    -3.739249    0.023795   -0.889185
H    -3.744029    0.036176    0.878566
H    -3.259869   -1.425525    0.006132
H     2.743762    0.642430   -0.006594
C     1.883431   -1.258975   -0.002280
C     0.752587   -2.240004    0.004035
H     2.887002   -1.673371   -0.007338
H     0.100399   -2.095945    0.871141
H     1.129333   -3.264012    0.024213
H     0.117194   -2.125889   -0.880292
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Frequencies

34.1982	69.4468	82.9976
104.5485	151.9286	200.217
250.711	289.7711	306.6979
324.3871	409.1065	534.7067
574.7658	635.8128	681.1763
706.7788	932.4593	960.5133
987.4712	1029.258	1038.608
1047.473	1053.54	1058.188
1114.215	1233.873	1263.133
1341.268	1406.208	1414.125
1419.395	1470.483	1479.383
1481.098	1483.227	1486.655
1496.555	1506.267	1539.001
2277.43	3031.436	3037.509
3040.123	3090.369	3094.515
3110.037	3114.626	3128.183
3130.235	3151.641	3179.969

i55
```
C    -1.832174   -1.027459    0.294101
C    -1.976529    0.427496   -0.093876
C    -0.944234    1.201752   -0.405272
C     0.501322    0.774355   -0.398992
C     1.309176    1.643816    0.578317
C     2.045808   -1.299279   -0.182349
C     0.660216   -0.716427   -0.098432
C    -0.409926   -1.412159    0.205409
H    -2.222355   -1.185851    1.307074
```

```
H   -2.446687   -1.652008   -0.366265
H   -2.984839    0.832025   -0.113842
H   -1.126255    2.240512   -0.671216
H    0.910820    0.949109   -1.405496
H    2.380118    1.441459    0.504479
H    0.989283    1.452946    1.606257
H    1.156258    2.705640    0.365251
H    2.505336   -1.061272   -1.147883
H    2.019234   -2.383358   -0.068929
H    2.697139   -0.891775    0.597145
```

Frequencies

63.2272	171.6267	216.8506
234.264	295.3513	315.9419
345.9251	448.276	491.5675
547.5946	585.6176	702.57
742.9648	830.7838	910.5149
920.0297	968.0207	980.5797
1006.253	1023.086	1048.66
1100.551	1120.489	1135.096
1185.898	1213.218	1217.628
1322.557	1343.922	1356.852
1406.857	1409.229	1419.42
1482.017	1486.027	1494.755
1502.479	1517.252	1746.614
1792.768	2998.561	3029.498
3041.133	3048.409	3055.457
3101.394	3123.094	3135.159
3146.202	3157.58	3185.183

i56
```
C    1.802012    0.843880    0.326858
C    1.868122   -0.573047   -0.160113
C    0.793044   -1.272431   -0.498857
C   -0.620226   -0.767255   -0.390429
C   -1.361395   -1.539469    0.716301
C   -1.919911    1.367834   -0.296189
C   -0.695825    0.733940   -0.149160
C    0.437005    1.438327    0.218254
H    2.156297    0.894121    1.367926
H    2.514954    1.461289   -0.237098
H    2.852570   -1.025493   -0.234881
H    0.907579   -2.297701   -0.842281
H   -1.130934   -0.978886   -1.338270
H   -2.412183   -1.244996    0.769014
H   -0.899774   -1.339254    1.686899
H   -1.316197   -2.616967    0.533148
H   -2.023377    2.431859   -0.116936
H   -2.805653    0.822915   -0.602383
H    0.339760    2.502442    0.414868
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Frequencies

60.0934	194.6038	241.9102
265.7611	281.857	385.6939
459.3989	509.9832	544.8379
566.5693	616.3426	709.1111
747.5971	754.4479	788.4498
858.7707	901.5408	935.5996
955.7088	993.389	1016.622
1033.654	1093.513	1102.582
1143.97	1208.148	1216.48
1248.952	1323.887	1343.717

1385.841	1407.678	1429.245
1437.184	1459.144	1482.403
1496.794	1505.535	1528.299
1763.894	2997.556	3026.35
3037.27	3045.019	3123.147
3130.025	3155.346	3161.859
3175.329	3187.244	3252.009

i57

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C    1.752409   -1.004388   -0.246496
C    2.023679    0.352115    0.047820
C    1.022097    1.211520    0.364237
C   -0.422837    0.805771    0.393032
C   -1.247973    1.697726   -0.564225
C   -2.033471   -1.186282    0.191679
C   -0.630693   -0.663922    0.113161
C    0.421450   -1.475082   -0.192817
H    2.558327   -1.682614   -0.497892
H    3.048911    0.707057    0.024206
H    1.242833    2.250627    0.589880
H   -0.817490    1.007279    1.405358
H   -2.319914    1.520721   -0.450533
H   -0.968543    1.498426   -1.602045
H   -1.058695    2.753936   -0.355565
H   -2.515084   -0.875752    1.126426
H   -2.055334   -2.276598    0.140942
H   -2.654314   -0.801958   -0.625546
H    0.231342   -2.525873   -0.393576
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Frequencies

68.8902	139.9691	220.6518
251.4679	321.5845	366.3992
400.3251	490.313	495.6913
575.5934	631.7645	685.3003
745.4153	789.1081	844.576
928.6815	956.4442	976.9808
986.1119	1025.324	1034.06
1060.452	1077.568	1114.829
1131.919	1191.853	1208.821
1293.82	1321.809	1344.886
1406.581	1412.707	1431.17
1437.083	1475.914	1492.745
1508.903	1516.525	1566.035
1637.747	2936.352	3029.681
3047.922	3083.334	3126.505
3130.74	3135.441	3169.965
3172.158	3194.202	3222.089

i58

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C   -1.308249   -1.310338    0.381411
C   -1.953805   -0.234350   -0.072245
C   -1.196830    0.843568   -0.797966
C    0.257387    0.978069   -0.284676
C    0.336006    1.709843    1.018427
C    2.390701   -0.463001   -0.275685
C    0.901650   -0.393327   -0.131794
C    0.140476   -1.439577    0.210170
H   -1.846652   -2.115964    0.869364
H   -3.029731   -0.142981    0.031532
H   -1.171174    0.593132   -1.868979
H    0.816439    1.548861   -1.034212
H    0.077294    1.198339    1.938586
H   -1.704900    1.807813   -0.713121
H    0.513519    2.778591    1.050072
H    2.696783   -0.199230   -1.294174
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```
H     2.773517   -1.460378   -0.050495
H     2.872221    0.254656    0.398042
H     0.598670   -2.408155    0.387537
```

Frequencies

89.6451	125.3166	180.7035
213.6583	242.9299	297.906
348.3659	480.2059	494.9519
502.7249	574.1649	621.4298
713.226	753.7958	845.1915
888.584	896.1875	930.7735
981.6005	1002.608	1039.888
1052.988	1063.464	1090.864
1118.27	1183.364	1201.356
1237.609	1291.254	1339.996
1353.699	1396.654	1410.362
1431.897	1455.443	1474.048
1481.838	1493.719	1696.68
1747.803	3004.104	3031.83
3059.444	3088.961	3093.9
3133.922	3152.468	3170.453
3181.997	3202.987	3265.023

i59
```
C    -2.022653   -0.661433    0.000005
C    -1.887146    0.826609    0.000000
C    -0.671401    1.431055   -0.000008
C     0.547628    0.707058   -0.000010
C     1.861521    1.430596    0.000007
C     0.493786   -0.726292   -0.000002
C    -0.704259   -1.367649    0.000004
H    -2.622008   -0.985653    0.867627
H    -2.622011   -0.985658   -0.867614
H    -2.793943    1.421946    0.000001
H    -0.621468    2.516678   -0.000010
H     2.387207   -1.279324   -0.880057
H     2.465914    1.177242   -0.878964
H     2.465728    1.177529    0.879193
H     1.712881    2.512095   -0.000177
H    -0.725904   -2.453750    0.000007
C     1.779671   -1.512588   -0.000003
H     1.583451   -2.585996    0.000056
H     2.387266   -1.279233    0.879985
```

Frequencies

59.2713	109.5737	167.7462
244.2136	264.5107	327.458
408.7265	423.5626	487.0681
566.9463	594.7329	714.3908
719.4709	766.9211	807.3322
920.2611	937.6841	962.6552
987.2894	1001.107	1030.136
1063.116	1084.44	1166.138
1191.368	1194.318	1255.596
1272.941	1324.997	1395.355
1419.066	1431.439	1446.477
1460.895	1477.354	1489.389
1498.722	1505.552	1566.236
1648.432	2957.822	2959.2

3020.934	3041.013	3069.693
3099.751	3130.199	3137.737
3169.509	3178.975	3193.834

i60

C	-1.575512	-1.013503	0.295140
C	-1.875962	0.149739	-0.389549
C	-0.910114	1.079560	-0.727819
C	0.531111	0.895165	-0.337638
C	0.856333	1.715838	0.928794
C	1.920295	-1.147467	-0.648525
C	0.841466	-0.572543	-0.130015
C	-0.166014	-1.337208	0.694845
H	-2.362614	-1.705122	0.573164
H	0.020829	-2.411905	0.614559
H	-2.908962	0.343246	-0.662455
H	-1.186561	1.994058	-1.241822
H	1.168456	1.269284	-1.146086
H	1.911164	1.605039	1.192941
H	0.247988	1.382514	1.773907
H	0.646947	2.776221	0.764936
H	2.131843	-2.200916	-0.495029
H	2.629803	-0.582341	-1.244888
H	-0.028515	-1.087566	1.759383

Frequencies

91.0635	131.6959	252.5526
257.8567	306.7181	412.5811
473.3233	481.9346	555.8515
605.1137	631.3471	729.4709
732.043	760.9625	858.8677
920.3038	936.9372	950.2305
954.3111	973.701	1000.525
1034.922	1083.832	1088.757
1152.203	1169.714	1212.964
1308.624	1315.529	1323.471
1344.235	1391.593	1410.921
1454.938	1465.158	1475.279
1499.207	1506.956	1521.494
1751.572	2986.544	3045.805
3060.223	3086.485	3125.651
3131.219	3147.414	3175.555
3197.401	3210.798	3232.955

i61

C	-1.919300	-0.812792	0.001771
C	-2.020385	0.538926	0.002150
C	-0.805224	1.406514	-0.003172
C	0.503512	0.665832	-0.005757
C	1.720470	1.540356	0.002859
C	1.859097	-1.457230	0.000074
C	0.547693	-0.704742	-0.001942
C	-0.656943	-1.451743	-0.000208
H	-2.817764	-1.421498	0.004168
H	-2.991185	1.022798	0.004835
H	-0.829566	2.093834	0.861282
H	-0.835252	2.088367	-0.871673
H	2.650940	0.984065	-0.107726
H	1.779426	2.110132	0.939209
H	1.670912	2.278418	-0.806561
H	2.438023	-1.256784	-0.906346
H	1.686355	-2.533605	0.050385
H	2.481355	-1.181698	0.856055
H	-0.606761	-2.534757	0.001722

Frequencies

76.1446	104.2886	141.1477

177.8148	299.1417	327.0682
394.3357	472.5252	503.8742
541.1058	566.1281	665.4653
722.4155	768.496	818.5197
909.383	931.5392	981.2972
987.3593	1019.131	1037.005
1062.995	1094.28	1161.686
1189.927	1203.673	1211.542
1272.417	1323.222	1409.572
1422.969	1427.139	1442.054
1442.982	1481.665	1487.554
1502.352	1511.524	1586.075
1634.398	2947.326	2947.561
3022.332	3047.17	3069.973
3109.399	3136.677	3153.588
3176.141	3199.785	3208.929

i62
```
C    -1.200191   -1.327331    0.270486
C    -1.781641   -0.338072   -0.400183
C    -1.041183    0.876226   -0.890938
C     0.298940    1.077048   -0.160419
C     0.105964    1.635402    1.212652
C     2.239264   -0.433428   -0.614467
C     1.031953   -0.254845   -0.090556
C     0.267380   -1.350633    0.608317
H    -1.793873   -2.173280    0.605156
H    -2.844033   -0.395495   -0.619678
H    -0.858751    0.777947   -1.967824
H     0.921778    1.769052   -0.738922
H    -0.826298    1.483836    1.745514
H    -1.661313    1.769978   -0.763826
H     0.952818    2.042472    1.752439
H     2.741254   -1.394796   -0.569074
H     2.767490    0.378463   -1.104401
H     0.695563   -2.325388    0.355544
H     0.382454   -1.238991    1.695720
```

Frequencies

111.3348	142.075	156.3536
231.8951	322.2327	393.4236
414.9299	454.6158	525.3066
558.0892	600.2061	680.9849
740.2909	765.5063	831.2974
905.7759	919.2996	934.0283
958.6378	972.7456	1006.418
1020.273	1026.323	1090.917
1115.438	1182.244	1222.746
1241.685	1291.582	1306.495
1336.441	1355.15	1372.53
1421.874	1456.598	1457.916
1471.067	1484.838	1741.568
1750.463	3015.826	3037.901
3051.564	3081.504	3086.17
3143.203	3152.897	3164.274
3188.552	3229.083	3265.375

SUPPORTING INFORMATION

i63

C	-1.318810	-1.258443	0.368974
C	-1.962024	-0.014033	-0.172566
C	-0.988800	0.908767	-0.820427
C	0.437618	0.924087	-0.372353
C	0.589894	1.732838	0.940135
C	2.235294	-0.807331	-0.385818
C	0.959639	-0.487011	-0.163303
C	-0.001737	-1.469369	0.349149
H	-1.980299	-2.019050	0.773055
H	-2.752690	-0.292468	-0.881086
H	-2.496138	0.495303	0.650749
H	-1.362306	1.729573	-1.423038
H	1.049946	1.413433	-1.136214
H	1.642211	1.795978	1.228638
H	0.041355	1.250137	1.753742
H	0.198475	2.745933	0.814451
H	2.609022	-1.807764	-0.193086
H	2.943505	-0.079647	-0.768570
H	0.400481	-2.408456	0.718618

Frequencies

82.3352	123.6349	222.5261
242.9635	269.955	356.2719
380.3199	459.3873	510.8141
582.0144	608.4186	718.332
740.9081	810.0308	855.4109
881.0453	914.2015	933.3452
950.2216	991.301	1005.877
1018.463	1054.442	1076.669
1142.624	1194.638	1198.178
1306.792	1321.578	1329.906
1378.179	1389.04	1410.064
1418.412	1457.493	1468.775
1492.115	1500.838	1698.62
1749.966	2938.416	3041.592
3041.691	3067.832	3124.089
3127.038	3146.894	3164.378
3189.582	3197.886	3234.044

i64

C	-1.075899	-1.428539	0.347428
C	-1.884584	-0.218881	-0.025383
C	-1.076318	0.751498	-0.887512
C	0.314031	1.006533	-0.279676
C	0.220996	1.727603	1.026117
C	2.380832	-0.396084	-0.312871
C	1.063219	-0.305440	-0.125339
C	0.257193	-1.461267	0.280974
H	-1.614454	-2.310109	0.682916
H	-2.791808	-0.528839	-0.553442
H	-2.223067	0.282739	0.891088
H	-0.949936	0.325030	-1.888009
H	0.881814	1.634131	-0.985746
H	0.990424	1.609837	1.779005
H	-1.610567	1.699386	-1.002223
H	-0.548202	2.477512	1.180392
H	2.908327	-1.332695	-0.164214
H	2.969481	0.462885	-0.618036
H	0.791170	-2.372421	0.535839

Frequencies

98.2183	177.2873	204.3675
238.8654	346.6837	365.0863
402.4627	475.6262	487.9737
595.226	625.8673	722.1366
733.7147	789.939	824.231

867.3449	909.8303	934.8445
967.278	979.6897	995.7219
1015.978	1035.797	1103.311
1123.435	1181.317	1206.441
1256.081	1293.541	1317.782
1348.105	1382.188	1387.546
1420.526	1455.36	1468.24
1477.426	1503.679	1697.014
1747.833	2970.897	3029.836
3052.747	3082.118	3101.997
3141.061	3147.972	3167.242
3190.67	3235.975	3255.938

i65
```
C     2.011360    0.442048   -0.033643
C     1.842855   -0.872713   -0.043279
C     0.496850   -1.523457    0.031937
C    -0.668145   -0.578470    0.019343
C    -2.028759   -1.211903   -0.005811
C    -1.580021    1.676858   -0.038922
C    -0.507725    0.807262    0.009319
C     0.882296    1.421353    0.057993
H     3.013618    0.857937   -0.086665
H     2.704905   -1.530656   -0.103781
H     0.441765   -2.150526    0.936139
H     0.386092   -2.236999   -0.798858
H    -2.545442   -1.014020   -0.952507
H    -2.669964   -0.831486    0.795958
H    -1.956849   -2.295455    0.111076
H    -1.419891    2.749286   -0.048723
H    -2.605472    1.332334   -0.073800
H     0.975329    2.158234   -0.748562
H     0.983643    1.995482    0.988105
```

Frequencies

60.5878	115.9373	135.6738
282.8607	351.939	385.7926
403.9908	496.4661	503.9493
519.1581	553.2676	675.8239
703.146	752.4286	821.1042
919.8121	928.7955	946.336
973.3148	1015.225	1019.244
1035.725	1041.7	1162.869
1196.972	1226.53	1227.289
1244.486	1293.841	1388.829
1402.523	1413.687	1428.887
1455.806	1473.443	1482.28
1493.617	1503.537	1544.57
1772.289	2985.799	3006.48
3029.598	3030.394	3058.637
3088.311	3124.104	3165.371
3165.918	3190.24	3259.912

i66
```
C     1.903267    0.697262   -0.007386
C     1.852314   -0.773847    0.296754
C     0.582337   -1.413678   -0.268316
C    -0.655629   -0.595633   -0.027407
C    -1.979865   -1.288921    0.053539
C    -1.648113    1.642781    0.094342
C    -0.558074    0.810994   -0.021258
```

```
C     0.786977    1.408837   -0.151445
H     2.872387    1.182272   -0.067288
H     2.734706   -1.280518   -0.103370
H     1.884709   -0.911808    1.386303
H     0.454065   -2.419128    0.143896
H     0.705203   -1.543809   -1.356097
H    -2.652024   -0.972282   -0.753110
H    -2.492626   -1.066262    0.996796
H    -1.864096   -2.372226   -0.015045
H    -1.524422    2.719444    0.089674
H    -2.655036    1.260150    0.202744
H     0.837844    2.477387   -0.337440
```

Frequencies

69.4271	122.7323	150.8837
283.936	344.1133	366.3408
412.5518	479.1818	504.8045
587.5145	604.7714	704.9733
716.4977	776.8796	806.2429
864.9555	910.0058	968.3573
981.0095	1004.047	1012.93
1049.411	1066.047	1174.299
1196.973	1199.756	1250.451
1284.487	1332.793	1359.669
1394.786	1415.035	1428.345
1459.243	1477.101	1484.967
1490.027	1502.934	1547.189
1731.69	2974.224	3023.633
3023.906	3074.669	3077.983
3096.246	3127.666	3167.181
3176.594	3199.892	3261.617

Transition states
i55 – i27
```
C     1.999966   -0.831286    0.168726
C     1.936847    0.631898   -0.221120
C     0.816654    1.367767   -0.161642
C    -0.446491    0.954907    0.429155
C    -1.696495    1.664492   -0.005016
C    -1.956790   -1.549842   -0.174029
C    -0.537030   -1.197090   -0.040191
C     0.672484   -1.445129    0.011165
H     2.745112   -1.338401   -0.451305
H     2.337439   -0.951452    1.206891
H     2.832881    1.057196   -0.661719
H     0.830385    2.351401   -0.632131
H    -0.419884    0.656416    1.473139
H    -1.803313    1.655132   -1.093851
H    -1.675977    2.716741    0.311214
H    -2.591162    1.214898    0.430539
H    -2.508101   -1.309922    0.739514
H    -2.060214   -2.620190   -0.364608
H    -2.422042   -1.006116   -0.999967
```

Frequencies

-648.673	70.1328	120.8732
147.9855	188.4376	226.5611
251.0372	304.6995	373.1673
407.0212	449.4957	509.0002
682.5443	709.7382	774.0343
806.7474	894.053	924.2519
971.1432	981.0407	1002.239
1042.535	1069.209	1115.446

1141.975	1162.154	1211.621
1245.021	1321.16	1338.503
1406.564	1418.153	1432.409
1466.883	1480.117	1482.011
1494.584	1502.259	1662.632
2098.952	3009.402	3030.41
3048.14	3085.071	3086.987
3116.332	3128.844	3129.987
3133.105	3159.493	3190.768

i55 – i56
```
C   -1.845114  -0.884311   0.262048
C   -1.864741   0.604726  -0.017375
C   -0.799789   1.342367  -0.326476
C    0.623652   0.837706  -0.438882
C    1.563629   1.595802   0.510421
C    1.669131  -1.704854  -0.122356
C    0.623801  -0.632327  -0.171139
C   -0.435081  -1.354460   0.136190
H   -2.246358  -1.084687   1.262321
H   -2.504664  -1.409060  -0.439138
H   -2.836591   1.087883   0.044899
H   -0.939858   2.406197  -0.504286
H    0.974755   1.019300  -1.465037
H    2.593388   1.246326   0.396795
H    1.259742   1.440046   1.548968
H    1.544953   2.669654   0.304770
H    2.087634  -2.066097  -1.062454
H    0.493402  -2.417353   0.197844
H    2.360669  -1.720108   0.720728
```

Frequencies

-2272.91	80.9049	167.0635
223.7253	248.1264	289.3499
393.5442	452.6943	471.839
503.5254	576.462	595.3902
714.2869	765.2025	835.8305
902.6916	940.4823	959.3893
973.4055	1014.029	1024.302
1049.393	1079.714	1086.851
1117.069	1129.428	1199.06
1219.367	1236.875	1316.546
1337.258	1393.264	1404.042
1423.196	1441.236	1475.69
1493.505	1507.424	1730.606
1798.703	1874.791	3011.336
3041.403	3046.304	3067.844
3078.862	3124.692	3129.703
3154.183	3172.636	3178.66

i55 – i57
```
C   -1.389600  -1.186113   0.521738
C   -1.901806  -0.198254  -0.434918
C   -1.078930   0.777688  -0.840747
C    0.340649   0.916509  -0.321219
C    0.397739   1.898919   0.862660
C    2.252757  -0.841446  -0.430095
C    0.872833  -0.470196   0.012046
C    0.021840  -1.290857   0.664766
H   -2.048803  -1.616865   1.270179
H   -0.731929  -2.263326   0.140100
H   -2.926295  -0.258669  -0.785532
H   -1.433581   1.534660  -1.535415
```

```
H    0.964129    1.333552   -1.122600
H    1.427324    2.019456    1.210534
H   -0.203300    1.520410    1.692703
H    0.012152    2.882551    0.577797
H    2.346146   -0.758409   -1.519749
H    2.497896   -1.862663   -0.135675
H    3.003368   -0.168191    0.002265
```

Frequencies

-1846.2	90.7592	144.4263
188.4574	233.9316	260.3305
321.0926	409.4825	464.6354
512.5208	563.9235	606.4394
717.6033	741.1045	810.0811
839.0832	910.9249	951.7275
985.1747	1013.127	1023.45
1035.623	1090.552	1099.165
1151.897	1187.083	1212.386
1223.668	1320.973	1338.783
1385.524	1402.384	1408.181
1413.133	1476.709	1484.731
1491.257	1496.493	1590.434
1669.029	2107.541	3018.369
3032.737	3044.878	3068.898
3121.391	3136.463	3139.696
3167.996	3172.407	3203.817

i57 – p42

```
C   -1.579692    1.058189   -0.469344
C   -2.006828   -0.130836    0.122447
C   -1.090969   -0.963237    0.734826
C    0.291545   -0.662436    0.686941
C    0.948891   -1.960035   -0.943629
C    2.150756    1.008005    0.300977
C    0.704836    0.612423    0.208993
C   -0.235011    1.427201   -0.398909
H   -2.295738    1.716351   -0.947913
H   -3.059862   -0.389759    0.119639
H   -1.417195   -1.880808    1.211695
H    0.962040   -1.203920    1.346923
H    2.025779   -1.824243   -0.960008
H    0.400501   -1.515218   -1.766162
H    0.604497   -2.936329   -0.618885
H    2.542949    0.844273    1.308922
H    2.293737    2.060510    0.048888
H    2.763767    0.412376   -0.384650
H    0.078356    2.381123   -0.812257
```

Frequencies

-576.404	85.7262	121.6788
128.5931	190.2386	218.8043
352.9577	401.1366	487.9325
522.7612	558.47	584.7065
638.3069	693.9742	738.9179
797.9556	860.9046	883.2599
947.7206	982.2728	992.4044
1010.342	1029.678	1053.781
1066.118	1100.838	1179.238
1194.852	1226.839	1325.71
1345.598	1419.889	1425.386
1431.607	1456.432	1493.174

1506.587	1533.495	1608.943
1639.367	3038.607	3089.198
3099.336	3136.433	3177.287
3181.492	3189.656	3206.647
3216.657	3245.086	3255.774

i57 – p89

C	1.962322	-0.696804	-0.027879
C	1.958242	0.694061	-0.032178
C	0.755437	1.374634	-0.010596
C	-0.474631	0.689367	0.070426
C	-1.762530	1.456378	-0.135118
C	-1.754052	-1.496066	-0.008591
C	-0.462717	-0.729367	-0.011290
C	0.756611	-1.391195	-0.030851
H	2.899994	-1.240495	-0.043415
H	2.892633	1.242961	-0.059604
H	0.745917	2.459692	-0.017039
H	-0.616343	0.717779	1.895451
H	-2.581612	1.056487	0.463944
H	-2.060654	1.406631	-1.188051
H	-1.632255	2.506758	0.129838
H	-2.297419	-1.330852	0.928714
H	-1.575692	-2.567468	-0.111702
H	-2.412532	-1.181180	-0.823663
H	0.765872	-2.476354	-0.058009

Frequencies

-902.203	152.4408	168.4286
198.5697	257.0256	329.5618
381.2164	427.9521	469.3768
481.9117	541.0198	551.481
600.3995	721.9146	750.9676
767.4685	840.6054	876.4618
956.1207	1003.28	1011.976
1021.598	1048.539	1073.48
1081.791	1152.662	1189.471
1215.513	1248.193	1313.935
1324.104	1417.791	1427.138
1473.083	1482.613	1498.328
1501.931	1515.21	1526.96
1625.846	1663.915	3040.144
3047.403	3100.918	3123.703
3140.016	3153.713	3185.924
3191.693	3205.033	3219.57

i56 – p92

C	1.693149	0.724329	0.411086
C	1.814638	-0.628941	-0.133677
C	0.736642	-1.299828	-0.540252
C	-0.660113	-0.753527	-0.403728
C	-1.380742	-1.505552	0.734519
C	-1.794269	1.468538	-0.387076
C	-0.694785	0.744273	-0.139938
C	0.492810	1.352703	0.437812
H	2.552182	1.169515	0.899323
H	2.553341	1.708501	-1.204107
H	2.802192	-1.069690	-0.208134
H	0.833106	-2.306768	-0.935319
H	-1.206195	-0.953709	-1.331913
H	-2.416092	-1.165856	0.817920
H	-0.878629	-1.318552	1.687373
H	-1.378550	-2.583823	0.551817
H	-1.840522	2.524591	-0.143972
H	-2.673838	1.026044	-0.843375
H	0.409031	2.357776	0.837909

SUPPORTING INFORMATION

Frequencies

-637.469	74.6023	183.8475
249.965	256.9286	275.5698
309.9347	386.6152	418.3131
494.0268	542.3589	586.8882
678.6169	699.427	751.1266
776.0074	847.3973	875.3501
925.0327	942.2589	961.7538
1000.12	1004.424	1017.203
1033.974	1091.523	1123.079
1186.742	1213.406	1308.083
1327.265	1353.325	1395.506
1415.001	1440.276	1472.932
1489.117	1506.763	1587.743
1677.753	1725.872	3045.581
3058.387	3127.569	3132.873
3152.807	3177.927	3188.536
3203.755	3216.21	3241.431

i56 – i60

C	-1.722837	-0.880754	0.346788
C	-1.916219	0.449845	-0.150618
C	-0.874170	1.207343	-0.551761
C	0.572523	0.813023	-0.384334
C	1.197936	1.616527	0.773119
C	1.976551	-1.249779	-0.346826
C	0.766436	-0.685642	-0.157120
C	-0.360638	-1.452213	0.317725
H	-2.498170	-1.412971	0.881706
H	-1.278327	-1.666232	-0.591463
H	-2.930237	0.823516	-0.240538
H	-1.059119	2.193739	-0.966574
H	1.112286	1.083106	-1.300294
H	2.269995	1.420522	0.853105
H	0.724396	1.340398	1.719191
H	1.050742	2.690022	0.620666
H	2.144890	-2.306176	-0.167898
H	2.825276	-0.659901	-0.675192
H	-0.199222	-2.416122	0.785466

Frequencies

-1867.87	41.0282	199.7926
249.4347	284.5468	374.0914
391.1589	494.7679	499.8633
559.467	637.3523	661.6015
686.6065	740.1532	756.7631
856.9842	860.7152	901.5351
930.4013	946.2036	968.5576
1014.044	1031.845	1091.15
1108.333	1140.843	1198.491
1237.459	1307.513	1323.984
1345.062	1384.223	1398.86
1411.947	1455.883	1469.264
1500.506	1501.607	1626.874
1628.493	2164.326	3034.668
3042.807	3120.072	3132.472
3151.51	3174.495	3198.871

3201.709	3224.5	3240.91

i56 – i63

C	-1.541060	-1.032849	0.403076
C	-1.907600	0.266918	-0.203637
C	-0.919001	1.131828	-0.640747
C	0.536038	0.857937	-0.367782
C	0.993450	1.666485	0.865271
C	2.040942	-1.129396	-0.443037
C	0.824830	-0.626858	-0.149193
C	-0.215703	-1.440964	0.423318
H	-2.324886	-1.611045	0.876946
H	-1.983192	-0.862817	-0.875545
H	-2.946465	0.574362	-0.156977
H	-1.193299	2.069898	-1.108698
H	1.132031	1.195548	-1.223060
H	2.063100	1.522900	1.041991
H	0.450193	1.335767	1.754647
H	0.800412	2.733614	0.722090
H	2.280601	-2.170158	-0.253050
H	2.819898	-0.508989	-0.873262
H	0.030230	-2.437687	0.771305

Frequencies

-1907.87	68.5834	177.7784
253.2398	280.9042	365.5492
401.8366	496.7523	539.4906
562.3296	641.4241	658.6207
679.8589	735.6887	742.693
819.1699	869.5061	879.7464
928.1142	954.3367	996
1007.072	1027.671	1082.467
1097.844	1124.394	1168.828
1209.05	1310.113	1319.86
1331.757	1378.116	1405.955
1410.777	1447.632	1497.637
1501.011	1519.382	1543.17
1621.672	1862.624	3039.429
3045.382	3121.042	3125.906
3151.111	3191.62	3200.36
3211.851	3222.282	3241.644

i60 – i62

C	-0.897526	-1.587065	0.182785
C	-1.668556	-0.694487	-0.455384
C	-1.249366	0.678002	-0.701002
C	0.174300	1.069503	-0.269420
C	-0.351301	1.769179	0.983793
C	2.349168	-0.097643	-0.525083
C	1.100093	-0.097205	-0.071288
C	0.501382	-1.281973	0.646741
H	-1.285079	-2.579140	0.391826
H	-2.675010	-0.971544	-0.754155
H	-1.643267	1.178537	-1.583369
H	0.618158	1.784815	-0.962731
H	-0.363997	1.187683	1.902884
H	-1.612659	1.443731	0.342814
H	-0.177929	2.835600	1.101441
H	3.002571	-0.953809	-0.391592
H	2.762323	0.762109	-1.042698
H	1.143086	-2.158093	0.520061
H	0.482635	-1.079756	1.728665

Frequencies

-2087.37	111.5735	134.5583
259.5418	362.4591	377.3579
457.558	491.1287	526.8496

573.0746	625.7845	697.1887
735.075	761.7134	860.1434
900.5105	916.1838	928.6873
936.018	941.4242	965.1615
994.8417	1006.237	1051.326
1085.363	1110.511	1186.513
1209.876	1262.099	1308.066
1322.861	1329.403	1340.623
1363.119	1430.499	1433.936
1461.944	1479.495	1671.512
1746.661	1806.575	3001.882
3093.5	3105.271	3115.203
3152.489	3155.804	3175.838
3198.011	3225.264	3237.53

i56 – i59

```
C    -1.945739   -0.469195    0.412671
C    -1.715283    0.821396   -0.338132
C    -0.496973    1.287495   -0.638716
C     0.703773    0.566169   -0.198791
C     1.645164    1.343358    0.701946
C     0.456159   -0.873681    0.111306
C    -0.745453   -1.380753    0.350961
H    -2.225919   -0.237452    1.450260
H    -2.815484   -0.983211   -0.010888
H    -2.595695    1.393826   -0.615508
H    -0.380285    2.239848   -1.148332
H     1.579376   -0.081765   -1.084890
H     2.571871    0.798532    0.896969
H     1.159783    1.541821    1.664186
H     1.904670    2.304294    0.250042
H    -0.906367   -2.454280    0.379502
C     1.682600   -1.436880   -0.506782
H     1.588965   -2.266203   -1.203518
H     2.613596   -1.402862    0.055396
```

Frequencies

-2270.95	125.7351	216.943
226.1106	257.9471	292.8471
422.5774	433.8952	461.5098
518.6717	548.6731	621.3228
726.9369	762.7291	811.1977
844.5057	888.8586	914.5954
962.4769	981.9821	1011.058
1016.457	1064.403	1072.084
1147.634	1161.74	1184.824
1219.603	1266.431	1307.201
1363.82	1381.431	1414.467
1421.736	1443.822	1477.333
1491.149	1500.936	1662.531
1694.181	1829.338	3010.845
3034.954	3068.442	3106.518
3115.279	3131.839	3163.799
3182.166	3187.069	3213.005

i57 – i58

```
C     1.310330   -1.411544   -0.252056
C     1.971774   -0.296327    0.128419
C     1.255576    0.914585    0.471579
```

```
C    -0.283157    0.902502    0.419772
C    -0.294030    1.881925   -0.753113
C    -2.402064   -0.498894    0.198258
C    -0.907892   -0.432301    0.114875
C    -0.141269   -1.477131   -0.236796
H     1.862954   -2.298708   -0.540785
H     3.056204   -0.272772    0.139253
H     1.689819    1.561954    1.231399
H    -0.745008    1.332336    1.313463
H    -0.497920    1.467070   -1.736733
H     1.170546    1.738882   -0.560104
H    -0.593969    2.911944   -0.578573
H    -2.742460   -0.279455    1.217149
H    -2.779280   -1.483869   -0.083510
H    -2.864101    0.248122   -0.457140
H    -0.612400   -2.422398   -0.490046
```

Frequencies

-2084.12	99.8991	164.9029
212.0589	251.5604	327.9831
382.8004	480.7927	532.575
554.875	576.6157	641.7938
726.5055	756.3375	855.6675
887.3802	896.2784	913.5612
939.9425	974.5201	984.8209
1041.697	1052.466	1064.798
1082.813	1134.586	1182.209
1205.865	1261.778	1321.402
1337.796	1343.285	1405.089
1415.492	1424.92	1449.948
1477.146	1494.862	1583.609
1718.996	1807.511	3029.538
3071.341	3083.943	3117.191
3134.572	3147.653	3178.683
3190.25	3208.712	3235.828

i41 – i43
```
C     2.187308   -1.141839    0.488991
C     1.219883   -0.436048   -0.469867
C    -0.194040   -0.895848   -0.304165
C    -1.252110   -0.173893    0.007003
C    -1.238984    1.297707    0.240164
C     0.168582    1.816365    0.062997
C     1.224084    1.067737   -0.252256
C    -2.286442   -1.256264    0.023428
H     2.187020   -2.220033    0.311812
H     1.892059   -0.962472    1.525819
H     3.207500   -0.771678    0.352649
H     1.554002   -0.637425   -1.496073
H    -1.113452   -1.969394   -0.306083
H    -1.606040    1.539324    1.246292
H    -1.919548    1.812409   -0.450863
H     0.312136    2.883996    0.204312
H     2.194306    1.549457   -0.356251
H    -2.673309   -1.590043    0.986932
H    -3.004370   -1.301646   -0.796315
```

Frequencies

-2257.96	92.3213	132.5987
230.9418	265.1303	332.8925
390.4603	430.9313	474.9883
509.0347	542.0029	595.6059
710.8333	765.7961	869.0018
910.1581	933.3812	944.2134
980.1544	993.0431	1022.653

1061.891	1073.543	1083.93
1109.986	1144.697	1211.094
1212.909	1238.213	1321.575
1332.7	1396.219	1406.242
1423.284	1440.948	1473.643
1491.931	1507.831	1730.244
1798.856	1876.092	3027.244
3030.138	3047.911	3050.411
3079.8	3126.091	3134.692
3147.35	3173.291	3180.721

i41 – i23

```
C    1.985871   -1.222011    0.730263
C    1.250896   -0.620339   -0.481585
C   -0.184054   -0.956234   -0.466198
C   -1.318186   -0.556852   -0.192448
C   -0.715195    1.379247    0.674807
C    0.466938    1.749623   -0.078664
C    1.390010    0.892169   -0.543046
C   -2.778072   -0.642163   -0.059486
H    1.884417   -2.309818    0.743779
H    1.571015   -0.823606    1.658886
H    3.048821   -0.970776    0.692747
H    1.707623   -1.030022   -1.389356
H   -0.595453    0.855261    1.616362
H   -1.564566    2.057385    0.645328
H    0.583165    2.803427   -0.326678
H    2.258505    1.274278   -1.071130
H   -3.127535   -1.630756   -0.365926
H   -3.084403   -0.474419    0.976307
H   -3.270837    0.108408   -0.682175
```

Frequencies

-662.454	89.9775	120.1652
138.1145	212.8344	250.9961
265.6432	321.1738	373.71
477.8076	493.9038	541.5471
623.1213	682.6367	711.9462
758.9769	852.8472	882.9627
954.9622	983.049	1022.281
1033.95	1058.302	1073.939
1092.174	1120.868	1182.087
1246.496	1321.863	1348.897
1396.947	1407	1411.872
1477.602	1487.312	1491.165
1497.178	1501.064	1652.383
2118.723	3049.107	3053.131
3055.153	3124.259	3131.02
3131.965	3133.758	3135.517
3145.224	3190.141	3222.425

i41 – i44

```
C    2.559755   -0.911906    0.274711
C    1.227995   -0.352331   -0.155834
C    0.005073   -1.041944    0.086846
C   -1.190572   -0.410137    0.132431
C   -1.162308    1.049267    0.551755
C    0.002780    1.741933   -0.122903
C    1.117714    1.085912   -0.462658
C   -2.494721   -1.026177   -0.263086
H    2.511544   -1.999435    0.358108
H    2.822490   -0.509668    1.258519
```

```
H    3.358121   -0.637605   -0.420691
H    0.751688   -1.231677   -1.011923
H   -1.079863    1.168586    1.642605
H   -2.103519    1.537733    0.275828
H   -0.082920    2.807481   -0.316301
H    1.951785    1.597248   -0.933588
H   -2.360347   -2.069286   -0.552227
H   -3.221776   -0.987738    0.557579
H   -2.941490   -0.483350   -1.105482
```

Frequencies

-1752.67	126.4231	142.2104
172.6486	214.0421	271.7403
309.3883	378.1212	470.9068
479.4508	515.3939	605.9577
674.5021	751.5409	850.6986
879.5642	918.6179	938.0802
977.5817	997.9389	1014.994
1037.714	1048.517	1124.87
1184.127	1196.959	1209.219
1246.176	1334.431	1366.081
1408.862	1410.546	1414.783
1466.414	1479.26	1484.354
1488.506	1501.019	1580.754
1681.477	2100.421	2991.661
3019.773	3042.949	3065.905
3069.213	3110.118	3138.924
3143.699	3169.886	3193.105

i41 – i42

```
C    1.780639   -1.479600    0.452658
C    1.387572   -0.311625   -0.461328
C    0.009904   -0.879953   -0.507412
C   -1.111558   -0.259555   -0.154244
C   -1.076671    1.253883   -0.050400
C    0.307008    1.797832    0.211246
C    1.424858    1.094928    0.052711
C   -2.398318   -0.953698    0.173517
H    2.567415   -2.159574    0.132572
H    0.563275   -2.008338    0.059439
H    1.711505   -1.295962    1.521758
H    1.913381   -0.386480   -1.419155
H   -1.743870    1.565113    0.764038
H   -1.493839    1.717845   -0.955034
H    0.364903    2.827437    0.553524
H    2.390566    1.546423    0.261745
H   -2.305841   -2.033016    0.044594
H   -2.698108   -0.748151    1.207628
H   -3.209989   -0.598565   -0.471599
```

Frequencies

-2069.87	120.1379	140.6607
197.2562	268.3864	330.4794
384.8618	439.1739	476.1277
503.5716	566.1955	642.9064
710.252	762.1869	869.3337
896.0747	918.748	949.2919
985.4364	1007.069	1008.438
1055.092	1077.899	1084.795
1137.008	1184.744	1203.802
1226.769	1242.506	1271.11
1347.156	1368.808	1413.066

1416.611	1433.269	1476.116
1487.4	1492.429	1713.003
1750.229	1893.042	3018.931
3029.702	3046.228	3056.489
3085.282	3113.369	3138.774
3165.011	3189.278	3226.753

i26 – i27

C	0.556434	1.487746	0.427320
C	-0.543035	1.240851	-0.570014
C	3.620089	-1.232251	-0.090192
C	2.546507	-0.262680	0.098632
C	1.665016	0.536490	0.262223
H	0.940105	2.507340	0.325026
H	0.157736	1.390089	1.444277
H	-0.501912	1.775529	-1.514921
H	3.327599	-2.000133	-0.810742
H	3.866320	-1.728754	0.851722
H	4.524748	-0.746201	-0.463905
C	-1.379922	0.037077	-0.463767
C	-2.591489	-0.001754	0.084922
C	-3.433825	-1.233502	0.214472
H	-0.951560	-0.893667	-0.848757
H	-3.018141	0.921285	0.474651
H	-3.654085	-1.445172	1.265867
H	-2.933781	-2.105951	-0.212313
H	-4.395676	-1.106226	-0.292487

Frequencies

-206.265	29.9783	85.4792
106.2903	149.3765	206.0593
213.2746	235.263	267.007
386.4025	398.1949	414.5719
519.0292	596.5429	749.7042
800.2959	880.4503	955.8666
995.9542	1030.236	1061.593
1063.619	1080.828	1120.346
1137.158	1167.345	1228.167
1302.709	1314.745	1336.229
1378.653	1422.841	1423.958
1471.609	1486.48	1489.103
1492.242	1503.413	1753.069
2389.274	3037.238	3038.108
3053.261	3077.394	3090.735
3097.197	3125.069	3126.21
3127.374	3150.299	3173.77

i23 – i22

C	-0.952475	-1.840494	-0.815870
C	-0.476750	-1.127452	0.461383
C	0.863384	-0.548808	0.265784
C	1.941432	-0.048281	0.089369
C	-1.429447	-0.045627	0.909595
C	3.250658	0.557082	-0.127671
H	-0.242617	-2.618084	-1.104599
H	-1.033708	-1.127611	-1.639332
H	-1.930768	-2.299234	-0.651023
H	-0.402933	-1.869422	1.264030
H	-1.585360	0.097055	1.973972
H	3.735718	0.128866	-1.008435
H	3.158585	1.634901	-0.284173
H	3.905138	0.394216	0.732201
C	-1.331859	2.074929	-0.371133
C	-1.956791	0.949795	-0.037039
H	-0.366556	2.328063	0.054857
H	-1.764423	2.770248	-1.082931

H   -2.921989   0.734136   -0.501076

Frequencies

-220.614	57.2186	70.0446
96.9033	136.2264	203.8132
255.1284	280.7871	309.3108
321.2251	411.0365	500.8419
535.2539	566.2176	707.2389
732.039	881.6223	958.1269
975.3099	1023.812	1035.484
1056.007	1060.265	1072.91
1105.723	1154.782	1186.641
1320.054	1323.481	1336.508
1358.337	1415.263	1418.588
1453.556	1485.467	1490.078
1502.787	1508.625	1706.9
2383.921	3051.766	3052.619
3055.668	3099.531	3122.514
3125.869	3134.12	3144.704
3151.683	3186.573	3243.347

i27 – p67

C	0.383360	0.799988	0.733918
C	-0.493402	0.952385	-0.482993
C	-1.701134	0.414511	-0.679889
C	-2.434585	-0.447976	0.232944
C	-3.656468	-0.930674	-0.034206
C	4.075839	-0.723727	-0.289575
C	2.774490	-0.180212	0.082772
C	1.701027	0.260673	0.389496
H	0.515744	1.783646	1.201065
H	-0.083135	0.162256	1.488129
H	-0.069282	1.567822	-1.271443
H	-2.202779	0.633003	-1.619973
H	-1.970907	-0.705485	1.180536
H	-4.146173	-0.730126	-0.982097
H	-5.043770	0.632273	0.807693
H	-4.161334	-1.603478	0.648176
H	4.028056	-1.205068	-1.269442
H	4.407610	-1.469227	0.437279
H	4.831210	0.064571	-0.334728

Frequencies

-431.65	21.5575	85.4697
106.0349	120.502	175.8886
185.2829	224.0796	258.9202
277.0812	374.0184	388.3777
401.63	517.7204	617.3967
667.9939	785.5561	832.1995
916.4187	942.1792	958.1979
1000.76	1030.517	1040.838
1059.366	1068.351	1171.916
1175.232	1242.421	1300.618
1323.165	1339.086	1403.231
1424.398	1474.781	1477.765
1489.347	1493.949	1656.87
1731.614	2398.888	3037.93
3052.375	3110.544	3124.488

| 3125.943 | 3157.689 | 3161.48 |
| 3187.046 | 3190.89 | 3255.218 |

i27 – p62

C	0.390653	-0.259463	-0.185089
C	-0.429711	0.780519	0.105680
C	-1.880247	0.760396	0.004666
C	-2.647428	-0.334245	0.056621
C	-4.137128	-0.336977	-0.063481
C	4.465305	-0.048165	0.020335
C	3.011981	-0.122533	-0.048798
C	1.811283	-0.178769	-0.099035
H	0.050471	-1.421311	1.506885
H	-0.015173	-1.144450	-0.666801
H	0.025603	1.702769	0.454929
H	-2.364516	1.730572	-0.088589
H	-2.174180	-1.301065	0.218606
H	-4.456605	-0.948303	-0.914222
H	-4.532818	0.671813	-0.200851
H	-4.600096	-0.771455	0.828415
H	4.856019	0.636099	-0.737443
H	4.913146	-1.030801	-0.146412
H	4.789898	0.311552	1.000090

Frequencies

-633.309	65.9431	77.5511
77.9833	144.2622	173.5288
196.3186	213.1493	308.5085
320.5516	327.6663	353.5749
374.0305	491.2644	501.8118
629.3672	796.3884	852.7737
893.5276	930.6576	987.6675
1005.933	1054.627	1061.295
1074.779	1077.744	1138.548
1213.37	1308.373	1322.751
1354.099	1362.738	1420.492
1422.234	1485.037	1486.189
1486.293	1495.345	1629.379
1724.995	2376.064	3037.027
3047.761	3095.714	3119.127
3122.874	3126.67	3149.805
3157.426	3179.257	3187.342

i27 – i28

C	-0.073494	0.316852	-0.793705
C	0.676483	1.395817	-0.063225
C	1.735724	0.935858	0.597776
C	1.923165	-0.540747	0.492062
C	3.157976	-1.056563	-0.199525
C	-3.918483	-0.479484	0.355486
C	-2.553210	-0.188356	-0.063148
C	-1.425325	0.057943	-0.411556
H	0.080806	0.305697	-1.875600
H	0.766194	-0.612739	-0.332018
H	0.360414	2.433226	-0.087407
H	2.419767	1.567684	1.158493
H	1.629296	-1.106186	1.379166
H	4.061838	-0.829927	0.381772
H	3.279590	-0.591067	-1.181906
H	3.116781	-2.140289	-0.332599
H	-4.213158	0.158574	1.192531
H	-4.015075	-1.520648	0.675605
H	-4.623479	-0.312250	-0.463030

Frequencies

-1927.95	28.0236	56.5201
89.8093	124.1275	183.6263

188

221.625	227.7892	320.3097
414.6718	458.3901	515.8068
600.6941	673.216	738.3825
812.7076	844.5452	905.5483
940.1271	998.4403	1015.219
1052.329	1057.623	1070.406
1099.665	1130.893	1162.588
1201.257	1297.114	1342.306
1369.936	1400.816	1414.705
1420.382	1483.941	1485.018
1489.62	1493.338	1637.701
1708.31	2335.45	3013.008
3042.571	3082.801	3090.111
3099.314	3111.746	3117.814
3124.266	3164.393	3201.086

i27 – p70

```
C   -0.438956   1.008657   -0.271366
C    0.489404   0.396151    0.759179
C    1.610473  -0.191078    0.434492
C    2.631461  -0.741888   -0.194969
C    3.954726  -0.069990   -0.412807
C   -4.212708  -0.637194   -0.064528
C   -2.880516  -0.049059   -0.146208
C   -1.782822   0.432060   -0.213108
H   -0.507574   2.088495   -0.095367
H   -0.016282   0.873878   -1.270431
H    0.179724   0.461042    1.796719
H    2.376462  -0.422068    2.255328
H    2.542057  -1.785972   -0.488735
H    4.736801  -0.560630    0.176120
H    3.916359   0.981466   -0.125713
H    4.248684  -0.137664   -1.464371
H   -4.169841  -1.630171    0.389657
H   -4.655783  -0.738615   -1.058340
H   -4.876987  -0.015714    0.541024
```

Frequencies

-706.3	36.5476	76.6762
94.9757	104.6284	125.2396
174.1632	199.6647	231.6612
278.212	335.3519	401.9397
464.0072	521.1897	559.3156
577.0155	717.7112	785.4796
857.5759	901.4405	953.5129
1044.07	1051.467	1061.411
1067.832	1106.064	1160.098
1174.901	1224.928	1299.14
1345.369	1403.388	1424.439
1446.684	1479.039	1481.43
1490.459	1492.665	1502.298
2024.157	2398.661	3041.584
3046.574	3049.615	3098.564
3104.487	3120.266	3124.386
3141.267	3159.288	3192.353

i23 – p11b

```
C   -0.736503   2.253538   1.013372
```

```
C    -0.542803   0.777685   -0.835683
C     0.762571   0.313316   -0.493132
C     1.882619  -0.044381   -0.235921
C    -1.114972  -1.860130    0.766973
C    -1.936104  -1.206778   -0.070385
C    -1.697959   0.041197   -0.758630
C     3.228785  -0.504719    0.077954
H     0.182223   2.809245    0.871681
H    -0.743746   1.481935    1.772293
H    -1.671632   2.758506    0.804522
H    -0.559521   1.654901   -1.474310
H    -0.127322  -1.492289    1.013612
H    -1.432364  -2.788867    1.227114
H    -2.917598  -1.640007   -0.249465
H    -2.567813   0.483942   -1.234545
H     3.752140   0.217230    0.710056
H     3.197967  -1.460831    0.606712
H     3.813862  -0.642141   -0.834956
```

Frequencies

-454.654	60.3109	65.504
79.1273	100.6977	124.9136
133.3906	217.7852	237.9251
328.8582	347.492	462.6498
486.3893	495.4361	531.7371
626.8207	678.9869	764.5301
814.1997	836.1372	935.0248
949.1405	957.0774	1040.984
1050.702	1055.796	1095.589
1161.451	1264.177	1341.877
1412.261	1415.673	1421.889
1431.557	1467.35	1482.877
1485.362	1518.792	1664.389
2369.804	3052.201	3107.381
3124.819	3125.783	3151.935
3170.296	3174.654	3191.362
3268.586	3277.441	3284.892

i23 – p12b

```
C     0.750425  -2.401990    0.026327
C     0.643756  -0.893417   -0.053400
C    -0.694225  -0.384393   -0.019001
C    -1.842384  -0.029327    0.037111
C     0.949174   2.242880   -0.196249
C     1.843978   1.336397    0.211984
C     1.745000  -0.110053    0.137236
C    -3.221366   0.434979    0.096056
H     0.119669  -2.878394   -0.725497
H     0.410053  -2.741756    1.009539
H     1.780751  -2.729615   -0.121295
H     0.773425  -0.819930   -2.049441
H     0.008523   1.963065   -0.652776
H     1.157451   3.301463   -0.090457
H     2.782508   1.700195    0.623950
H     2.689071  -0.640899    0.227566
H    -3.837957  -0.086071   -0.640487
H    -3.650177   0.254025    1.084969
H    -3.279473   1.507456   -0.106452
```

Frequencies

-797.355	67.3379	74.8498
82.5379	150.8688	179.5288
221.9535	236.7976	311.8458
323.3858	358.6326	393.4491
434.3968	527.0753	579.8926
640.4893	658.3615	698.8963

889.6687	959.9726	962.2734
1014.92	1040.94	1054.183
1056.235	1059.487	1072.193
1141.012	1234.427	1346.223
1407.719	1409.231	1422.441
1460.072	1481.389	1483.925
1487.983	1495.865	1596.312
1689.245	2371.67	3051.426
3053.282	3121.705	3127.507
3128.098	3151.45	3155.104
3172.029	3179.229	3268.214

i23 – p51
```
C    -0.862395    2.229992    0.561554
C    -0.605897    1.092724   -0.444083
C     0.738601    0.541084   -0.280675
C     1.843893    0.100801   -0.122623
C    -0.989650   -2.375645    0.296927
C    -1.507964   -1.205385   -0.020314
C    -1.705187    0.046363   -0.334531
C     3.181096   -0.447764    0.070128
H    -0.118312    3.019832    0.441939
H    -0.802819    1.847063    1.582441
H    -1.855618    2.660296    0.408156
H    -0.676271    1.516450   -1.454167
H    -0.716195   -3.089999   -0.472182
H    -0.905145   -2.683675    1.333602
H    -3.382434   -1.788271   -0.047005
H    -2.710811    0.409849   -0.519155
H     3.877460    0.326845    0.400705
H     3.169053   -1.236418    0.826425
H     3.566113   -0.874985   -0.859053
```

Frequencies

-827.114	53.9123	76.1408
99.0737	115.8236	137.5999
198.8685	265.8817	308.0634
313.7698	330.5654	356.5741
474.7501	500.4999	523.465
591.4954	666.8415	728.2389
865.8591	900.6914	914.5277
990.8491	1025.279	1062.058
1063.384	1078.9	1093.305
1132.899	1209.922	1306.445
1325.468	1378.732	1413.879
1423.798	1472.18	1489.657
1492.645	1501.346	1504.03
2016.765	2399.06	3035.007
3050.635	3052.229	3123.022
3126.18	3130.922	3144.006
3151.437	3190.087	3240.644

i60 – p92
```
C    -1.521994   -1.100060    0.259769
C    -1.923136    0.190485   -0.272464
C    -1.009187    1.109280   -0.605092
C     0.463803    0.893877   -0.379329
C     0.901375    1.693936    0.866356
C     2.034085   -1.040039   -0.523570
C     0.822945   -0.571940   -0.212949
C    -0.216958   -1.451009    0.328996
H    -2.287288   -1.792740    0.591166
```

```
H    -2.980596   0.394988   -0.397779
H    -1.315415   2.076992   -0.990818
H     1.015673   1.290682   -1.237854
H     1.978471   1.589331    1.018958
H     0.389168   1.320402    1.756672
H     0.663160   2.754691    0.749194
H     2.302257  -2.075048   -0.340332
H     2.790357  -0.401634   -0.968642
H     0.067514  -2.455441    0.623778
H     0.071105  -1.049398    2.425349
```

Frequencies

-539.357	91.7519	182.6301
248.4347	263.7779	288.5515
291.1251	378.9163	408.5593
487.2556	538.6738	594.4689
690.212	709.2114	749.3814
769.1191	843.6976	876.6406
929.9407	946.6879	962.7575
994.9451	1011.199	1017.429
1036.727	1089.157	1118.393
1187.067	1208.075	1310.733
1321.774	1348.635	1396.57
1415.738	1441.361	1472.4
1495.545	1502.967	1584.172
1695.313	1728.213	3045.871
3062.666	3128.763	3134.206
3152.799	3181.757	3190.975
3204.48	3216.316	3241.635

i60 – p45
```
C    -1.680753  -0.793477    0.478701
C    -1.931251   0.287201   -0.276380
C    -0.860161   1.032101   -0.898154
C     0.439933   0.625972   -0.783422
C     1.219079   1.895933    1.100983
C     1.859535  -1.357351   -0.550754
C     0.744937  -0.699956   -0.224864
C    -0.278113  -1.269943    0.733658
H    -2.491692  -1.331834    0.957862
H    -2.952050   0.622808   -0.424618
H    -1.095944   1.940024   -1.441667
H     1.209984   1.106659   -1.376417
H     2.199230   1.443072    1.183201
H     0.465476   1.601121    1.820460
H     1.155682   2.900822    0.702563
H     2.059440  -2.355483   -0.175799
H     2.603939  -0.913450   -1.203551
H    -0.233603  -2.362884    0.722384
H     0.000304  -0.973729    1.756977
```

Frequencies

-426.696	84.3232	102.431
131.032	133.9118	271.3754
387.538	442.3999	456.472
478.762	487.739	555.4402
596.9006	680.1701	723.4316
774.3275	777.3318	822.3496
900.8317	933.4964	939.1143
957.8238	972.4066	992.1449
998.2941	1034.153	1170.663
1198.212	1216.871	1314.201

1342.814	1395.102	1416.252
1423.873	1435.983	1451.064
1466.835	1501.226	1674.701
1719.279	2997.751	3086.336
3104.722	3152.319	3180.793
3190.386	3202.992	3213.558
3239.799	3275.63	3277.953

i60 – p91

```
C   -2.052852  -0.218885   0.070541
C   -1.696293   1.058250   0.244640
C   -0.314042   1.470211   0.095344
C    0.700649   0.579820  -0.078949
C    2.136939   1.025909  -0.045324
C    1.303354  -1.777545   0.328613
C    0.387028  -0.863596   0.002972
C   -1.038458  -1.254083  -0.315701
H   -3.090598  -0.523771   0.153414
H   -2.438206   1.811648   0.484481
H   -0.085002   2.530487   0.132872
H    0.541361   0.608675  -2.157353
H    2.737008   0.496103  -0.788128
H    2.573378   0.826630   0.939273
H    2.214212   2.096863  -0.238299
H    1.035963  -2.823918   0.430331
H    2.341754  -1.521317   0.500166
H   -1.114146  -1.400328  -1.405144
H   -1.273669  -2.221565   0.135576
```

Frequencies

-596.191	110.1633	180.4688
247.3335	305.0586	341.75
356.4798	385.2942	426.726
482.798	504.8166	522.7963
605.5943	699.9361	725.1769
761.9676	831.9702	884.3678
926.1948	941.621	963.4952
991.483	1002.562	1020.11
1058.981	1093.309	1170.031
1198.178	1224.289	1302.528
1347.112	1400.112	1421.266
1439.806	1450.19	1462.776
1493.787	1504.798	1592.098
1698.439	1724.852	2991.683
3046.878	3095.938	3116.683
3148.678	3165.956	3184.873
3193.726	3214.972	3252.272

i63 – p92

```
C   -1.339391  -1.278090   0.298357
C   -1.879515  -0.052856  -0.297148
C   -1.045765   0.919202  -0.726570
C    0.421360   0.892949  -0.401950
C    0.667151   1.772931   0.844510
C    2.227993  -0.823617  -0.332432
C    0.941796  -0.511983  -0.149935
C   -0.018194  -1.493111   0.355596
H   -2.036143  -2.024455   0.662119
H   -2.932200  -0.022912  -0.554206
H   -2.523338   0.741808   1.418851
H   -1.439012   1.801506  -1.220887
H    0.980351   1.331130  -1.234916
H    1.736048   1.816368   1.067384
H    0.146388   1.354569   1.709632
H    0.298479   2.789254   0.681458
```

```
H    2.611182   -1.807546   -0.083412
H    2.934198   -0.104394   -0.734554
H    0.371446   -2.427885    0.745967
```

Frequencies

-704.703	80.8786	187.0485
239.073	254.0354	318.1027
342.4554	387.9266	411.2764
506.5267	526.1854	591.4929
689.7235	711.1465	748.0169
786.496	837.6965	875.9343
926.0169	942.2297	962.9668
1002.103	1006.218	1017.911
1030.77	1083.482	1113.63
1186.172	1208.229	1307.134
1323.999	1349.009	1392.866
1413.862	1438.19	1473.834
1488.578	1501.453	1607.162
1683.387	1727.646	3047.165
3064.707	3129.721	3136.903
3149.253	3178.851	3188.676
3203.848	3213.175	3238.068

i63 – p44
```
C   -1.515650   -1.006305    0.508042
C   -1.982414    0.271883   -0.119959
C   -0.894775    1.017278   -0.824274
C    0.420765    0.664873   -0.727560
C    1.169835    1.824428    1.057289
C    2.032161   -1.176571   -0.401017
C    0.802784   -0.676125   -0.234525
C   -0.254519   -1.433536    0.442455
H   -2.260783   -1.603948    1.024593
H   -2.804242    0.057108   -0.817369
H   -2.435600    0.914222    0.651497
H   -1.166341    1.933598   -1.338151
H    1.146129    1.178217   -1.349936
H    2.232523    1.634916    0.958004
H    0.659411    1.289329    1.849903
H    0.835786    2.838219    0.866475
H    2.289815   -2.166319   -0.040660
H    2.810002   -0.610506   -0.902222
H    0.024175   -2.380390    0.895159
```

Frequencies

-543.241	86.711	127.0801
136.0797	163.3504	310.3749
362.0672	378.7669	498.1422
522.3617	553.9525	584.8938
609.7129	698.6608	739.0523
782.3972	805.7419	866.408
896.4431	905.2197	948.1201
956.5025	968.3961	990.5966
1020.798	1022.63	1166.43
1206.341	1210.323	1324.839
1378.992	1387.898	1418.087
1429.144	1436.271	1456.696
1466.208	1553.672	1688.308
1752.352	2992.696	3025.71

3093.351	3156.449	3176.827
3182.662	3198.52	3201.621
3245.851	3256.395	3261.518

i63 – p90

C	-1.951483	-0.591295	-0.000535
C	-1.857785	0.900058	0.064781
C	-0.454200	1.405431	0.088928
C	0.643141	0.621157	-0.066785
C	2.024510	1.212421	0.064620
C	1.539120	-1.689519	0.080393
C	0.494533	-0.857239	-0.006225
C	-0.877117	-1.377058	-0.026751
H	-2.944627	-1.028879	-0.019715
H	-2.385819	1.342256	-0.793543
H	-2.400338	1.270566	0.945770
H	-0.321158	2.481672	0.153074
H	0.594001	0.657863	-1.962286
H	2.706047	0.816297	-0.690626
H	2.441814	0.977549	1.049009
H	1.989660	2.297062	-0.047037
H	1.385452	-2.761544	0.135575
H	2.563629	-1.340502	0.098955
H	-0.992971	-2.456074	-0.059737

Frequencies

-882.197	88.9677	207.8301
264.087	306.8398	348.3443
397.6477	415.8812	455.0253
478.5698	520.2005	572.3268
610.6723	711.1345	737.442
795.0924	813.0424	835.4868
912.7638	916.3929	964.911
968.9442	1009.488	1011.477
1065.608	1092.002	1173.479
1202.921	1217.186	1308.536
1385.729	1394.505	1417.054
1441.338	1457.796	1470.349
1490.746	1513.463	1633.591
1690.768	1759.764	3005.06
3029.387	3051.728	3122.2
3145.387	3169.178	3176.825
3178.335	3201.869	3257.743

i59 – p89

C	1.945607	0.605740	-0.043523
C	1.880897	-0.795142	-0.094064
C	0.649909	-1.423396	-0.044448
C	-0.540953	-0.696698	0.003725
C	-1.863900	-1.410559	0.065417
C	-0.487091	0.710620	-0.029648
C	0.746685	1.339405	-0.078588
C	-1.755431	1.522292	-0.016323
H	2.388580	0.827305	1.729388
H	2.887228	1.110527	-0.225475
H	2.793361	-1.378149	-0.134759
H	0.602992	-2.507937	-0.051250
H	-2.485266	-1.175419	-0.804981
H	-2.433849	-1.117257	0.952800
H	-1.725580	-2.492394	0.097708
H	0.792095	2.423123	-0.108262
H	-2.415937	1.248252	-0.844679
H	-1.540857	2.589137	-0.094845
H	-2.317111	1.359238	0.909071

Frequencies

-922.567	97.4069	163.3641

181.2285	251.9813	328.8149
343.3888	392.9145	425.3748
452.4356	512.2259	558.6361
594.3974	725.3581	753.645
801.6425	841.2384	879.9568
964.2487	1012.974	1018.896
1045.965	1050.738	1063.508
1074.301	1147.973	1186.776
1212.982	1258.451	1314.475
1327.722	1419.089	1430.018
1471.67	1482.195	1500.392
1505.744	1508.839	1532.101
1620.779	1664.283	3038.481
3046.371	3095.488	3105.561
3138.241	3141.269	3184.667
3190.216	3203.048	3216.304

i59 – p90
```
C     1.960764   -0.759366   -0.063851
C     1.916282    0.733445   -0.000903
C     0.771467    1.410269    0.071188
C    -0.539112    0.754274    0.097645
C    -1.664928    1.486790    0.169376
C    -0.547330   -0.721225    0.031279
C     0.606592   -1.394040   -0.041769
C    -1.868930   -1.435940    0.044386
H     2.500632   -1.075642   -0.967714
H     2.563756   -1.147455    0.769435
H     2.863210    1.263991   -0.016457
H     0.780742    2.495207    0.114621
H    -1.617091    2.568320    0.229472
H    -2.648596    1.037509    0.212698
H    -2.186513    1.747123   -2.237777
H     0.581169   -2.479635   -0.091939
H    -2.424393   -1.218882    0.962286
H    -1.727750   -2.515761   -0.021914
H    -2.493993   -1.120024   -0.796820
```

Frequencies

-305.656	81.506	100.2686
145.9496	200.5688	252.7962
317.1345	349.5888	410.8423
425.0422	490.5259	571.1206
609.4146	723.5827	735.6721
801.056	835.8363	842.8175
906.0866	918.131	971.9805
972.4758	1013.943	1017.422
1071.606	1090.68	1177.762
1197.571	1217.568	1303.928
1382.203	1394.295	1421.352
1446.569	1458.792	1468.417
1485.177	1506.831	1661.587
1716.693	1767.401	3013.519
3031.03	3042.251	3103.247
3139.228	3171.263	3171.633
3178.205	3201.177	3264.5

SUPPORTING INFORMATION

i58 – p91

C	-1.748586	-1.015073	-0.124387
C	-2.041530	0.284750	-0.037332
C	-0.973901	1.275239	0.317540
C	0.427898	0.814544	-0.036084
C	1.437737	1.717834	-0.120629
C	2.086598	-1.144619	0.090647
C	0.673621	-0.642561	0.054580
C	-0.378645	-1.481730	0.039692
H	-2.522938	-1.746225	-0.328404
H	-3.059438	0.640636	-0.152613
H	-1.172555	2.251829	-0.128209
H	-1.004253	1.421610	1.409024
H	-0.005591	0.751094	-1.913793
H	2.471594	1.417982	-0.234142
H	1.228185	2.781491	-0.130243
H	2.613738	-0.887248	-0.834266
H	2.110757	-2.229758	0.201168
H	2.646316	-0.699437	0.919153
H	-0.204965	-2.552281	0.088166

Frequencies

-852.6	115.2765	189.6519
240.8575	337.5072	342.9298
397.2302	423.2048	477.582
482.3932	510.5467	525.7552
589.7565	666.9608	725.4236
739.8048	827.6523	867.22
895.931	936.1205	960.9433
991.8483	1001.857	1023.427
1069.943	1088.596	1170.702
1195.638	1223.015	1306.61
1338.825	1395.372	1418.825
1438.976	1446.099	1466.199
1487.837	1502.69	1596.877
1668.015	1734.562	2995.926
3040.772	3100.908	3108.363
3139.643	3169.29	3183.451
3194.091	3213.208	3264.736

i44 – p1

C	2.571276	-0.988934	0.057746
C	1.251869	-0.267261	-0.006475
C	0.047639	-0.973064	-0.019363
C	-1.182711	-0.331769	-0.054609
C	-1.206299	1.076774	-0.031085
C	-0.001768	1.794717	-0.090875
C	1.208427	1.129110	-0.056436
C	-2.472451	-1.101413	-0.046174
H	2.450437	-2.057262	-0.131526
H	3.028190	-0.874488	1.045703
H	3.276482	-0.590467	-0.676473
H	0.074782	-2.059372	-0.010249
H	-1.651154	1.278065	1.781992
H	-2.146099	1.593434	-0.195778
H	-0.027712	2.877331	-0.139435
H	2.136630	1.691430	-0.079720
H	-2.303894	-2.168385	-0.202153
H	-2.980732	-0.973949	0.915751
H	-3.152826	-0.745295	-0.824489

Frequencies

-813.404	130.2682	146.1397
192.1847	210.2601	281.8157
339.1612	375.3894	417.5071
459.0084	523.5133	544.3855
563.8394	723.1647	740.1261

810.679	896.5279	932.4744
961.7882	1005.676	1018.746
1027.746	1038.664	1071.678
1073.983	1122.841	1188.085
1199.543	1286.895	1313.801
1348.486	1425.873	1427.933
1463.881	1495.778	1498.296
1498.994	1520.146	1530.435
1631.7	1669.819	3042.011
3043.34	3106.603	3106.818
3135.89	3138.341	3178.488
3183.47	3189.62	3213.181

i44 – i32

```
C    2.554331   -1.023593   -0.022257
C    1.229715   -0.322594    0.012474
C    0.051566   -0.987909    0.076594
C   -1.231111   -0.333792    0.144937
C   -1.209876    1.180504    0.071905
C    0.056966    1.833636   -0.066084
C    1.222548    1.144571   -0.060067
C   -2.510978   -1.053462   -0.154580
H    2.436936   -2.108498    0.013996
H    3.180873   -0.719836    0.824492
H    3.106856   -0.768442   -0.933763
H    0.051573   -2.075480    0.074332
H   -1.292408    0.498095    1.153870
H   -2.142588    1.695437   -0.117411
H    0.064742    2.913466   -0.174335
H    2.169241    1.665883   -0.147544
H   -2.485000   -2.079817    0.220424
H   -3.369053   -0.553240    0.304724
H   -2.700135   -1.091736   -1.236315
```

Frequencies

-2649.02	135.388	139.0415
180.0321	193.1311	265.5705
373.0116	389.6796	418.454
472.5566	537.1573	609.9229
687.2009	703.8616	764.8061
839.5881	875.3774	961.7865
972.493	977.6797	1031.792
1052.018	1061.235	1072.368
1137.486	1183.212	1210.635
1268.646	1295.083	1333.81
1398.886	1420.017	1426.279
1456.139	1477.724	1484.802
1497.176	1501.538	1592.285
1642.022	2200.072	3005.927
3024.949	3078.188	3078.497
3119.904	3130.043	3169.692
3184.537	3205.102	3221.885

i44 – p48

```
C    2.580437   -0.932217   -0.000739
C    1.221315   -0.297129   -0.014546
C    0.089982   -1.008290   -0.160159
C   -1.232480   -0.393495   -0.134161
C   -1.294781    1.116003   -0.244546
C   -0.009805    1.814178    0.092471
C    1.146343    1.156801    0.176980
```

```
C    -2.345851   -1.134222   -0.030850
H     2.520739   -2.011307   -0.151367
H     3.084172   -0.744924    0.953545
H     3.214765   -0.509019   -0.786690
H     0.136937   -2.089741   -0.252854
H    -2.112086    1.504569    0.370345
H    -1.554660    1.379088   -1.280852
H    -0.044235    2.890442    0.227168
H     2.067756    1.689765    0.391330
H    -2.615419   -1.141448    2.437501
H    -3.330146   -0.679699   -0.003505
H    -2.298772   -2.217504   -0.011331
```

Frequencies

-285.166	55.5996	95.5616
131.1956	171.9012	209.3735
294.0776	305.719	424.7324
458.3531	526.7927	547.3947
555.6475	700.6811	711.5805
763.4032	866.4372	884.6174
895.9389	941.2144	955.851
975.5056	1013.077	1026.281
1051.983	1072.072	1194.169
1206.672	1230.22	1318.415
1349.019	1373.51	1418.757
1446.219	1446.598	1457.528
1489.135	1498.158	1672.73
1679.165	1752.193	3002.854
3039.746	3086.233	3098.748
3140.4	3157.851	3176.172
3177.563	3201.572	3247.522

i44 – p46
```
C     2.439600   -1.011851    0.176390
C     1.284075   -0.328040    0.110320
C    -0.014306   -1.001846    0.084340
C    -1.177297   -0.347736    0.007889
C    -1.226806    1.154310   -0.055406
C     0.115367    1.816683   -0.024655
C     1.257586    1.134851    0.049906
C    -2.500402   -1.052466   -0.025136
H     2.923395   -1.366514   -2.224589
H     2.451525   -2.094119    0.240251
H     3.395397   -0.501584    0.211146
H    -0.009283   -2.087858    0.127918
H    -1.844026    1.530367    0.773726
H    -1.768210    1.459685   -0.962901
H     0.132601    2.901429   -0.068542
H     2.209556    1.656192    0.067077
H    -2.381730   -2.134921    0.046011
H    -3.139056   -0.720881    0.800998
H    -3.037066   -0.825225   -0.952987
```

Frequencies

-289.866	94.8668	113.8081
129.308	149.949	208.9093
294.1842	341.5081	420.3231
443.5712	487.6937	538.146
589.8688	710.6859	716.0306
801.0208	882.3129	885.405
905.4548	931.1049	952.4072
974.445	1010.542	1017.781
1051.433	1070.194	1179.569

1203.263	1231.298	1319.134
1361.649	1402.113	1423.045
1441.017	1457.92	1465.898
1483.318	1495.794	1664.855
1716.76	1771.165	3007.258
3025.629	3034.867	3091.908
3136.477	3162.004	3175.011
3178.985	3202.096	3252.451

i42 – p46

C	-2.421531	-1.136642	-0.190329
C	-1.300544	-0.401691	0.068038
C	0.035405	-1.021374	0.044487
C	1.166906	-0.316212	-0.000944
C	1.155854	1.188577	-0.009352
C	-0.213447	1.793648	-0.052193
C	-1.328643	1.070497	-0.005321
C	2.518699	-0.963906	-0.043501
H	-2.379897	-2.218084	-0.245780
H	-3.392347	-0.663149	-0.276019
H	-1.474207	-0.451940	1.902168
H	0.072955	-2.107124	0.055779
H	1.747622	1.550173	-0.862179
H	1.692606	1.556487	0.877939
H	-0.274745	2.875434	-0.120452
H	-2.301696	1.549873	-0.032762
H	2.445084	-2.052252	-0.010449
H	3.055814	-0.681939	-0.955804
H	3.132615	-0.634865	0.802251

Frequencies

-1032.25	86.1258	131.5271
199.6325	289.7893	338.9441
389.9388	441.6174	444.2318
472.591	506.2286	550.6103
585.3708	633.2826	711.0316
775.9906	855.6448	875.334
887.1441	927.8453	952.7319
969.5903	1009.442	1016.842
1047.588	1068.539	1176.549
1205.891	1233.377	1317.918
1350.582	1394.25	1416.804
1433.224	1460.431	1462.017
1479.804	1493.786	1578.38
1723.731	1774.213	3006.534
3028.09	3033.831	3090.965
3136.891	3160.131	3178.314
3179.195	3204.384	3257.458

i26 – p58

C	-0.688290	1.600667	-0.078365
C	0.654344	1.391352	-0.125260
C	-3.486956	-1.376847	-0.003892
C	-2.482898	-0.321489	-0.027543
C	-1.655793	0.552277	-0.041052
C	1.295288	0.104113	-0.014028
C	2.623722	-0.064009	-0.043591
C	3.320559	-1.381002	0.064509
H	-0.886039	2.197710	1.872163
H	-1.070158	2.600676	-0.254547
H	1.297897	2.261134	-0.224475
H	-3.255301	-2.116512	0.766534
H	-3.533087	-1.892752	-0.966533
H	-4.476347	-0.963975	0.207029

H	0.645564	-0.761378	0.096878
H	3.258200	0.814332	-0.155550
H	3.918238	-1.580765	-0.831286
H	2.609242	-2.199769	0.191574
H	4.011939	-1.389076	0.913550

Frequencies

-733.384	60.5379	64.6562
92.4232	133.8134	180.2078
186.5572	210.3493	286.439
307.0579	322.2651	390.2932
428.9263	472.6301	560.625
647.3312	784.636	793.7256
864.9401	952.7709	982.6634
1023.173	1056.045	1059.187
1066.165	1089.111	1139.73
1188.531	1247.315	1299.366
1332.313	1416.712	1419.209
1436.349	1482.018	1483.163
1488.619	1492.053	1595.676
1709.536	2374.927	3038.113
3051.113	3095.84	3122.613
3127	3130.575	3154.677
3171.235	3179.374	3196.844

i26 – p66

C	0.756373	1.745721	0.064527
C	-0.706700	1.392189	0.004240
C	3.334921	-1.465862	-0.028903
C	2.421588	-0.328953	0.003859
C	1.672983	0.608909	0.031307
C	-1.214613	0.160602	-0.055400
C	-2.639925	-0.116529	-0.112435
C	-3.162887	-1.349737	-0.159421
H	0.990924	2.422596	-0.766432
H	0.939815	2.329082	0.975598
H	-1.382395	2.245416	0.013572
H	3.305309	-1.961021	-1.002522
H	3.068296	-2.200867	0.734356
H	4.362552	-1.143677	0.155998
H	-0.539047	-0.692161	-0.062591
H	-3.307666	0.742561	-0.103325
H	-3.449992	-1.882361	2.010875
H	-2.527036	-2.228438	-0.202193
H	-4.231196	-1.509179	-0.239978

Frequencies

-460.324	63.1107	80.283
95.8616	130.5196	175.4787
190.7384	220.1168	230.8339
286.6533	297.8531	399.2311
428.9736	474.424	622.8897
681.8778	768.1662	839.3094
949.8199	960.0107	976.6611
1000.957	1011.981	1051.84
1055.553	1065.349	1174.948
1193.707	1243.214	1288.611
1315.868	1345.541	1375.985
1416.948	1455.435	1463.924
1487.464	1491.29	1662.055

1741.58	2400.118	3033.71
3054.764	3060.205	3127.474
3128.264	3152.782	3159.272
3161.526	3170.901	3252.182

i26 – p71

C	-0.732998	1.875004	-0.143303
C	0.749530	1.712505	0.096430
C	-2.861782	-1.642156	0.069140
C	-2.118002	-0.390034	-0.000960
C	-1.500664	0.636688	-0.063869
C	1.383961	0.557731	0.154680
C	2.037922	-0.507256	0.537246
C	2.717520	-1.528323	-0.325060
H	-1.123854	2.598879	0.581367
H	-0.879896	2.331251	-1.130859
H	1.331177	2.631164	0.123154
H	-2.744993	-2.110199	1.049717
H	-2.505880	-2.346348	-0.686952
H	-3.927900	-1.472639	-0.100809
H	1.038251	0.150064	-1.778050
H	2.079618	-0.673462	1.613122
H	3.781869	-1.590967	-0.079417
H	2.614068	-1.284082	-1.382935
H	2.284617	-2.518619	-0.154164

Frequencies

-700.038	39.01	63.9897
92.7965	134.5883	144.4588
166.6448	214.8182	240.1689
312.3927	352.7889	399.5619
465.9734	535.5596	554.0418
639.747	689.6221	770.8972
875.332	890.6296	955.3649
982.4265	1066.372	1067.674
1068.617	1100.195	1159.551
1191.196	1246.697	1299.443
1363.927	1414.686	1429.624
1456.274	1476.687	1488.162
1492.709	1495.033	1509.297
2025.228	2403.999	3027.018
3044.206	3049.295	3060.783
3106.117	3120.116	3123.491
3137.8	3153.059	3157.763

i57 – p92

C	-1.435327	-1.244619	0.369550
C	-1.963683	-0.042028	-0.266408
C	-1.146972	0.942171	-0.648255
C	0.332591	0.909254	-0.372023
C	0.639499	1.876364	0.791910
C	2.146608	-0.790545	-0.177242
C	0.848512	-0.480039	-0.038067
C	-0.112950	-1.449534	0.474096
H	-2.133613	-1.991873	0.730137
H	-3.033041	0.034568	-0.429047
H	-1.542312	1.839863	-1.113927
H	0.866590	1.274191	-1.255885
H	1.716328	1.920917	0.972977
H	0.148107	1.533314	1.705933
H	0.279561	2.883893	0.565754
H	2.862285	-0.073420	-0.565448
H	2.180195	-1.625078	-2.452332
H	2.533175	-1.753683	0.137716
H	0.273050	-2.368843	0.902749

Frequencies

-341.02	75.2243	122.1266
148.2039	213.5066	244.9626
269.138	385.1294	398.7726
485.9235	532.36	593.2865
688.6154	713.7967	748.7213
785.5087	849.7743	876.048
917.6896	944.3029	966.6132
1012.139	1014.271	1022.855
1033.637	1085.824	1118.964
1194.527	1215.481	1305.979
1326.215	1347.645	1394.79
1414.941	1441.607	1477.296
1489.165	1503.764	1652.721
1670.78	1737.585	3047.313
3059.93	3129.169	3135.945
3149.576	3179.502	3184.215
3200.822	3213.02	3239.513

i57 – i61

```
C   -1.951552  -0.753869   0.070204
C   -2.012495   0.598437   0.060270
C   -0.830535   1.393942  -0.085371
C    0.521152   0.697067  -0.138237
C    1.736348   1.530313   0.147020
C    1.826098  -1.472434  -0.008867
C    0.508884  -0.749302  -0.046970
C   -0.664181  -1.432893   0.006439
H   -2.855779  -1.343400   0.160760
H   -2.965373   1.106989   0.161243
H   -0.836440   2.463194   0.080643
H   -0.176099   1.108173  -1.155844
H    2.646720   1.090729  -0.265222
H    1.882184   1.662440   1.228222
H    1.630106   2.529582  -0.285559
H    2.436263  -1.225530  -0.883867
H    1.677270  -2.552872   0.012466
H    2.404284  -1.190174   0.876945
H   -0.645446  -2.516699   0.043283
```

Frequencies

-2578.99	129.585	160.3242
211.2737	227.9527	306.1681
320.2891	387.488	485.12
498.4871	544.3036	627.6194
666.9581	715.7621	757.3442
815.6946	829.0173	942.7006
976.0321	977.5816	1040.534
1052.674	1064.576	1089.822
1164.971	1177.858	1187.83
1245.893	1285.944	1339.588
1388.156	1417.766	1431.457
1449.221	1479.743	1489.282
1501.428	1508.19	1602.11
1624.12	2207.358	3002.992
3036.722	3079.658	3095.086
3127.405	3142.058	3187.973

3195.263	3216.683	3224.988

i60 – i65

C	-2.014931	-0.309450	0.161600
C	-1.738274	1.007780	0.226903
C	-0.420278	1.503811	-0.044800
C	0.721708	0.555771	-0.151887
C	2.109791	1.099356	0.011961
C	1.381650	-1.769731	0.263005
C	0.439298	-0.860036	-0.051202
C	-0.991392	-1.295986	-0.326836
H	-3.010362	-0.674043	0.389067
H	-2.508541	1.725044	0.487316
H	-0.179176	2.552655	0.073267
H	0.089845	1.103457	-1.178274
H	2.836763	0.540337	-0.581585
H	2.415656	1.040943	1.063720
H	2.159523	2.148820	-0.288264
H	1.133867	-2.822151	0.340955
H	2.410573	-1.494078	0.461055
H	-1.113232	-1.428666	-1.414353
H	-1.160352	-2.281414	0.114635

Frequencies

-1847.83	112.2591	163.6331
206.6018	287.6738	340.2404
411.8862	484.8128	490.6468
504.0791	583.2446	676.1754
702.0131	720.3827	787.7469
826.0289	859.2834	928.0052
957.3779	961.068	984.0233
1011.949	1044.993	1090.985
1157.575	1179.944	1217.175
1243.414	1267.392	1343.418
1378.155	1404.516	1418.43
1447.007	1461.807	1483.867
1487.636	1510.248	1627.216
1641.817	2113.394	2971.442
3027.813	3086.92	3099.891
3130.867	3164.66	3192.779
3210.375	3224.647	3250.574

i63 – i66

C	-1.914720	-0.656664	-0.021367
C	-1.899005	0.830060	0.206471
C	-0.560077	1.436853	-0.080164
C	0.677386	0.600992	-0.150114
C	2.000326	1.282946	0.051455
C	1.601745	-1.677155	0.132552
C	0.552750	-0.845151	-0.038899
C	-0.811175	-1.396468	-0.121182
H	-2.887174	-1.137467	-0.065696
H	-2.680453	1.308821	-0.394784
H	-2.181570	1.022986	1.255883
H	-0.417434	2.506250	0.011207
H	0.081492	0.991192	-1.192061
H	2.798389	0.801297	-0.517924
H	2.281387	1.263694	1.111495
H	1.950324	2.329226	-0.260081
H	1.448719	-2.748436	0.192710
H	2.618260	-1.318336	0.233118
H	-0.895327	-2.471704	-0.246379

Frequencies

-1937.58	95.5769	152.805
178.6183	276.5919	344.0032
371.8422	413.2542	479.1491

515.9629	606.8483	620.5796
683.6586	713.1391	783.4806
822.2699	853.4916	904.5774
938.4088	973.9034	1002.193
1018.289	1035.933	1084.721
1152.514	1192.806	1207.877
1249.723	1263.362	1358.834
1375.217	1410.277	1418.924
1444.46	1461.387	1477.799
1489.19	1508.708	1633.282
1743.941	2206.18	2950.614
3024.768	3048.532	3098.407
3127.753	3169.196	3174.699
3197.315	3211.888	3258.601

i22 – p12a
```
C    0.011388   2.462021  -0.148999
C    0.207816   0.977399   0.062630
C   -0.983568   0.179304   0.037677
C   -2.005183  -0.454273  -0.005594
C   -3.238420  -1.228610  -0.046040
C    1.443451   0.404550  -0.025184
C    2.939973  -1.534276  -0.054645
C    1.709469  -1.013547   0.001967
H   -0.760331   2.855388   0.513811
H   -0.308801   2.643381  -1.179937
H    0.939978   3.006791   0.029387
H    0.247240   1.153940   2.043616
H   -3.177313  -2.019466  -0.797768
H   -3.432905  -1.695584   0.922905
H   -4.089896  -0.589701  -0.291967
H    2.302277   1.068725  -0.083534
H    3.819876  -0.901547  -0.122978
H    3.102427  -2.605253  -0.035893
H    0.847888  -1.672086   0.071490
```

Frequencies

-842.787	38.2006	79.2918
114.4109	153.5891	201.3979
202.797	217.705	301.8623
343.7145	395.9521	396.4519
442.8788	470.2454	582.9638
626.8769	677.3833	684.9146
895.0792	946.3382	952.5153
1040.087	1042.021	1053.789
1058.116	1060.476	1065.004
1186.103	1249.569	1327.978
1378.273	1417.038	1420.165
1455.131	1483.343	1483.704
1484.475	1499.963	1594.629
1679.121	2371.09	3047.065
3047.499	3119.5	3121.689
3123.429	3149.118	3149.434
3166.334	3178.814	3245.029

i22 – p51
```
C    0.132824   2.188725   0.002906
C    0.169382   0.684100   0.322080
C   -1.163771   0.083264   0.200673
```

```
C   -2.257534   -0.397891    0.081512
C   -3.584799   -0.986070   -0.058751
C    1.140719   -0.033920   -0.591718
C    3.220115   -1.376920    0.219371
C    2.269543   -0.573280   -0.175784
H   -0.562927    2.702288    0.669403
H   -0.195440    2.352605   -1.026533
H    1.128671    2.620463    0.126105
H    0.516223    0.553142    1.351947
H   -3.808663   -1.190372   -1.108651
H   -3.654613   -1.927221    0.492022
H   -4.352112   -0.309384    0.325313
H    0.925071   -0.007584   -1.657522
H    2.999504   -2.427705    0.381040
H    4.231271   -1.033926    0.397483
H    3.214145    1.139641    0.047656
```

Frequencies

-755.859	45.5504	92.7904
109.601	113.7112	143.4732
201.7214	257.3249	295.2384
302.938	354.919	404.2594
485.2115	521.0052	529.1748
551.378	671.3943	767.2522
871.3403	904.7654	919.6897
1015.993	1021.358	1058.791
1064.86	1090.617	1099.452
1152.516	1195.636	1271.174
1336.931	1386.05	1411.412
1421.858	1476.411	1488.709
1490.904	1497.058	1503.09
2009.099	2392.801	3051.129
3052.827	3074.526	3122.825
3125.708	3135.66	3143.339
3154.145	3164.649	3248.086

i22 – p11a
```
C   -0.047722    2.490482    0.787739
C   -0.199351    0.777410   -0.828285
C    1.005293    0.108844   -0.446203
C    2.025745   -0.447077   -0.134019
C    3.261773   -1.123572    0.238242
C   -1.446434    0.241039   -0.631559
C   -2.956001   -1.398273    0.394095
C   -1.723226   -0.920285    0.169449
H    0.925107    2.884149    0.518737
H   -0.101771    1.854470    1.661793
H   -0.916377    3.095386    0.557181
H   -0.089542    1.574032   -1.555541
H    3.070364   -1.899833    0.983120
H    3.723792   -1.596694   -0.632107
H    3.980751   -0.417446    0.661371
H   -2.294382    0.760518   -1.069371
H   -3.833870   -0.918324   -0.028098
H   -3.119015   -2.281027    1.000584
H   -0.865522   -1.426640    0.605581
```

Frequencies

-459.116	31.1864	75.7164
89.3454	96.8847	107.7155
159.1556	210.362	238.2858
331.3089	343.7246	445.2314
477.7449	488.4891	520.9179
647.619	663.3789	765.9889
808.497	840.6676	922.3735

943.0231	948.6316	1040.763
1054.799	1058.685	1120.656
1194.561	1252.336	1320.568
1393.024	1414.744	1418.869
1419.098	1469.533	1483.781
1485.35	1529.146	1649.165
2372.078	3046.018	3099.043
3117.188	3121.368	3147.94
3166.41	3172.785	3191.933
3243.904	3268.07	3275.615

i25 – i24

```
C   -0.655416   1.762053  -0.398259
C    0.090969   0.746163   0.416683
C   -3.597064  -0.993537  -0.119000
C   -2.240815  -0.556824   0.191163
C   -1.218008   0.132435   0.247817
C    1.252824   0.055905  -0.218476
C    2.419103  -0.145055   0.381960
C    3.597296  -0.828850  -0.240286
H   -1.137390   2.596405   0.090759
H   -0.545874   1.763917  -1.474251
H    0.298392   1.059502   1.440819
H   -4.133947  -0.242010  -0.710811
H   -4.167587  -1.174124   0.796054
H   -3.584800  -1.926635  -0.688754
H    1.095879  -0.291862  -1.238518
H    2.547976   0.204715   1.405525
H    4.467482  -0.165137  -0.265178
H    3.380208  -1.145971  -1.262813
H    3.886320  -1.712540   0.337550
```

Frequencies

-700.876	55.3394	70.7605
93.8991	131.3711	172.325
204.5231	222.3892	302.7348
357.0691	411.8085	442.7523
462.4775	631.1452	678.2832
741.46	844.5476	893.1707
962.4513	1005.797	1033.048
1056.463	1073.726	1075.431
1100.003	1157.017	1204.153
1215.957	1277.789	1338.779
1388.144	1413.39	1421.518
1444.449	1478.64	1479.544
1485.102	1498.477	1774.592
2095.793	3016.668	3035.504
3088.344	3095.993	3101.81
3113.229	3122.094	3143.788
3148.58	3167.433	3290.284

i25 – i26

```
C   -0.962762   1.916603  -0.205328
C    0.019825   1.022477   0.497868
C   -2.512248  -1.838029   0.046787
C   -2.284985  -0.412378  -0.192833
C   -1.560564   0.602529  -0.122400
C    1.146091   0.424759  -0.176312
C    2.138061  -0.245182   0.430167
C    3.300188  -0.869817  -0.275536
H   -1.420391   2.700877   0.393704
H   -0.677810   2.256745  -1.199901
```

```
H    0.009527    1.034872    1.581838
H   -3.341001   -1.990209    0.743452
H   -1.617631   -2.314679    0.467947
H   -2.765464   -2.354858   -0.882838
H    1.166562    0.523067   -1.261955
H    2.111471   -0.347808    1.513951
H    4.249389   -0.446682    0.070886
H    3.236735   -0.719336   -1.356044
H    3.346972   -1.947760   -0.085516
```

Frequencies

-701.11	54.6974	94.5143
121.4832	143.4689	168.4809
204.0315	220.5273	294.7982
377.387	438.2329	464.2463
472.0977	705.7474	787.2157
834.6956	905.7316	964.1279
988.679	1021.363	1036.351
1058.58	1061.39	1076.946
1124.287	1166.714	1204.992
1216.75	1287.194	1326.995
1400.986	1411.594	1422.974
1466.799	1477.254	1480.043
1484.682	1499.935	1680.433
2023.66	3016.697	3031.102
3086.175	3093.835	3099.914
3119.087	3121.157	3137.907
3151.468	3174.465	3201.897

i21 – i20
```
C   -0.200508    2.479859   -0.122719
C    0.182483    1.181716    0.508042
C   -0.578096   -0.340575   -0.185881
C   -1.692570   -0.873460   -0.203070
C   -3.113210   -1.093619    0.045532
C    0.813072    0.076603   -0.293727
C    2.994501   -1.121553   -0.172439
C    1.836529   -0.780276    0.375020
H   -1.018522    2.962473    0.417774
H   -0.525699    2.331299   -1.156544
H    0.645262    3.181293   -0.140070
H    0.269833    1.112493    1.586196
H   -3.543459   -0.295343    0.662988
H   -3.670889   -1.132013   -0.894178
H   -3.275209   -2.043985    0.561422
H    1.109190    0.373716   -1.302029
H    3.267326   -0.797354   -1.172289
H    3.709543   -1.739863    0.357938
H    1.579408   -1.124893    1.374252
```

Frequencies

-691.94	68.2826	72.4299
93.1778	113.4864	148.1398
169.9794	232.5035	273.5478
355.167	405.1755	420.0963
509.5641	633.8991	705.2862
803.904	892.3163	957.819
965.3427	1026.958	1032.562
1037.66	1056.512	1075.041
1123.751	1171.898	1195.485
1217.173	1290.153	1333.524
1392.315	1412.502	1422.629

1466.405	1478.554	1479.95
1484.882	1495.764	1738.823
2094.605	3003.027	3014.624
3079.021	3086.806	3089.562
3112.092	3117.705	3145.65
3163.716	3194.782	3237.916

i22 – i21

C	-0.209450	2.656187	0.301885
C	-0.283081	1.330579	-0.429182
C	0.783071	0.367936	-0.240835
C	1.861866	-0.260113	-0.195499
C	2.647445	-1.443077	0.155537
C	-0.865223	0.142498	0.288462
C	-2.282633	-1.877777	0.231774
C	-1.607395	-0.896069	-0.382621
H	0.495642	3.328017	-0.192437
H	0.128460	2.508709	1.330344
H	-1.192533	3.133447	0.323463
H	-0.618244	1.423640	-1.463309
H	3.422584	-1.194804	0.885279
H	2.008863	-2.225936	0.584406
H	3.144832	-1.857017	-0.725671
H	-0.925340	0.208937	1.370202
H	-2.321038	-1.947095	1.314495
H	-2.819226	-2.630462	-0.332739
H	-1.591601	-0.868421	-1.471164

Frequencies

-677.938	64.3133	114.7092
121.1741	140.812	183.2409
187.8126	225.2432	273.6728
389.5294	411.9428	462.9856
524.7569	674.8537	697.3104
848.8798	885.4552	891.8357
972.0638	1011.092	1022.244
1029.713	1057.559	1102.946
1108.608	1168.607	1216.348
1228.119	1295.331	1326.205
1399.461	1407.947	1423.533
1469.1	1476.075	1482.235
1488.833	1504.753	1647.155
2017.117	3018.006	3054.919
3095.505	3105.709	3120.708
3135.952	3140.167	3149.832
3159.008	3182.929	3248.809

i25 – p80

C	-0.808367	1.748552	-0.348654
C	0.090721	0.806825	0.451531
C	-3.187760	-1.352078	0.068501
C	-2.216387	-0.464691	0.082601
C	-1.298631	0.428147	0.078612
C	1.228140	0.128533	-0.206629
C	2.372731	-0.172503	0.397579
C	3.531034	-0.860652	-0.255781
H	-1.198166	2.624717	0.158432
H	-0.582460	1.885979	-1.401678
H	0.242289	1.073110	1.494361
H	-4.725452	-0.432231	-0.997665
H	-3.887345	-1.423248	0.894201
H	-3.216902	-2.131596	-0.684973
H	1.083450	-0.135335	-1.253784
H	2.495200	0.091646	1.447155
H	4.431197	-0.238877	-0.215074
H	3.320808	-1.088042	-1.303437

H   3.768503   -1.798911   0.255902

Frequencies

-535.825	55.7384	97.247
154.044	165.3685	202.409
211.9318	232.9843	284.4196
349.5621	403.0078	439.0292
472.3919	585.9455	654.7479
695.7424	825.3926	878.6398
901.0098	938.9723	953.3081
986.6819	1003.502	1027.891
1039.024	1059.94	1073.933
1106.938	1123.276	1198.095
1274.718	1337.326	1344.174
1401.678	1423.34	1461.261
1484.478	1498.556	1531.624
1770.056	2103.357	3034.501
3094.662	3120.71	3124.874
3140.908	3145.46	3146.852
3153.094	3216.857	3232.961

i21 – p57

```
C   -0.259929    2.514033   -0.166706
C    0.054582    1.181932    0.470783
C   -0.616286   -0.043791    0.004421
C   -1.669517   -0.766663   -0.082053
C   -2.778825   -1.471484   -0.146266
C    0.831436    0.118899   -0.308450
C    2.932774   -1.197033   -0.184529
C    1.822314   -0.736147    0.378184
H   -1.145826    2.960981    0.290690
H   -0.458354    2.394394   -1.234622
H    0.577289    3.206745   -0.046041
H    0.270151    1.213856    1.536844
H   -3.432369   -1.401427   -1.008879
H   -2.984321   -2.250491    0.579756
H   -4.192449   -0.316682    0.868964
H    1.063123    0.371750   -1.340890
H    3.182953   -0.969063   -1.216193
H    3.627708   -1.819530    0.366550
H    1.592800   -0.989016    1.411520
```

Frequencies

-532.061	70.063	101.6295
135.9221	186.5264	203.7211
216.9787	233.923	291.0935
337.4394	396.2953	424.8611
487.6786	586.9315	637.5285
687.5167	757.81	849.3569
885.3485	900.4299	948.8351
1004.596	1019.351	1029.159
1043.608	1047.332	1101.115
1127.104	1148.173	1205.904
1291.643	1314.728	1337.877
1412.539	1423.162	1463.994
1493.085	1501.4	1536.081
1733.729	2100.148	3045.364
3122.007	3124.159	3137.283

3143.254	3147.543	3148.037
3159.408	3233.744	3241.38

i63 – i64

C	1.105246	1.417276	0.365270
C	1.891791	0.355215	-0.344373
C	1.139572	-0.942932	-0.536873
C	-0.387725	-0.974061	-0.353402
C	-0.255257	-1.815086	0.924977
C	-2.350504	0.551055	-0.408930
C	-1.057934	0.358302	-0.137388
C	-0.227011	1.425437	0.430407
H	1.665157	2.247749	0.784844
H	2.180427	0.758028	-1.327385
H	2.837400	0.172869	0.177065
H	1.517522	-1.594618	-1.323135
H	-0.893501	-1.517890	-1.152580
H	-0.424303	-1.292607	1.864302
H	1.103516	-1.711535	0.605071
H	-0.601113	-2.845999	0.891634
H	-2.832530	1.502529	-0.209984
H	-2.962275	-0.234921	-0.838979
H	-0.739373	2.265158	0.891009

Frequencies

-2133.45	72.7119	89.8653
230.0865	347.3123	359.4505
383.3599	486.4488	514.5417
615.3928	630.2951	712.4955
744.4671	760.1385	823.8544
873.2638	895.8865	924.7138
939.6483	957.258	984.1451
993.3272	1023.289	1051.707
1072.265	1126.85	1193.341
1222.346	1247.587	1305.307
1322.826	1345.659	1365.214
1374.104	1423.073	1426.966
1468.096	1474.564	1697.935
1747.844	1832.969	2997.278
3066.295	3097.106	3106.511
3145.049	3153.082	3170.068
3194.572	3217.584	3241.159

i44 – i42

C	2.546173	-1.093085	0.131794
C	1.286540	-0.331332	-0.099767
C	-0.008563	-1.004834	-0.049101
C	-1.174022	-0.345796	-0.007476
C	-1.228092	1.160885	-0.009704
C	0.121986	1.814321	0.040808
C	1.266025	1.123504	-0.000261
C	-2.496654	-1.049374	0.044635
H	2.504151	-2.166560	0.247800
H	3.469750	-0.557042	0.297229
H	1.960018	-0.704650	-1.075227
H	-0.008514	-2.092182	-0.041695
H	-1.844032	1.504154	0.835480
H	-1.776064	1.500878	-0.903385
H	0.149572	2.896678	0.115388
H	2.218290	1.644069	0.043768
H	-2.379895	-2.134769	0.028193
H	-3.047930	-0.777152	0.952197
H	-3.125705	-0.759155	-0.805317

Frequencies

-1901.63	94.6846	157.5561
208.965	272.435	325.7562

389.7556	394.3652	445.6912
480.5318	515.5395	535.3167
599.9757	695.331	760.0535
864.4184	874.7863	924.9794
954.0732	963.7108	991.5061
1001.541	1037.806	1068.51
1147.336	1164.272	1202.68
1230.428	1266.938	1331.045
1353.33	1418.105	1426.802
1432.429	1449.497	1473.732
1481.767	1498.085	1676.316
1747.826	2214.912	2975.978
2995.256	3022.161	3076.085
3126.365	3160.201	3167.561
3175.074	3191.316	3299.586

i61 – p89

```
C     1.917690  -0.789016  -0.029208
C     1.971248   0.589043  -0.086818
C     0.778131   1.330545  -0.039689
C    -0.471931   0.681226  -0.059672
C    -1.735262   1.495017  -0.068191
C    -1.833217  -1.441287   0.030123
C    -0.514027  -0.715272   0.003073
C     0.682919  -1.431336   0.028750
H     2.831206  -1.372742  -0.036919
H     2.922493   1.105512  -0.136376
H     0.812999   2.399097  -0.225889
H     0.769378   1.838126   1.735994
H    -2.267151   1.396376   0.884630
H    -2.421125   1.168295  -0.855173
H    -1.522113   2.554102  -0.221106
H    -2.461444  -1.097822   0.857542
H    -1.687144  -2.516810   0.141532
H    -2.397019  -1.272653  -0.893052
H     0.646616  -2.515006   0.078625
```

Frequencies

-875.241	133.9551	170.2394
176.7251	249.2751	306.1203
319.4907	391.037	428.3219
507.6452	518.9267	528.3246
591.8561	731.2204	757.0609
777.0609	840.7193	903.6292
986.8827	1011.346	1016.806
1024.164	1058.725	1076.477
1080.768	1146.164	1190.155
1212.88	1248.932	1311.154
1326.048	1420.027	1429.409
1467.88	1486.642	1503.329
1503.946	1506.322	1535.776
1639.095	1652.832	3042.019
3045.498	3102.054	3106.267
3137.915	3140.503	3183.328
3187.79	3201.423	3219.364

i61 – p91

```
C    -1.873760  -0.881211  -0.073711
```

```
C   -2.049256   0.439722   -0.031669
C   -0.886577   1.363687    0.176087
C    0.471710   0.748018   -0.093559
C    1.525828   1.526303   -0.378554
C    1.943440  -1.348625    0.054840
C    0.582273  -0.716180    0.020645
C   -0.539572  -1.460776    0.033637
H   -2.720002  -1.550406   -0.183716
H   -3.040430   0.876090   -0.094163
H   -0.907119   1.687593    1.228708
H   -1.007185   2.277589   -0.412271
H    2.519858   1.123444   -0.526168
H    2.257006   2.035289    1.971542
H    1.410168   2.597643   -0.502210
H    2.477142  -1.183372   -0.886851
H    1.866538  -2.425431    0.212847
H    2.556620  -0.922180    0.854747
H   -0.457110  -2.541899    0.091234
```

Frequencies

-291.42	60.6646	98.5363
136.5172	178.9797	255.6071
320.6706	346.4931	422.0123
477.1714	497.1547	526.3931
599.5422	707.1316	721.8685
775.8809	833.0751	897.6493
918.1677	939.3839	957.4924
988.3545	1004.672	1023.237
1072.418	1090.937	1170.212
1195.856	1224.383	1302.999
1345.457	1401.655	1422
1439.192	1445.457	1454.569
1492.274	1510.261	1670.974
1678.899	1740.919	2991.085
3044.205	3090.434	3104.668
3140.747	3163.197	3179.58
3189.79	3212.92	3251.578

i58 – i61

```
C    1.847176  -0.899921    0.100222
C    2.033868   0.426820    0.052119
C    0.886233   1.353093   -0.226163
C   -0.458655   0.729789    0.075447
C   -1.618187   1.651856    0.071000
C   -1.968273  -1.306747   -0.069958
C   -0.593666  -0.706686   -0.031256
C    0.529215  -1.480758   -0.029440
H    2.692411  -1.563830    0.249207
H    3.025743   0.855020    0.147974
H    0.895164   1.643038   -1.292932
H    0.997875   2.293052    0.326007
H   -2.630982   1.276332    0.065748
H   -1.435976   2.715056    0.003433
H   -0.925776   1.113508    1.161915
H   -2.539858  -1.054037    0.831309
H   -1.918772  -2.394178   -0.141089
H   -2.538607  -0.928653   -0.925705
H    0.432514  -2.559980   -0.077686
```

Frequencies

-1886	110.2806	182.7969
229.0476	307.3228	312.1633
391.4825	422.5516	477.5337
499.7301	535.9729	558.5266
626.1857	715.2539	724.9999
807.2525	831.9661	925.8088

953.9181	986.7969	994.4701
1006.88	1056.427	1083.248
1163.806	1170.543	1195.641
1235.455	1258.851	1304.709
1364.547	1415.275	1427.657
1439.626	1456.351	1481.05
1485.505	1503.106	1580.299
1697.482	2219.586	2932.001
3026.924	3056.321	3082.433
3138.074	3180.661	3186.539
3192.01	3208.552	3306.054

i65 – p94
```
C    1.892781   0.500765   0.232669
C    1.804002  -0.736786  -0.239263
C    0.501192  -1.427180  -0.535388
C   -0.703260  -0.654870  -0.052156
C   -1.805038  -1.267017   0.402457
C   -1.521216   1.603045  -0.593810
C   -0.577876   0.819799  -0.074370
C    0.698900   1.369785   0.519125
H    2.869724   0.929581   0.435334
H    2.710027  -1.303993  -0.431454
H    0.501186  -2.428451  -0.093194
H    0.416621  -1.574175  -1.621360
H   -1.900111  -2.347608   0.376767
H   -2.665079  -0.697855   0.736051
H   -1.288242  -1.533316   2.525502
H   -1.413352   2.682929  -0.605378
H   -2.419856   1.185313  -1.033737
H    0.875087   2.383875   0.148236
H    0.577086   1.458453   1.607644
```

Frequencies

-436.69	90.6785	100.0636
164.2462	204.4834	303.2061
327.3354	387.1232	429.5378
477.8041	556.745	614.8632
665.9761	725.0617	735.2061
807.8369	845.2916	924.7283
937.3654	943.2813	947.2653
977.2686	982.2623	996.6657
1026.528	1038.503	1198.065
1204.553	1228.791	1249.13
1335.063	1350.204	1360.593
1420.481	1444.889	1460.116
1472.406	1476.791	1678.954
1727.71	1760.528	3018.246
3019.307	3082.571	3086.141
3153.245	3154.456	3169.248
3193.037	3243.862	3247.162

i65 – p91
```
C    2.031177   0.333674  -0.107281
C    1.739692  -0.958497  -0.249295
C    0.367446  -1.434640  -0.083736
C   -0.690374  -0.586521  -0.007993
C   -2.097601  -1.103666   0.019465
C   -1.425904   1.754219  -0.182394
C   -0.446616   0.861614   0.008527
C    0.971301   1.317256   0.291129
H    3.048131   0.694054  -0.219181
```

```
H     2.509934   -1.682941   -0.488007
H     0.423514   -1.956228    2.001867
H     0.182727   -2.499113   -0.183682
H    -2.641601   -0.811740   -0.884788
H    -2.647086   -0.699224    0.874950
H    -2.110348   -2.192583    0.085124
H    -1.215606    2.818253   -0.202979
H    -2.458849    1.459663   -0.321595
H     1.149755    2.292600   -0.169171
H     1.064700    1.476621    1.376936
```

Frequencies

-528.051	84.9352	162.0033
192.1585	236.0055	258.4387
345.5232	348.4012	426.9111
489.78	499.3102	521.4254
602.5372	703.8086	724.4145
758.3789	832.0498	911.0075
919.275	943.8715	964.9204
984.2217	1006.984	1022.335
1062.773	1085.81	1173.268
1197.271	1232.449	1305.061
1351.897	1399.335	1417.883
1433.531	1455.782	1466.582
1482.793	1501.13	1622.318
1685.459	1729.115	2994.564
3043.084	3089.166	3104.362
3141.877	3166.463	3188.375
3195.608	3216.827	3255.892

i66 – p93
```
C     1.820496    0.776256    0.169077
C     1.872784   -0.724419    0.108102
C     0.611266   -1.303373   -0.544660
C    -0.627734   -0.665112    0.025763
C    -1.625185   -1.377404    0.563195
C    -1.753828    1.532884   -0.193439
C    -0.635592    0.816693   -0.031210
C     0.679785    1.463229    0.086112
H     2.759629    1.308369    0.286791
H     2.760013   -1.043972   -0.446908
H     1.985941   -1.126016    1.123475
H     0.573784   -2.388141   -0.423596
H     0.649692   -1.090610   -1.620139
H    -2.472234   -0.899222    1.041262
H    -1.575339   -2.459966    0.608567
H    -2.985657   -1.636802   -1.244209
H    -1.722780    2.617113   -0.213039
H    -2.718438    1.058048   -0.328922
H     0.693443    2.548668    0.119076
```

Frequencies

-373.146	99.9384	150.5166
159.427	215.915	294.2311
346.1682	379.7846	432.1884
480.0022	560.5635	636.774
698.9195	735.0875	772.9096
787.7895	822.6353	880.9626
899.1813	937.9104	945.0298
974.8504	989.8999	1008.289
1049.056	1056.974	1185.013
1196.473	1233.791	1270.897

1339.628	1350.537	1368.669
1419.096	1450.17	1466.993
1484.306	1498.317	1681.539
1696.289	1744.362	3032.341
3042.631	3083.983	3114.119
3157.148	3158.935	3175.232
3197.947	3247.589	3249.468

i66 – p90

```
C    -1.921327   -0.658696    0.000514
C    -1.864959    0.829733   -0.129005
C    -0.470355    1.374403   -0.056825
C     0.643528    0.612860   -0.058235
C     2.005492    1.241916   -0.053270
C     1.600710   -1.666382    0.000752
C     0.531581   -0.855205   -0.004326
C    -0.825756   -1.413051    0.053246
H    -2.902453   -1.121094    0.041638
H    -2.316852    1.131559   -1.085194
H    -2.489804    1.298297    0.640464
H    -0.384541    1.767781    2.031769
H    -0.366782    2.452395   -0.141694
H     2.593241    0.915964   -0.916965
H     2.561128    0.958648    0.846352
H     1.931252    2.329931   -0.080285
H     1.476383   -2.742714    0.045189
H     2.615887   -1.292396   -0.039684
H    -0.910953   -2.491842    0.141312
```

Frequencies

-483.179	87.1012	179.4866
195.1063	249.3655	326.4438
341.9851	353.5698	417.3765
438.7442	489.9442	569.9656
609.6856	718.232	724.946
796.5573	834.3837	878.1226
908.354	917.6054	966.1606
975.3632	1009.992	1017.689
1063.438	1087.18	1178.762
1204.083	1217.75	1306.983
1382.643	1394.863	1415.621
1445.499	1463.405	1466.293
1479.777	1502.186	1666.751
1676.401	1757.76	3014.663
3041.92	3056.717	3103.471
3141.651	3168.033	3174.956
3176.043	3200.127	3257.754

i62 – p94

```
C    -1.722525   -0.842877    0.250617
C    -1.889937    0.385427   -0.224721
C    -0.749912    1.297778   -0.594717
C     0.558963    0.809805   -0.000675
C     1.260474    1.547309    0.887718
C     1.866724   -1.228869   -0.579142
C     0.768521   -0.666193   -0.088284
C    -0.377188   -1.474532    0.482228
H    -2.591878   -1.444080    0.500628
H    -2.893199    0.772979   -0.375654
H    -0.673990    1.345846   -1.686928
H    -0.953539    2.316797   -0.253085
H     1.607028    1.331213   -1.491145
H     1.028365    2.593622    1.056355
H     2.114821    1.126572    1.405063
H     1.983845   -2.307745   -0.600082
```

```
H     2.674016  -0.627107  -0.981168
H    -0.360902  -2.485381   0.063215
H    -0.225281  -1.589809   1.564666
```

Frequencies

-916.499	90.731	107.606
265.1762	331.1706	386.392
432.0202	466.0749	498.4603
538.6567	572.0273	626.6255
655.3217	697.9304	724.3357
763.5581	847.6608	919.5345
924.253	936.8285	947.0019
971.9985	979.4963	993.4957
1026.028	1036.757	1189.386
1197.138	1229.291	1246.748
1324.691	1345.073	1352.577
1413.509	1439.958	1456.617
1471.99	1479.226	1633.741
1740.875	1757.86	3018.23
3046.231	3085.087	3093.946
3154.006	3154.663	3163.97
3188.74	3245.954	3254.186

i24 – p83

```
C    0.181566   2.060936  -0.190338
C   -0.003767   0.724683   0.001591
C   -3.768356  -0.899359   0.010880
C   -2.434538  -0.313006   0.016281
C   -1.337446   0.177190   0.030272
C    1.096235  -0.253226  -0.235554
C    2.332524  -0.133406   0.236192
C    3.449268  -1.087182  -0.048972
H   -0.645199   2.755052  -0.108254
H    1.172874   2.455246  -0.376497
H    0.113491   0.702890   1.845822
H   -4.463204  -0.280613  -0.562091
H   -4.155431  -0.993798   1.028658
H   -3.750245  -1.895276  -0.438312
H    0.826588  -1.111262  -0.847174
H    2.560540   0.704307   0.893522
H    4.287918  -0.572872  -0.529452
H    3.125438  -1.897763  -0.705421
H    3.834320  -1.525696   0.877091
```

Frequencies

-1084.65	53.0968	81.0607
84.5229	146.3999	179.561
209.0603	222.9421	306.3341
362.1149	395.7056	431.1275
472.5286	494.5317	585.7814
589.9186	675.227	766.4909
828.8732	893.5948	921.0573
987.5423	1005.162	1053.218
1058.238	1074.595	1078.55
1133.717	1271.127	1333.33
1352.095	1413.528	1421.576
1424.814	1483.899	1485.194
1488.151	1499.739	1577.324
1757.073	2384.779	3038.869

3053.244	3097.672	3124.949
3128.681	3129.34	3155.143
3160.557	3170.36	3274.144

i24 – i53

C	0.108783	2.535780	0.156220
C	-0.055385	1.073489	-0.112935
C	3.251369	-1.327183	0.038149
C	2.071993	-0.472106	-0.010022
C	1.098838	0.236307	-0.049441
C	-1.394403	0.478710	-0.060134
C	-1.664931	-0.827451	0.004364
C	-3.045344	-1.403394	0.052308
H	1.101101	2.936021	0.297448
H	-0.770765	3.133896	0.348195
H	0.024098	1.871543	-1.062199
H	3.957641	-0.978455	0.795847
H	3.766567	-1.341193	-0.926119
H	2.972695	-2.354814	0.284839
H	-2.217956	1.191204	-0.080779
H	-0.835574	-1.530784	0.032787
H	-3.210371	-2.101342	-0.775454
H	-3.809022	-0.623703	-0.003360
H	-3.203940	-1.967281	0.977743

Frequencies

-1886.36	70.021	81.1181
110.6754	137.5683	192.8035
195.2386	212.4672	304.1911
346.4242	378.1488	421.9614
446.9638	542.1935	616.3591
642.6813	674.6049	831.0033
916.1869	988.4166	996.7801
1038.999	1053.556	1062.974
1066.439	1131.443	1174.392
1240.461	1335.623	1350.473
1370.804	1418.358	1422.03
1425.426	1483.855	1484.265
1490.234	1500.264	1725.25
2226.032	2356.426	3035.697
3047.59	3093.102	3118.526
3120.554	3121.532	3152.591
3172.206	3181.332	3312.782

i24 – p76'

C	-0.077131	2.175335	0.424417
C	0.370937	1.269573	-0.484235
C	3.504421	-1.258418	0.255916
C	2.385999	-0.361381	-0.006152
C	1.463748	0.382118	-0.211999
C	-1.224097	-0.384813	-0.539528
C	-2.336457	-0.192692	0.124416
C	-3.477618	-1.172740	0.216598
H	-0.817794	2.914824	0.145308
H	0.251697	2.144130	1.455941
H	0.122856	1.409867	-1.531910
H	4.308243	-0.736180	0.780960
H	3.911321	-1.655540	-0.677344
H	3.188971	-2.102760	0.874379
H	-0.831952	-1.203890	-1.129778
H	-2.459457	0.747183	0.665119
H	-3.662682	-1.447350	1.259706
H	-3.270779	-2.084100	-0.347583
H	-4.399244	-0.728079	-0.171394

Frequencies

| -404.233 | 31.308 | 40.2178 |

72.2661	119.1558	137.7181
148.1111	193.8192	211.5912
279.1884	337.5515	416.0307
421.852	545.2494	611.6168
685.5833	724.83	854.5564
882.5898	917.1181	932.2989
975.5019	1043.045	1055.941
1058.969	1063.926	1117.111
1189.708	1283.235	1291.006
1406.578	1417.829	1434.018
1484.576	1485.715	1486.736
1490.239	1571.688	1707.96
2381.503	3037.545	3045.601
3102.395	3110.702	3117.382
3119.918	3134.812	3160.409
3171.786	3222.06	3262.388

i24 – i49

```
C    0.454582    1.729359   -0.444016
C   -0.049105    0.681364    0.481647
C   -3.851959   -0.747509   -0.157085
C   -2.504306   -0.239572    0.072266
C   -1.395616    0.178265    0.266533
C    1.071501   -0.091846   -0.146829
C    2.297788   -0.292929    0.434270
C    3.436201   -0.982733   -0.244574
H    1.175759    2.451709   -0.090878
H    0.017176    1.840035   -1.426324
H    0.139260    0.901209    1.533229
H   -4.591381    0.051466   -0.061682
H   -4.101143   -1.528960    0.565010
H   -3.940915   -1.173080   -1.159700
H    0.831459   -0.581054   -1.085369
H    2.481777    0.126263    1.421192
H    3.126467   -1.415907   -1.198938
H    3.843868   -1.787985    0.375967
H    4.263162   -0.290091   -0.445779
```

Frequencies

-620.909	30.9774	72.6258
101.4861	140.3848	171.4596
225.8155	258.2777	323.3951
332.345	424.5795	504.6534
550.9474	581.65	645.3572
722.0038	750.7462	920.9125
942.6903	989.3868	1034.423
1057.848	1058.625	1066.138
1095.824	1162.239	1186.738
1216.196	1284.795	1303.112
1389.546	1418.624	1420.269
1450.142	1480.214	1485.589
1486.116	1490.789	1553.467
2397.461	3015.954	3047.522
3070.855	3103.934	3115.05
3120.359	3121.045	3152.855
3174.93	3186.562	3300.346

i26 – i51

```
C    -0.783481    1.662131   -0.038894
C     0.692984    1.438284   -0.000726
C    -3.455483   -1.410085   -0.000207
C    -2.500232   -0.310088   -0.014892
C    -1.714987    0.608874   -0.037277
C     1.307708    0.143699    0.036043
C     2.635183   -0.078287   -0.036083
C     3.269091   -1.432773   -0.005395
H    -0.032823    1.716701    1.040871
H    -1.113860    2.666718   -0.270969
H     1.300103    2.313283   -0.204725
H    -4.368186   -1.129627    0.532276
H    -3.029376   -2.283056    0.501289
H    -3.733082   -1.708788   -1.015206
H     0.635195   -0.708141    0.125062
H     3.306305    0.773986   -0.130909
H     3.840998   -1.626516   -0.919748
H     2.518586   -2.220584    0.095811
H     3.971446   -1.524496    0.830832
```

Frequencies

-1899.29	14.8655	60.0113
101.3931	140.9841	175.3859
194.1904	214.2174	280.4855
325.6377	417.1796	432.6248
463.8449	630.4405	632.8219
767.8351	793.9642	865.7521
951.1495	984.5627	1005.223
1050.039	1055.662	1056.231
1122.146	1180.153	1216.658
1254.033	1296.826	1322.923
1394.114	1413.103	1422.915
1433.796	1480.983	1482.163
1486.468	1500.26	1664.446
2158.358	2309.706	3024.263
3038.943	3078.035	3106.561
3115.037	3115.48	3144.307
3152.364	3190.56	3207.861

i20 – p56

```
C     1.935434    2.014396   -0.182456
C     1.082238    1.182570    0.421308
C    -0.983820    0.007076   -0.168418
C    -2.180786    0.043883   -0.083038
C    -3.635449    0.087354    0.008517
C     0.482596   -0.037417   -0.241360
C     1.813571   -2.164504   -0.181543
C     1.013229   -1.295602    0.417093
H     2.324025    2.888177    0.327114
H     2.169683    1.914170   -1.237600
H     3.800473    1.105091    0.130635
H     0.813360    1.334488    1.463629
H    -3.961462    0.927077    0.627116
H    -4.082628    0.202591   -0.981836
H    -4.025035   -0.832525    0.451355
H     0.783981   -0.044323   -1.294664
H     2.130866   -2.028715   -1.211113
H     2.180947   -3.042849    0.336573
H     0.703704   -1.449719    1.448177
```

Frequencies

-555.122	19.5252	58.089
64.1833	107.2126	120.6593
194.2709	274.502	284.0213
288.1595	348.1583	399.7415
437.6573	501.0328	508.4644

672.2954	711.9374	839.7523
924.2463	962.8754	972.5236
978.812	1021.32	1036.452
1058.38	1058.91	1121.175
1162.424	1186.241	1278.067
1309.436	1314.088	1332.13
1419.933	1451.064	1454.851
1485.569	1485.78	1673.447
1735.53	2391.629	3048.598
3058.28	3121.905	3122.471
3146.42	3149.53	3166.463
3171.24	3238.959	3244.197

i20 – p52
```
C    -0.455767   2.487324  -0.009515
C    -1.175632   1.195097  -0.172558
C     0.807246  -0.219565   0.020326
C     1.995392  -0.401782   0.015162
C     3.436226  -0.618965   0.026843
C    -0.622684  -0.043765  -0.011503
C    -2.632033  -1.518510   0.178927
C    -1.419763  -1.270504  -0.299876
H    -0.694313   3.172582  -0.828228
H     0.625121   2.345329   0.030536
H    -0.769881   2.979268   0.919659
H    -2.244234   1.234981  -0.361925
H     3.907542  -0.168903  -0.850472
H     3.886241  -0.176543   0.919167
H     3.665819  -1.687158   0.026105
H    -0.750758  -0.113824   1.842644
H    -3.110123  -0.845402   0.883783
H    -3.176163  -2.410877  -0.107066
H    -0.937157  -1.985436  -0.961044
```

Frequencies

-1018.14	39.8905	75.8256
93.1071	104.1372	152.7733
186.1962	224.6894	287.8987
357.8082	387.8319	449.3025
485.1192	491.9889	566.6703
598.3199	702.3454	718.3526
827.8035	932.9502	960.1001
1014.472	1025.086	1049.788
1056.042	1058.19	1104.576
1142.632	1235.327	1320.311
1371.041	1413.404	1420.131
1450.227	1478.124	1483.864
1484.667	1485.668	1607.125
1723.441	2379.393	3025.837
3047.121	3088.988	3119.115
3123.169	3140.89	3150.11
3171.203	3182.479	3244.258

i20 – p55
```
C     2.439122   1.607038   0.055804
C     0.998410   1.316237   0.307477
C    -1.142466   0.266389  -0.246145
C    -2.323279   0.102240  -0.088549
C    -3.756239  -0.088129   0.099176
C     0.264053   0.450851  -0.445164
C     2.111760  -2.055958  -0.104901
```

```
C      0.955345   -1.600704    0.309040
H      2.642102    2.681537    0.098320
H      2.758742    1.234274   -0.920449
H      3.067667    1.130662    0.818203
H      0.542824    1.746434    1.194677
H     -4.009676   -0.110790    1.162048
H     -4.322212    0.723296   -0.365803
H     -4.085149   -1.029659   -0.347705
H      0.658093    0.121917   -1.403490
H      2.710923   -1.517069   -0.836616
H      2.527067   -2.996864    0.258893
H      0.229383   -1.971525    1.021501
```

Frequencies

-439.308	26.7367	36.3346
76.9504	100.4483	108.65
146.4725	190.3021	227.802
266.1204	288.3003	346.3028
389.8076	480.67	516.8319
743.1554	797.5262	818.1608
909.0538	930.9505	941.0516
962.2251	1042.846	1055.645
1058.178	1091.075	1133.27
1198.669	1293.588	1315.076
1397.293	1414.673	1419.554
1479.936	1484.327	1485.796
1488.306	1601.57	1666.725
2379.793	3024.1	3045.714
3085.284	3086.66	3117.238
3119.734	3120.073	3155.674
3166.164	3178.282	3227.48

i28 – p62
```
C     -0.441044   -0.257617   -0.204714
C      0.379502    0.783637    0.013676
C      1.833520    0.745159   -0.053836
C      2.606398   -0.348580    0.088186
C      4.091454   -0.360758   -0.113933
C     -4.509091   -0.093942    0.083502
C     -3.057030   -0.147932   -0.018774
C     -1.856296   -0.183987   -0.100153
H     -0.029439   -1.221731   -0.492820
H     -0.068774    1.745182    0.247537
H      2.327868    1.704431   -0.192054
H      2.130904   -1.316139    0.234265
H      2.609661   -0.376877    2.232959
H      4.497182    0.652616   -0.149394
H      4.338129   -0.857960   -1.058468
H      4.599500   -0.909420    0.682465
H     -4.817266    0.213487    1.086202
H     -4.950103   -1.072069   -0.123089
H     -4.922144    0.622601   -0.631322
```

Frequencies

-554.66	17.6207	57.9122
74.8069	97.4317	173.9806
180.2781	215.9292	297.9989
310.5401	323.8618	350.9459
367.7778	483.4311	500.1522
628.2023	804.5761	857.0527
889.074	925.5661	994.0412
1006.323	1053.522	1057.991
1063.268	1076.485	1133.352

1217.839	1306.911	1318.576
1341.235	1359.447	1418.795
1420.311	1483.284	1483.841
1484.635	1497.179	1655.945
1702.033	2368.379	3037.944
3045.257	3103.936	3116.396
3121.267	3130.583	3151.205
3160.265	3164.122	3179.194

i28 – p10b

C	0.235239	-0.038070	0.238013
C	-0.486213	-1.019450	-0.339857
C	-1.924190	-1.173406	-0.244253
C	-2.728682	-0.543419	0.641097
C	-3.165812	1.694365	-0.349503
C	4.289759	0.322463	-0.051700
C	2.842531	0.190427	0.049432
C	1.646331	0.073376	0.128827
H	-0.265170	0.731995	0.819797
H	0.042917	-1.746065	-0.949860
H	-2.381516	-1.830825	-0.978395
H	-2.325689	0.008312	1.482381
H	-3.792047	-0.745517	0.661735
H	-3.813282	1.384211	-1.158635
H	-2.132388	1.914722	-0.582777
H	-3.615552	2.173858	0.511079
H	4.605050	0.354306	-1.097945
H	4.792311	-0.522494	0.426502
H	4.631591	1.239781	0.433786

Frequencies

-316.226	34.4931	53.9666
68.648	90.4149	106.9324
135.5282	230.8644	244.6229
302.6584	321.5832	410.326
433.2614	466.7155	507.691
564.642	690.1544	709.9888
835.5559	878.9647	904.5886
984.1552	990.3963	1016.852
1053.542	1058.006	1081.604
1219.149	1300.722	1322.495
1341.515	1411.28	1418.382
1419.263	1448.865	1483.303
1484.179	1581.41	1672.928
2361.117	3044.708	3105.446
3115.239	3120.883	3161.813
3162.307	3169.172	3183.231
3256.091	3278.204	3284.263

i28 – p75

C	0.541509	0.975612	0.543677
C	-0.548498	0.744877	-0.175577
C	-1.662703	0.299312	-0.684659
C	-2.451929	-0.838309	-0.083251
C	-3.851941	-0.398924	0.349805
C	4.177655	-0.741876	-0.151724
C	2.878223	-0.131020	0.092614
C	1.799765	0.367196	0.284916
H	0.496195	1.717090	1.338104
H	-0.227362	2.315636	-1.479227
H	-2.069122	0.765263	-1.578478
H	-1.903472	-1.252189	0.766141
H	-2.534025	-1.634978	-0.831151
H	-4.414766	0.011366	-0.493572

```
H     -3.794610   0.372792   1.121436
H     -4.417414  -1.243138   0.751774
H      4.090612  -1.564768  -0.865185
H      4.601092  -1.137602   0.774947
H      4.880393  -0.010676  -0.559598
```

Frequencies

-676.741	22.9131	48.0666
55.8433	103.1194	123.0575
180.3763	233.0412	247.3007
295.7836	374.2865	400.961
437.7849	496.8686	547.8252
579.9048	773.7587	807.3243
811.6808	892.6947	907.1474
1019.222	1053.711	1057.916
1088.487	1107.809	1146.458
1211.005	1278.851	1316.432
1357.357	1417.329	1417.686
1455.491	1482.733	1484.015
1490.113	1501.917	1509.294
2018.038	2367.217	3043.834
3046.535	3046.901	3100.208
3118.109	3123.091	3123.396
3127.825	3150.788	3164.16

i28 – p73

```
C     -0.405633  -0.235799   0.231052
C      0.456316   0.867683  -0.160537
C      1.785434   0.919588  -0.003561
C      2.685512  -0.125423   0.582766
C      3.663177  -0.684266  -0.457457
C     -4.272987  -0.218916  -0.286324
C     -2.965679  -0.227046  -0.118982
C     -1.716754  -0.233519   0.052628
H      0.042229  -1.112473   0.691353
H     -0.046281   1.713338  -0.620326
H      2.292401   1.814462  -0.359948
H      2.111188  -0.943465   1.023483
H      3.256227   0.327175   1.402101
H      4.268036   0.114286  -0.896358
H      3.123105  -1.178434  -1.268802
H      4.342564  -1.410562  -0.004857
H     -5.116810   0.757792   1.764890
H     -4.878245  -1.073810  -0.004957
H     -4.770722   0.617877  -0.764087
```

Frequencies

-416.986	28.1036	59.5736
88.229	128.7598	162.0007
204.251	246.8039	263.625
272.0476	312.1851	444.4471
495.8503	548.8352	583.5605
620.6914	789.3338	811.5847
881.6123	882.516	893.5122
945.8706	1026.346	1034.366
1036.517	1077.02	1098.679
1176.353	1279.47	1291.085
1309.85	1346.356	1415.555
1427.994	1465.762	1493.907
1502.964	1511.646	1676.455

1722.097	2155.96	3043.952
3044.532	3099.966	3123.441
3127.903	3147.029	3149.998
3167.423	3184.834	3234.797

i32 – i46

```
C    1.713527   -1.352083    0.705071
C    1.335061   -0.476427   -0.489505
C   -0.123430   -0.967447   -0.432992
C   -1.184526   -0.044474   -0.057262
C   -0.881669    1.240321    0.239510
C    0.467968    1.765599    0.106529
C    1.497593    0.995995   -0.268293
C   -2.578005   -0.595396    0.045427
H    2.302631   -2.249073    0.531472
H    0.280604   -1.680748    0.614544
H    1.844521   -0.851974    1.660818
H    1.853440   -0.785767   -1.400129
H   -0.380979   -1.749886   -1.146359
H   -1.669415    1.919534    0.549419
H    0.623671    2.823640    0.290169
H    2.487066    1.420245   -0.405009
H   -2.630855   -1.380504    0.807329
H   -2.893548   -1.045297   -0.901924
H   -3.296247    0.183309    0.308761
```

Frequencies

-2067.58	113.8235	155.9103
186.4156	306.4653	315.2591
376.3981	496.8198	516.4395
551.9153	574.3348	640.3661
751.5521	764.6443	867.9395
878.0117	891.6811	911.2746
937.2668	987.9683	1008.848
1036.272	1064.018	1073.869
1086.38	1119.603	1198.395
1201.705	1264.143	1313.186
1333.22	1351.543	1409.926
1420.168	1427.97	1446.527
1484.125	1504.929	1615.945
1711.299	1802.317	3036.919
3084.116	3094.269	3116.895
3136.672	3140.215	3174.525
3188.156	3203.476	3236.081

i40 – p39

```
C   -0.621885    1.979504   -0.917444
C   -0.306022    1.035420    0.211783
C    0.963533    0.385115    0.167670
C    2.038574   -0.154361    0.093355
C    3.337148   -0.811221    0.023622
C   -1.197216    0.740826    1.180991
C   -1.707432   -1.889732   -0.635010
C   -2.448736   -1.183482    0.177990
H   -0.637521    1.440048   -1.869607
H    0.139326    2.760542   -0.996984
H   -1.595757    2.449812   -0.771280
H    3.226604   -1.897320    0.079066
H    3.847595   -0.568380   -0.911483
H    3.976984   -0.495119    0.851748
H   -2.137948    1.275038    1.243175
H   -0.935232    0.086554    2.002473
H   -0.676139   -1.611894   -0.846972
H   -2.086408   -2.786243   -1.128819
H   -3.469294   -1.265444    0.530944
```

Frequencies

-217.495	29.8809	42.4948
60.4565	88.6166	118.884
151.9119	169.189	209.7074
270.1477	311.9894	368.7445
384.7903	564.1677	581.7369
666.0592	767.7432	794.6094
881.7655	894.8866	940.2772
952.1478	1029.027	1052.472
1058.834	1066.696	1082.415
1096.801	1336.22	1395.226
1411.261	1420.828	1429.159
1480.495	1483.525	1484.167
1497.182	1624.975	1669.685
2350.279	3041.593	3045.199
3081.291	3107.402	3116.201
3120.971	3138.206	3164.443
3166.127	3222.813	3262.493

i43 – i43

```
C    1.971790  -1.051431   0.702565
C    1.302066  -0.424355  -0.527311
C   -0.037467  -1.097938  -0.217075
C   -1.248351  -0.307381   0.006729
C   -1.060792   1.122441   0.462748
C    0.209548   1.757873  -0.030685
C    1.254752   1.071675  -0.478844
C   -2.471445  -0.835329  -0.138951
H    2.573401  -1.945120   0.555802
H    0.597339  -1.466053   0.917732
H    2.288698  -0.382499   1.499116
H    1.742836  -0.757823  -1.469822
H   -0.184532  -2.050771  -0.722755
H   -1.054234   1.145485   1.561823
H   -1.923992   1.720597   0.157660
H    0.262626   2.841798   0.016743
H    2.151868   1.598924  -0.791730
H   -3.366599  -0.251663   0.048249
H   -2.608018  -1.866204  -0.447870
```

Frequencies

-2165.52	60.7954	118.64
262.4279	315.0911	369.255
445.2902	502.3564	515.5107
534.493	618.4768	687.8781
725.4465	754.0378	861.4746
876.5846	891.2934	912.1135
925.4888	941.8443	974.3769
1009.8	1023.531	1040.565
1067.506	1132.87	1199.38
1223.497	1262.349	1296.673
1323.583	1340.933	1354.521
1381.374	1417.684	1430.209
1459.5	1469.655	1672.154
1754.213	1793.176	3020.33
3083.238	3084.957	3116.316
3147.839	3154.058	3164.483

3188.572	3229.87	3241.776

i43 – i31

C	2.596336	-0.766865	-0.063852
C	1.226432	-0.192119	-0.067011
C	0.107313	-1.002160	0.545173
C	-1.235661	-0.492414	0.089302
C	-1.442680	0.985937	0.304999
C	-0.219407	1.786510	-0.062007
C	0.989476	1.224933	-0.239242
C	-2.144971	-1.275499	-0.478828
H	2.738201	-1.784809	0.270671
H	3.450519	-0.124994	-0.232828
H	1.712764	-0.712444	-1.103252
H	0.185630	-0.906854	1.639450
H	0.219639	-2.064090	0.309282
H	-1.688150	1.165990	1.362487
H	-2.307571	1.330536	-0.269571
H	-0.340264	2.857306	-0.185394
H	1.834073	1.848874	-0.519910
H	-3.097941	-0.882891	-0.818855
H	-1.967919	-2.336562	-0.623277

Frequencies

-1921.19	108.8761	122.9647
295.7295	303.0672	377.5359
402.3093	431.5755	455.5412
498.5672	569.2789	607.9886
685.4042	734.915	746.5165
846.1497	913.8467	926.5536
933.6758	945.8867	976.3568
982.8839	1005.185	1020.259
1164.086	1182.212	1212.474
1224.983	1268.991	1305.697
1337.573	1352.874	1357.46
1430.365	1451.157	1463.071
1472.454	1487.258	1660.465
1756.941	2218.157	2989.824
3002.9	3081.66	3093.389
3145.814	3162.973	3174.16
3197.318	3231.175	3296.881

i64 – p93

C	-1.544331	-1.119233	0.257015
C	-1.932040	0.326814	0.123833
C	-0.872198	1.115395	-0.656258
C	0.499078	0.816740	-0.087707
C	1.152708	1.695918	0.703156
C	2.098448	-1.085635	-0.218111
C	0.849632	-0.635961	-0.075305
C	-0.283924	-1.544053	0.142833
H	-2.334310	-1.837807	0.453141
H	-2.900272	0.408296	-0.379350
H	-2.064305	0.763246	1.122276
H	-0.909795	0.804755	-1.704222
H	-1.074429	2.187963	-0.618086
H	1.416008	1.273009	-1.685874
H	2.042722	1.406188	1.249247
H	0.831275	2.730010	0.768348
H	2.321666	-2.145464	-0.158907
H	2.921790	-0.408139	-0.413002
H	-0.054590	-2.601968	0.229686

Frequencies

-891.223	101.2717	195.4092
280.3845	336.2005	376.6336
415.0825	455.8093	464.7037

512.0301	574.4008	636.0287
676.1316	722.8035	741.2856
773.9955	818.8253	880.613
897.159	915.3183	936.3984
973.9305	986.5555	1010.721
1045.309	1052.616	1183.375
1195.167	1231.371	1269.696
1333.399	1355.329	1366.393
1414.998	1445.161	1462.444
1480.905	1499.063	1634.052
1691.578	1742.101	3030.593
3062.348	3083.899	3118.625
3150.807	3154.329	3168.282
3190.99	3246.208	3248.613

i64 – i66
```
C   1.779517  -0.854866  -0.130965
C   1.845371   0.634281  -0.330522
C   0.725436   1.325352   0.451109
C  -0.620130   0.680058   0.173755
C  -1.736537   1.522462  -0.327356
C  -1.815954  -1.494487  -0.016167
C  -0.675169  -0.781771   0.092510
C   0.621861  -1.479432   0.087199
H   2.701358  -1.425040  -0.188031
H   2.815290   1.022004  -0.006439
H   1.758779   0.863819  -1.400522
H   0.964545   1.243406   1.517615
H   0.688070   2.390422   0.208619
H  -1.500410   1.105671   0.949336
H  -2.602096   1.063569  -0.783665
H  -1.588920   2.591394  -0.393169
H  -1.784462  -2.575539  -0.083226
H  -2.795294  -1.031090  -0.026135
H   0.596770  -2.558197   0.208234
```

Frequencies

-1880.06	69.7722	158.6233
301.8543	327.4739	373.2424
416.4202	430.0289	467.1663
526.0853	602.9086	642.5552
693.4922	696.4871	734.0221
798.7535	847.7477	866.8094
898.0906	962.8746	986.1467
1011.214	1035.409	1050.448
1168.919	1185.903	1195.874
1220.402	1273.558	1293.178
1355.289	1367.034	1396.92
1433.22	1442.369	1465.447
1481.234	1496.705	1629.061
1728.041	2251.904	3032.579
3042.679	3090.995	3102.079
3167.49	3175.085	3175.797
3198.286	3255.557	3299.282

i62 – i65
```
C  -1.967778  -0.449391  -0.106563
C  -1.812783   0.844819   0.140793
C  -0.471404   1.498855   0.287200
```

```
C     0.678272    0.609530   -0.124648
C     2.000317    1.262137   -0.242867
C     1.563123   -1.640764    0.357427
C     0.538992   -0.833844    0.031455
C    -0.830561   -1.416731   -0.260770
H    -2.968571   -0.859785   -0.208758
H    -2.685414    1.480882    0.256860
H    -0.449851    2.432374   -0.288638
H    -0.323380    1.801156    1.335680
H     1.133052    0.954956   -1.246338
H     2.075585    2.329438   -0.083886
H     2.898645    0.676444   -0.371694
H     1.424605   -2.714043    0.430476
H     2.550500   -1.255932    0.581261
H    -0.842736   -1.811623   -1.286082
H    -1.001512   -2.281526    0.388949
```

Frequencies

-1883.03	76.8589	121.3506
287.0946	344.1362	385.6645
404.7238	448.9249	500.8074
509.7121	563.4202	666.447
668.1427	707.555	730.5337
822.4576	869.8529	916.1518
930.7502	962.2312	976.8588
995.9974	1025.02	1038.265
1190.357	1190.514	1211.893
1234.395	1259.173	1260.229
1345.741	1371.683	1412.895
1425.86	1451.339	1463.483
1468.56	1486.483	1652.593
1766.174	2228.233	2992.909
3023.357	3045.822	3074.392
3162.41	3165.079	3183.499
3192.231	3251.228	3302.61

i61 – i59

```
C    -2.011353   -0.644016   -0.000131
C    -1.922340    0.782179   -0.054903
C    -0.726571    1.414570   -0.016087
C     0.544131    0.678759    0.014760
C     1.795675    1.508304    0.030869
C     0.536136   -0.684816   -0.010799
C    -0.708401   -1.411342    0.017710
C     1.804373   -1.501899   -0.048880
H    -1.446067   -1.137740    1.047764
H    -2.925053   -1.175901   -0.225996
H    -2.841743    1.353609   -0.127010
H    -0.685901    2.498523   -0.035674
H     1.890703    2.086258   -0.896581
H     2.701587    0.913441    0.147657
H     1.765068    2.233641    0.851910
H    -0.739159   -2.472419   -0.192055
H     2.466541   -1.180072   -0.856448
H     1.584039   -2.560195   -0.198386
H     2.360082   -1.409577    0.889579
```

Frequencies

-2559.64	68.1267	122.8508
158.777	194.3903	334.1495
347.1179	388.4631	468.6198
500.8913	537.6963	602.387
634.0805	720.7755	736.8569
779.4976	822.5083	919.078
966.4483	980.5958	1000.439

1035.019	1063.956	1103.264
1161.339	1183.232	1203.817
1222.336	1264.875	1343.537
1397.196	1412.937	1422.911
1452.771	1482.752	1489.368
1504.298	1515.478	1604.237
1621.661	2215.431	3027.613
3050.342	3076.621	3115.2
3138.953	3151.44	3184.207
3204.168	3214.806	3232.175

i23 – p13b

```
C     0.583254   1.658267  -0.292408
C     0.177777   0.222179  -0.033441
C    -1.241300   0.001712   0.017798
C    -2.435542  -0.137973   0.040558
C     3.292306  -0.065715   0.387545
C     2.450020  -0.877266  -0.257360
C     0.997486  -0.861777  -0.173080
C    -3.880605  -0.319441   0.080868
H     0.328737   2.300820   0.552083
H     0.026660   2.021504  -1.160977
H     1.648745   1.747398  -0.495964
H     0.443704   0.307406   1.909897
H     2.940313   0.700011   1.070097
H     4.364756  -0.177040   0.277417
H     2.867987  -1.680178  -0.861392
H     0.514704  -1.834827  -0.191377
H    -4.395287   0.632974  -0.066562
H    -4.208417  -1.008903  -0.701187
H    -4.192279  -0.729078   1.045088
```

Frequencies

-858.267	81.1469	87.1037
93.4495	123.0161	175.7035
245.9518	261.7752	309.7831
328.6366	375.5354	441.6256
481.5075	542.3448	566.281
575.8526	637.9993	784.3345
884.8722	908.8469	968.844
1012.989	1043.938	1052.655
1060.504	1064.799	1071.263
1112.151	1286.863	1333.7
1376.753	1418.807	1421.61
1460.693	1485.881	1487.333
1492.58	1498.24	1611.606
1694.987	2375.612	3051.814
3062.111	3123.412	3127.546
3128.618	3154.833	3164.446
3177.989	3185.04	3252.489

i23 – p10b

```
C    -0.457646   2.134455   0.363590
C    -0.211548  -0.123193  -0.361863
C     1.207587  -0.194599  -0.230568
C     2.405599  -0.249732  -0.132110
C    -3.246131  -0.138869  -0.511005
C    -2.494558  -0.869544   0.325244
C    -1.054970  -0.815531   0.463306
C     3.855884  -0.326992  -0.012139
H     0.084222   2.626668  -0.434809
H     0.044305   2.028445   1.316022
```

```
H    -1.538896    2.197946    0.366227
H    -0.583663    0.255523   -1.308360
H    -2.817764    0.594523   -1.186426
H    -4.322272   -0.259347   -0.541756
H    -3.001422   -1.565625    0.988751
H    -0.620348   -1.329592    1.314607
H     4.290474    0.666068    0.129288
H     4.142349   -0.946680    0.841113
H     4.297713   -0.763890   -0.911384
```

Frequencies

-434.399	73.194	81.353
91.9073	104.6961	119.3062
145.9493	244.3191	265.6693
280.3398	322.0877	470.2711
473.0821	495.0972	513.4364
566.83	635.745	759.9232
831.1159	856.0304	928.1155
943.3733	1010.658	1036.586
1059.328	1063.072	1078.766
1211.78	1281.354	1321.475
1341.321	1408.229	1423.439
1425.418	1457.033	1484.093
1490.451	1556.487	1670.931
2373.225	3046.915	3103.126
3116.913	3122.185	3159.158
3171.034	3177.049	3196.76
3250.264	3273.772	3283.01

i22 – p10a
```
C    -0.105740    2.321913    0.341135
C    -0.122346    0.149364   -0.567129
C     1.246095   -0.149783   -0.289086
C     2.401814   -0.400035   -0.067126
C     3.799782   -0.710830    0.203331
C    -1.155306   -0.479741    0.077115
C    -3.568699   -0.868710    0.344049
C    -2.532859   -0.314892   -0.302029
H     0.668304    2.758117   -0.278916
H     0.159991    2.066735    1.358899
H    -1.130819    2.618736    0.154710
H    -0.323310    0.646067   -1.512032
H     4.044508   -0.517037    1.250834
H     4.012727   -1.762682   -0.004434
H     4.460107   -0.100977   -0.418026
H    -0.934995   -1.089626    0.948939
H    -3.417515   -1.492792    1.219445
H    -4.589296   -0.715809    0.014707
H    -2.726141    0.305560   -1.175687
```

Frequencies

-463.285	77.1538	90.311
95.4546	106.829	137.7538
141.1876	231.1453	246.662
294.5719	351.5192	429.6709
471.4328	477.4695	508.1363
553.0914	636.4882	779.3521
823.5596	859.0443	912.3985
943.0451	964.7813	1025.568
1064.884	1066.722	1193.241
1196.992	1281.054	1286.234
1328.487	1412.299	1420.349

1426.128	1448.604	1490.381
1492.942	1558.951	1653.015
2373.699	3047.017	3102.287
3118.534	3121.815	3150.433
3162.617	3170.114	3178.692
3254.103	3273.669	3276.793

i22 – p13a

C	0.294432	1.968816	-0.129570
C	0.099917	0.485007	0.097240
C	-1.259366	0.028962	0.052584
C	-2.410125	-0.314690	-0.016119
C	-3.801629	-0.740031	-0.089252
C	1.106659	-0.436219	0.049511
C	3.458385	-1.101182	-0.074293
C	2.517866	-0.149878	-0.056937
H	-0.473360	2.534696	0.398445
H	0.199742	2.189656	-1.197516
H	1.269245	2.314852	0.213218
H	0.123376	0.680329	2.090810
H	-4.213503	-0.554349	-1.084634
H	-3.893393	-1.808325	0.120646
H	-4.412412	-0.196445	0.635889
H	0.828825	-1.483713	0.124652
H	3.199384	-2.153017	-0.000581
H	4.510032	-0.857042	-0.164693
H	2.825223	0.888653	-0.135212

Frequencies

-802.1	53.3202	84.2582
102.447	125.0733	137.4017
232.6133	245.1222	319.057
347.2357	390.9437	408.6733
430.3745	447.7475	567.3875
585.3752	669.892	747.2375
907.2396	920.825	947.4886
1009.569	1029.899	1053.434
1055.542	1060.185	1072.013
1209.782	1271.138	1338.615
1359.123	1419.793	1422.854
1453.575	1482.952	1484.351
1488.736	1501.566	1600.691
1676.926	2374.231	3052.321
3057.309	3121.985	3129.123
3133.499	3156.81	3161.719
3181.581	3192.147	3252.942

i22 – i40

C	-0.047697	2.511735	0.154452
C	-0.126594	1.033795	-0.121146
C	1.038962	0.241302	-0.055721
C	2.038168	-0.437378	-0.015185
C	3.244811	-1.252111	0.042164
C	-1.475883	0.389664	-0.105140
C	-2.923769	-1.592350	0.100170
C	-1.708149	-1.021049	0.003254
H	0.862054	2.943424	-0.265036
H	-0.050310	2.697728	1.235060
H	-0.907234	3.035905	-0.273037
H	-0.846566	0.742814	-1.186870
H	3.532076	-1.460839	1.076666
H	3.087584	-2.209225	-0.462034
H	4.082036	-0.747763	-0.447355
H	-2.309549	1.075788	0.003855
H	-3.833220	-0.999370	0.103346
H	-3.032314	-2.665881	0.190049

SUPPORTING INFORMATION

H   -0.823653   -1.654225   0.008267

Frequencies

-1888.45	77.4451	119.1902
125.6842	146.8035	170.8521
198.4122	202.8065	304.6798
328.2525	374.2137	440.4662
528.9557	606.2964	614.9477
672.8307	797.5803	870.0327
920.3792	1016.107	1028.814
1044.446	1053.868	1060.202
1062.849	1153.966	1231.967
1255.861	1308.289	1354.388
1376.043	1423.097	1426.173
1479.145	1487.134	1489.887
1492.217	1499.883	1635.898
2151.685	2312.698	3030.994
3042.683	3099.456	3110.471
3118.757	3140.749	3149.982
3161.839	3194.522	3248.003

i50 – i54

C	-0.742142	2.449387	-0.230715
C	-0.575209	0.973313	-0.076109
C	3.238440	-0.487011	0.150523
C	1.882059	0.038856	0.061694
C	0.755331	0.460375	-0.001488
C	-1.712234	0.185973	0.440032
C	-1.910342	-1.129524	0.304769
C	-1.051142	-2.099309	-0.446013
H	-1.730494	2.871312	-0.109907
H	0.130757	3.081037	-0.306127
H	-0.783708	1.457888	-1.202026
H	3.948547	0.303922	0.404898
H	3.554115	-0.933841	-0.796280
H	3.301824	-1.256495	0.924286
H	-2.456160	0.762073	0.986254
H	-2.788823	-1.547276	0.790209
H	-0.394016	-1.600885	-1.159195
H	-1.674359	-2.817199	-0.986790
H	-0.416248	-2.672894	0.238513

Frequencies

-1897.41	42.2928	76.4064
92.8183	124.9533	147.9953
241.4041	286.2079	314.2588
351.4057	388.3736	448.1398
522.6485	541.2383	618.1881
636.6538	702.4231	769.2143
900.7886	966.7214	992.344
1041.301	1053.882	1057.98
1062.931	1120.755	1183.506
1242.558	1275.763	1363.045
1408.622	1420.684	1422.373
1445.189	1484.004	1488.746
1491.615	1508.348	1713.885
2232.11	2352.647	3044.414
3047.538	3103.485	3115.654

3123.039	3148.122	3155.901
3172.441	3180.262	3304.383

i50 – p85

```
C    0.574815   1.693315  -0.350575
C    0.145049   0.413096  -0.168071
C   -3.857223  -0.393267   0.215294
C   -2.436664  -0.099105   0.079969
C   -1.264792   0.149630  -0.014125
C    0.984543  -0.763072  -0.528672
C    2.267155  -0.963021  -0.227485
C    3.156487  -0.087819   0.600658
H    1.601985   1.899285  -0.622256
H   -0.095309   2.528883  -0.193024
H    0.404425   0.278270   1.676893
H   -4.451418   0.220258  -0.466335
H   -4.196398  -0.193815   1.235037
H   -4.057485  -1.443889  -0.008049
H    0.459193  -1.524640  -1.097582
H    2.720679  -1.875223  -0.607233
H    2.582674   0.592089   1.234733
H    3.814265   0.517669  -0.033082
H    3.801163  -0.697420   1.238940
```

Frequencies

-1037.93	70.5485	96.837
112.6067	161.0802	197.1946
247.3367	281.538	327.5424
353.9621	427.8242	455.3333
509.4099	546.5822	562.2248
592.6741	666.1539	766.1176
788.251	885.9443	904.5538
972.5493	1011.55	1052.368
1067.501	1076.026	1080.404
1118.466	1280.851	1289.872
1407.13	1418.711	1426.255
1448.254	1487.981	1489.419
1494.563	1502.966	1577.773
1743.886	2383.785	3034.272
3051.29	3097.56	3124.331
3124.538	3125.509	3163.025
3174.039	3188.28	3277.651

i26 – p59

```
C   -0.583071   0.730845   0.098097
C    0.467230  -0.118304  -0.044883
C   -4.487663  -0.468403   0.011595
C   -3.093938  -0.045399   0.042703
C   -1.942931   0.304055   0.059772
C    1.846267   0.287297   0.085162
C    2.883289  -0.544000  -0.074805
C    4.320885  -0.156110   0.046548
H   -0.400544   1.747494   0.436572
H   -0.571537   1.654703  -1.724379
H    0.268724  -1.155950  -0.299695
H   -4.572629  -1.544373   0.182384
H   -4.940745  -0.242642  -0.957338
H   -5.066355   0.044845   0.783641
H    2.033456   1.334150   0.320238
H    2.680035  -1.587168  -0.312467
H    4.819142  -0.739254   0.828071
H    4.432948   0.903779   0.285046
H    4.857099  -0.355474  -0.887199
```

Frequencies

-746.876	42.459	67.4798
75.2688	123.8349	181.0244

188.774	214.3964	301.2491
316.13	328.3749	377.927
403.9855	445.8739	498.9875
586.7643	811.3429	816.1785
897.7684	953.668	964.5777
1027.287	1055.368	1059.037
1069.817	1111.176	1191.181
1208.487	1262.823	1310.986
1347.213	1366.701	1421.537
1422.526	1482.582	1483.719
1488.351	1492.556	1622.594
1719.322	2376.575	3038.701
3051.048	3096.53	3121.835
3125.626	3129.685	3147.857
3152.64	3168.981	3178.603

i26 – i47
```
C   -0.651154   1.665728   0.180037
C    0.768993   1.221087  -0.075469
C   -3.497140  -1.306746  -0.018218
C   -2.485200  -0.258502   0.054177
C   -1.657821   0.609513   0.111854
C    1.160344  -0.017581  -0.355222
H   -0.699822   2.144490   1.165695
H   -0.909302   2.452014  -0.539968
H    1.511387   2.014592  -0.020544
H   -3.336085  -2.059904   0.757118
H   -3.470178  -1.807789  -0.988962
H   -4.497503  -0.888726   0.119038
H    0.394652  -0.797630  -0.403530
C    2.556488  -0.419222  -0.582458
C    3.367076  -1.004342   0.523558
H    2.915658  -0.502247  -1.604152
H    2.968135  -1.979062   0.845653
H    3.345613  -0.359362   1.410018
H    4.407922  -1.155987   0.230077
```

Frequencies

-227.462	45.4063	78.2081
105.2774	115.6084	154.2141
197.681	223.8489	268.523
385.1998	385.6379	405.3118
477.3204	631.5186	760.0224
791.4507	934.8134	969.6002
974.0122	993.0054	1004.008
1058.883	1064.773	1107.623
1145.4	1175.31	1241.893
1278.462	1345.495	1353.602
1381.441	1404.718	1420.635
1477.377	1478.248	1483.641
1487.596	1493.946	1752.104
2399.378	2983.782	3036.457
3049.132	3051.133	3063.723
3087.99	3119.799	3124.775
3125.813	3163.134	3175.454

i27 – p63
```
C    0.424882   1.774779  -0.000612
```

```
C    -0.926508    1.716409   -0.145133
C    -1.804504    0.562955   -0.186523
C    -1.506298   -0.705441    0.128124
C    -2.483647   -1.833804    0.061980
C     3.089490   -1.319466   -0.074594
C     2.130389   -0.223702   -0.040464
C     1.326893    0.672131   -0.011201
H     0.892630    2.752567   -0.059794
H     0.521039    2.129656    2.034404
H    -1.426797    2.676946   -0.226958
H    -2.827506    0.780803   -0.488812
H    -0.502674   -0.950009    0.460780
H    -2.130546   -2.611462   -0.623763
H    -3.466852   -1.498969   -0.276804
H    -2.599355   -2.307682    1.042421
H     3.206461   -1.765355    0.916703
H     4.069660   -0.967433   -0.405271
H     2.759762   -2.102224   -0.762377
```

Frequencies

-681.488	40.8668	60.9302
75.7392	147.4066	184.3783
190.5036	212.1257	284.771
299.6759	322.5214	394.5599
399.5174	506.924	570.2239
677.5444	760.9364	836.8752
868.2452	914.1283	990.7455
1007.442	1045.821	1055.183
1059.418	1071.263	1140.882
1175.745	1278.604	1359.571
1363.241	1419.219	1421.877
1463.484	1481.512	1484.255
1485.553	1497.038	1600.017
1715.694	2369.151	3033.97
3048.193	3091.911	3118.544
3125.76	3126.116	3147.149
3173.455	3191.231	3209.729

i51 – i49
```
C     0.617668    1.645536   -0.380354
C    -0.118601    0.826496    0.622116
C    -3.760031   -0.817519   -0.179401
C    -2.458306   -0.229346    0.109027
C    -1.385803    0.266948    0.358695
C     1.235737    0.296355   -0.492713
C     2.452723   -0.064309    0.077937
C     3.010180   -1.447700    0.020118
H     1.261863    2.421188    0.026678
H     0.037225    1.983842   -1.233436
H     0.235521    0.845171    1.644435
H    -4.563422   -0.087670   -0.044656
H    -3.959471   -1.665798    0.480563
H    -3.803029   -1.177159   -1.210965
H     0.763940   -0.390093   -1.188051
H     2.980201    0.669642    0.683099
H     2.456261   -2.070441   -0.687032
H     2.966647   -1.942393    0.999667
H     4.062856   -1.445052   -0.282859
```

Frequencies

-636.694	31.0526	67.2573
101.7015	125.3151	151.6665
224.6161	268.9138	298.9496
329.0584	470.1778	475.5618
536.5989	664.565	729.9173
804.8913	860.1235	936.643

1006.494	1023.095	1031.211
1051.585	1055.615	1074.38
1136.908	1182.285	1201.365
1228.289	1275.706	1325.824
1393.025	1416.974	1421.637
1478.61	1481.783	1482.525
1486.164	1489.616	1527.061
2317.498	3008.689	3040
3065.677	3108.233	3113.482
3114.294	3115.112	3154.81
3180.561	3196.126	3210.303

i28 – i29
```
C    -0.488266   -0.823521   -0.202021
C     0.546164   -0.325672    0.484675
C    -4.315495    0.594521   -0.003316
C    -2.949241    0.092657   -0.070879
C    -1.818777   -0.316503   -0.120386
H    -0.329569   -1.668539   -0.867743
H     0.356766    0.523903    1.145678
H    -4.683422    0.583192    1.025899
H    -4.985535   -0.019285   -0.610196
H    -4.370983    1.622572   -0.370672
C     1.921048   -0.834926    0.395234
C     2.931852   -0.169025   -0.482712
C     3.349408    1.223989    0.024300
H     2.254487   -1.558089    1.134915
H     2.515571   -0.059138   -1.492128
H     3.819318   -0.802744   -0.568451
H     3.792332    1.160448    1.021702
H     2.486633    1.892973    0.078924
H     4.084231    1.675581   -0.647289
```

Frequencies

-261.257	29.2906	47.7186
75.345	101.4178	192.1654
216.2347	256.7633	280.0457
319.0405	406.1406	496.8438
520.945	548.1284	788.8562
819.0437	861.2438	906.8928
980.3585	996.8463	1047.871
1055.256	1058.648	1118.873
1142.637	1206.115	1274.803
1287.648	1328.031	1339.739
1376.873	1409.341	1419.44
1484.181	1484.466	1487.205
1502.48	1508.704	1709.151
2376.933	3026.452	3042.288
3045.602	3085.306	3091.632
3117.087	3121.029	3121.175
3124.904	3160.196	3162.815

i46 – p3
```
C     2.302233   -1.141484    0.430802
C     1.285507   -0.407841   -0.096483
C    -0.086959   -1.027387   -0.324724
C    -1.253676   -0.128150    0.010111
C    -1.077076    1.190302    0.137487
C     0.244328    1.802696    0.016601
C     1.353811    1.065138   -0.101721
C    -2.590920   -0.794439    0.109237
H     3.263944   -0.687301    0.641436
```

```
H      2.204719   -2.210117    0.584691
H      1.910359   -0.489288   -1.825601
H     -0.163098   -1.961840    0.240645
H     -0.194421   -1.309974   -1.379489
H     -1.927391    1.835159    0.335502
H      0.317748    2.883827    0.060709
H      2.334410    1.526034   -0.141553
H     -2.603022   -1.525102    0.925362
H     -2.817757   -1.344088   -0.811723
H     -3.388979   -0.070324    0.282163
```

Frequencies

-1043.92	2.8064	164.5115
208.2094	299.5194	349.1665
401.1164	442.0477	459.7755
497.3512	520.8204	568.3627
601.6951	645.864	733.2284
778.6745	866.7306	872.324
885.8368	930.4575	948.915
977.7673	996.9777	1012.84
1069.15	1082.195	1182.036
1204.386	1244.121	1318.533
1335.797	1371.474	1418.677
1426.981	1455.573	1469.548
1482.61	1498.557	1592.528
1683.764	1753.847	3032.025
3036.057	3079.445	3089.924
3135.188	3156.031	3183.545
3195.261	3214.354	3252.762

i46 – i8
```
C      2.504129   -1.100319   -0.062013
C      1.265707   -0.290618   -0.058315
C     -0.024002   -1.012370    0.255773
C     -1.258162   -0.184726   -0.003396
C     -1.166562    1.154853   -0.054263
C      0.103936    1.840955    0.053087
C      1.269445    1.145570    0.047080
C     -2.555166   -0.927303   -0.090553
H      3.470289   -0.614188   -0.074113
H      2.433932   -2.175397    0.023378
H      1.746800   -0.637670   -1.149096
H     -0.009114   -1.308116    1.321501
H     -0.074927   -1.956839   -0.300451
H     -2.067105    1.747952   -0.183389
H      0.116419    2.923472    0.100430
H      2.223089    1.664366    0.067024
H     -2.724617   -1.519152    0.817484
H     -2.550336   -1.632559   -0.929575
H     -3.400377   -0.248129   -0.217596
```

Frequencies

-1923.02	100.265	160.4954
207.3102	273.589	338.902
389.7862	418.985	454.8873
485.2579	509.7905	551.1014
608.8231	721.8751	743.3296
858.2369	878.1892	921.3654
942.095	949.6715	976.6657
1003.918	1061.991	1079.723
1163.351	1171.66	1190.125
1248.294	1267.435	1323.928

1345.187	1403.611	1419.802
1443.167	1463.503	1482.038
1486.101	1492.988	1577.809
1715.075	2219.542	2927.681
3026.18	3040.194	3079.342
3134.908	3177.311	3181.324
3185.96	3214.767	3299.286

i43 – p43

C	2.500788	-0.816940	-0.051465
C	1.262391	-0.267186	-0.028605
C	0.081996	-1.002558	0.583663
C	-1.232448	-0.449948	0.103113
C	-1.377217	1.038866	0.288661
C	-0.110944	1.777391	-0.055399
C	1.068050	1.179601	-0.225787
C	-2.172793	-1.204344	-0.451924
H	2.655694	-1.863684	0.183921
H	3.362180	-0.241038	-0.370612
H	0.792705	-0.734993	-1.804074
H	0.147762	-0.854260	1.670809
H	0.155543	-2.074190	0.391441
H	-1.639038	1.256155	1.334799
H	-2.205343	1.418222	-0.316902
H	-0.187250	2.853685	-0.176417
H	1.941446	1.762233	-0.502463
H	-3.106489	-0.778380	-0.804577
H	-2.036140	-2.273038	-0.579463

Frequencies

-943.487	105.0668	133.6113
326.6864	328.0199	398.3069
428.9727	443.359	456.3744
512.7863	544.5876	569.2341
643.11	702.0127	741.7473
784.7106	859.9835	879.9815
920.3994	937.8576	939.2927
950.7662	999.0535	1010.103
1017.357	1026.677	1176.732
1205.42	1238.495	1299.056
1317.063	1337.993	1359.038
1400.355	1454.854	1460.581
1469.639	1486.124	1609.791
1729.824	1759.817	3007.091
3023.643	3091.109	3124.171
3149.249	3155.322	3169.464
3192.862	3235.767	3250.377

i20 – p54

C	0.957234	2.051723	0.709309
C	1.195869	1.254176	-0.527758
C	-0.935925	0.028089	-0.485855
C	-2.054845	-0.171429	-0.092116
C	-3.411112	-0.406409	0.387754
C	0.390557	0.252436	-0.982464
C	2.462807	-1.552804	0.522401
C	1.284883	-1.646207	-0.039594
H	1.685538	1.785956	1.485186
H	-0.042408	1.878219	1.111010
H	1.077119	3.122356	0.515570
H	2.126470	1.427364	-1.060831
H	-4.063028	0.437210	0.146504
H	-3.835542	-1.302810	-0.071202
H	-3.422202	-0.544299	1.471955
H	0.613564	-0.191710	-1.947199

H	3.017018	-0.615874	0.517588
H	2.937329	-2.400591	1.016938
H	0.569332	-2.453271	-0.135579

Frequencies

-434.595	45.4317	82.2247
88.0829	93.2088	109.6301
134.9277	197.3907	221.1702
266.1079	343.9467	356.8756
416.3729	517.2518	602.767
719.8921	791.9487	799.6389
909.2754	916.7702	946.1862
950.5987	1047.667	1052.544
1058.456	1087.256	1101.287
1171.472	1258.261	1390.436
1399.607	1415.633	1438.022
1480.281	1484.908	1489.397
1489.836	1581.808	1671.354
2378.403	3031.504	3050.515
3088.966	3095.992	3120.806
3125.026	3138.966	3173.682
3175.347	3191.172	3228.673

i20 – p53

C	2.478547	-1.434451	-0.129401
C	1.006740	-1.250170	0.007573
C	-1.106873	-0.076263	0.040737
C	-2.308243	-0.057590	0.011080
C	-3.765221	-0.044139	-0.011626
C	0.334642	-0.060951	0.040694
C	2.014634	1.802702	0.192724
C	0.947651	1.238543	-0.358540
H	2.941589	-1.561373	0.857838
H	2.957890	-0.579954	-0.610004
H	2.698787	-2.339269	-0.701540
H	0.413294	-2.145407	0.168104
H	-4.152588	-0.820885	-0.675728
H	-4.170927	-0.217851	0.988278
H	-4.137903	0.920546	-0.364594
H	0.478605	0.204759	1.895509
H	2.512254	1.358511	1.048476
H	2.408000	2.740058	-0.183546
H	0.439740	1.734775	-1.182242

Frequencies

-973.727	54.9598	77.7853
105.4467	124.7403	193.9196
210.8763	240.8866	299.8534
334.2505	405.7076	430.0644
473.9674	509.9587	519.2085
569.1114	728.2473	755.0862
832.5555	933.6977	973.8319
989.5589	1029.341	1054.298
1056.272	1061.378	1104.115
1139.457	1260.157	1335.234
1353.127	1414.822	1419.834
1458.076	1475.529	1483.453
1486.861	1493.335	1607.789
1728.772	2382.693	3022.497

3049.75	3092.696	3121.933
3123.796	3139.469	3151.133
3164.769	3188.261	3246.692

i40 – p49

C	-0.549728	2.328425	-0.400714
C	-0.390332	1.060505	0.010682
C	0.890158	0.427263	-0.005134
C	1.947661	-0.146651	0.002418
C	3.231396	-0.834252	0.003020
C	-1.545073	0.225121	0.527313
C	-1.732140	-2.218308	-0.002776
C	-1.840672	-0.948246	-0.366169
H	-0.282622	3.488614	1.524732
H	-1.532407	2.786174	-0.417389
H	0.280551	2.900997	-0.795097
H	3.812393	-0.569139	0.890188
H	3.089842	-1.917645	0.000374
H	3.817496	-0.563688	-0.878692
H	-2.429752	0.865498	0.602888
H	-1.306135	-0.131467	1.534460
H	-1.415607	-2.494355	0.998846
H	-1.953323	-3.025929	-0.691478
H	-2.148061	-0.702202	-1.380673

Frequencies

-406.423	33.74	48.7313
60.8679	114.9912	133.429
157.647	223.9563	246.3977
316.2391	349.7461	394.0397
438.3622	568.6378	600.7756
643.6699	732.3038	782.8881
918.7324	945.3402	949.1915
964.977	976.3001	1041.957
1053.923	1057.459	1083.426
1132.256	1243.981	1312.25
1334.56	1341.75	1417.99
1442.66	1454.172	1482.31
1482.796	1483.738	1664.694
1738.558	2369.241	3047.057
3048.128	3098.321	3119.289
3123.535	3142.778	3158.375
3160.564	3235.783	3257.668

i40 – p50

C	-0.223922	2.550779	0.102111
C	-0.233273	1.050468	-0.007033
C	0.874771	0.342769	0.076736
C	1.935923	-0.338014	0.151695
C	3.042656	-1.049905	0.212100
C	-1.586578	0.406224	-0.213009
C	-2.219155	-1.949188	0.336702
C	-1.559703	-1.078542	-0.413999
H	0.781675	2.935467	0.268382
H	-0.865835	2.874812	0.928536
H	-0.625836	3.000328	-0.812382
H	4.004001	-0.578721	0.385347
H	3.012177	-2.132915	0.160604
H	3.733159	-1.176899	-2.037075
H	-2.050138	0.886916	-1.086479
H	-2.225960	0.661236	0.641581
H	-2.829932	-1.628092	1.175795
H	-2.170494	-3.014695	0.142778
H	-0.947135	-1.434982	-1.238911

Frequencies

-368.754	36.3281	77.1832

92.6951	127.4912	147.3141
160.2883	214.4195	226.9791
306.4079	376.8117	411.0406
425.0189	555.7382	573.7382
596.5217	632.4943	734.6214
880.2168	904.5933	935.3421
959.3042	996.3756	1033.917
1034.337	1047.461	1126.648
1161.315	1209.5	1261.23
1329.191	1358.145	1412.914
1445.808	1454.19	1475.531
1488.708	1489.913	1719.681
1746.038	2191.595	3016.325
3037.873	3056.496	3095.861
3146.676	3148.767	3157.387
3171.401	3235.654	3240.07

i53 – p82

```
C    0.084520   2.428453  -0.177933
C   -0.063421   1.092212  -0.109372
C    3.223925  -1.341621   0.040362
C    2.048040  -0.483102  -0.015474
C    1.088424   0.240357  -0.060855
C   -1.397012   0.477759  -0.069843
C   -1.638691  -0.830154   0.008700
C   -3.002541  -1.440834   0.054447
H    1.063903   2.885845  -0.230503
H    0.137830   3.056690   2.133312
H   -0.781721   3.077811  -0.236829
H    3.702225  -1.277289   1.021049
H    3.956622  -1.043555  -0.713559
H    2.955832  -2.385423  -0.139281
H   -2.229617   1.177321  -0.106792
H   -0.793365  -1.514172   0.046656
H   -3.139165  -2.152185  -0.766461
H   -3.786623  -0.683366  -0.012706
H   -3.145389  -2.000106   0.984919
```

Frequencies

-382.64	79.9315	109.258
113.0521	122.8832	135.8928
188.4983	205.9088	211.8894
218.9841	313.541	388.9082
397.4874	455.0025	623.9136
646.1045	676.5823	753.2916
856.6109	926.4862	927.8379
1008.972	1012.513	1057.907
1063.339	1074.854	1085.743
1136.177	1303.746	1337.618
1367.273	1421.448	1421.895
1440.946	1484.453	1487.732
1490.127	1498.341	1649.621
1748.303	2378.8	3040.502
3052.342	3100.568	3123.762
3127.636	3128.05	3163.674
3168.163	3169.762	3268.068

SUPPORTING INFORMATION

i53 – p86

C	0.149837	2.500690	-0.044567
C	0.006925	1.000554	0.004871
C	3.156574	-1.299068	0.188340
C	2.091687	-0.522934	0.132892
C	1.077469	0.222409	0.070855
C	-1.360689	0.465754	-0.023416
C	-1.693466	-0.826304	0.012840
C	-3.093396	-1.346243	-0.016332
H	1.196408	2.802386	-0.026625
H	-0.362113	2.957393	0.808879
H	-0.314936	2.895875	-0.953723
H	3.060199	-2.377372	0.250592
H	4.154568	-0.876721	0.229426
H	3.678561	-1.732135	-2.182911
H	-2.150686	1.212951	-0.079002
H	-0.896847	-1.566162	0.068266
H	-3.240525	-2.018920	-0.867656
H	-3.824748	-0.537983	-0.085848
H	-3.309523	-1.928463	0.885701

Frequencies

-365.932	35.5011	74.7027
112.4982	130.1924	157.9593
161.384	178.6927	198.1131
230.6495	305.5986	377.4702
436.2956	469.8005	557.6145
599.977	623.0446	736.1143
828.9437	856.9317	933.8628
1008.484	1016.274	1035.519
1052.553	1071.67	1101.32
1174.294	1238.672	1334.475
1361.463	1410.04	1417.965
1448.756	1481.43	1485.487
1492.922	1493.053	1694.71
1732.838	2160.702	3038.469
3041.398	3097.437	3103.232
3128.318	3151.908	3153.298
3156.178	3163.255	3239.311

i53 – p88

C	0.013915	2.299939	-0.059437
C	-0.025012	0.797180	0.083670
C	3.579017	-1.126527	-0.058546
C	2.290582	-0.448452	-0.011910
C	1.217890	0.095681	0.031039
C	-1.165845	0.129025	0.183989
C	-2.218561	-0.545779	0.553930
C	-3.247990	-1.191518	-0.327418
H	0.673139	2.729769	0.699258
H	-0.983814	2.725820	0.048150
H	0.411380	2.573893	-1.040994
H	4.110771	-1.013653	0.889874
H	4.208595	-0.714752	-0.851255
H	3.446271	-2.194358	-0.248070
H	-1.612654	0.572165	-1.862287
H	-2.363665	-0.654488	1.629095
H	-3.300843	-2.265275	-0.125115
H	-3.014270	-1.043920	-1.382305
H	-4.238883	-0.772506	-0.128248

Frequencies

-527.801	57.871	92.5154
100.5609	120.761	149.2959
154.6799	182.6298	228.5547
273.1973	297.7758	371.3872
460.3482	478.0067	489.4643

572.3388	607.0486	676.1201
823.2983	872.4283	1003.031
1054.141	1056.767	1061.159
1064.504	1068.227	1105.122
1232	1294.971	1406.064
1410.744	1420.06	1439.668
1482.923	1486.862	1488.209
1491.001	1492.618	1512.187
2028.121	2367.776	3046.89
3051.194	3052.404	3110.85
3121.406	3123.469	3125.895
3128.476	3149.821	3153.062

i53 – p12a
```
C     0.161495   2.503743  -0.043748
C    -0.109365   1.023072   0.009665
C     3.238536  -1.326507  -0.019973
C     2.037973  -0.501128  -0.011006
C     1.042304   0.175448  -0.000516
C    -1.359473   0.523287   0.063605
C    -1.697522  -0.883671   0.117466
C    -2.956628  -1.342856   0.163937
H     0.779121   2.811476   0.804960
H    -0.769078   3.073649  -0.025198
H     0.711443   2.759547  -0.954043
H     3.739121  -1.291393   0.951118
H     3.944806  -0.976912  -0.777096
H     2.994057  -2.368874  -0.237870
H    -2.188897   1.226760   0.066694
H    -0.870152  -1.587961   0.109521
H    -3.168628  -2.402443   0.238291
H    -3.511661  -1.606946  -2.054686
H    -3.804058  -0.665230   0.201730
```

Frequencies

-367.19	78.7441	97.9086
105.1915	132.4796	158.1846
177.4349	204.7996	230.473
280.501	306.7367	370.1766
392.9105	462.1125	593.2645
619.1588	677.4165	722.6434
915.8686	948.8868	952.7457
1041.446	1047.178	1056.97
1060.635	1064.136	1071.701
1185.851	1255.263	1325.285
1378.779	1417.799	1423.991
1459.249	1480.609	1486.313
1490.27	1497.216	1656.213
1698.147	2367.997	3045.607
3050.087	3110.843	3123.066
3123.695	3141.634	3156.163
3171.591	3187.577	3253.248

i53 – i54
```
C     0.369066   2.541430   0.256965
C     0.432693   1.066535  -0.045157
C    -3.160799  -0.895482  -0.021172
C    -1.880379  -0.199918  -0.034338
C    -0.816286   0.362136  -0.046912
C     1.580238   0.421634  -0.300035
H    -0.257681   3.057174  -0.476127
```

```
H    1.365202   2.987516   0.240496
H   -0.076135   2.712569   1.241151
H   -3.825177  -0.504792  -0.796248
H   -3.659530  -0.772856   0.943712
H   -3.023085  -1.964688  -0.199363
H    2.502511   1.007087  -0.277679
C    1.686084  -1.014551  -0.585414
C    1.787636  -2.009236   0.519654
H    1.569486  -1.356646  -1.609082
H    0.840218  -2.067419   1.076212
H    2.555947  -1.723922   1.248366
H    2.018728  -3.009315   0.147016
```

Frequencies

-242.065	69.9868	91.9464
122.6563	128.6786	149.1504
180.7098	187.2968	304.5033
314.5049	353.0573	419.7422
482.9155	607.1665	630.8362
649.9328	837.0431	922.5731
990.5672	1014.651	1061.027
1063.246	1066.191	1071.999
1105.92	1153.574	1219.533
1339.645	1391.112	1408.063
1420.041	1426.937	1475.677
1478.848	1487.465	1490.034
1491.5	1500.955	1710.388
2375.12	2995.202	3048.431
3049.804	3054.78	3097.922
3114.031	3120.202	3125.041
3126.515	3142.868	3182.176

i54 – p87

```
C   -0.928847  -2.365592   0.294132
C   -0.607486  -0.926961  -0.031038
C    3.120401   0.207466  -0.271569
C    1.863322  -0.180296  -0.186949
C    0.653624  -0.523529  -0.096526
C   -1.749900  -0.046382  -0.292764
C   -1.810811   1.284513  -0.163053
C   -0.724850   2.201788   0.303699
H   -1.484048  -2.822523  -0.531779
H   -1.562735  -2.421149   1.184653
H   -0.023272  -2.945300   0.469196
H    3.373905   1.217138  -0.576635
H    3.934570  -0.486642  -0.093981
H    3.594631   1.026797   1.975692
H   -2.655956  -0.564818  -0.598890
H   -2.759054   1.754184  -0.412367
H   -0.099589   2.526484  -0.535578
H   -0.061804   1.713035   1.020530
H   -1.149366   3.096743   0.763564
```

Frequencies

-369.083	45.2278	74.2422
104.0268	120.9096	135.3467
160.5343	185.5847	256.3357
296.5459	312.8616	364.7561
497.5633	523.3996	559.6774
591.9835	652.3116	729.8193
749.9379	859.3713	932.4095
992.6322	1004.524	1033.177
1050.916	1064.2	1087.795

1160.466	1223.025	1299.727
1403.867	1407.695	1445.465
1457.439	1485.234	1486.206
1487.995	1498.366	1694.513
1719.472	2172.283	3040.788
3043.047	3102.731	3107.157
3138.184	3150.163	3155.527
3160.49	3181.577	3237.358

i54 – p84
```
C   -0.776356  -2.331881  -0.272566
C   -0.609925  -1.005086  -0.104045
C    3.225485   0.412183   0.064983
C    1.860097  -0.090268  -0.003098
C    0.724026  -0.481282  -0.057108
C   -1.791318  -0.144402   0.072004
C   -1.907276   1.186861   0.097537
C   -0.867698   2.251410  -0.070217
H   -1.768865  -2.765502  -0.319937
H   -0.748481  -3.154075   1.990087
H    0.070125  -2.990530  -0.418498
H    3.765091   0.197505  -0.860840
H    3.768785  -0.054099   0.890673
H    3.233078   1.494061   0.220975
H   -2.709633  -0.713356   0.194075
H   -2.914906   1.565118   0.258743
H   -1.225207   3.006078  -0.777264
H    0.084176   1.864536  -0.425191
H   -0.696367   2.765054   0.882241
```

Frequencies

-360.284	50.5411	66.5412
80.2933	120.7931	133.289
147.6699	187.5279	250.7723
305.4416	333.2753	353.6426
413.633	532.6337	619.7326
641.0412	713.9394	740.7816
807.02	902.2903	928.626
979.8398	1021.935	1053.589
1058.289	1078.163	1079.994
1122.821	1295.573	1361.287
1410.569	1416.043	1428.884
1462.986	1480.307	1487.866
1493.24	1498.543	1636.302
1742.12	2377.128	3043.902
3050.188	3097.41	3122.834
3124.769	3147.41	3170.404
3176.196	3184.374	3270.553

i54 – p88
```
C   -0.129992  -2.240935   0.357874
C   -0.101726  -0.779673  -0.022797
C    3.556317   1.044126   0.032005
C    2.250768   0.398491   0.007028
C    1.163855  -0.117638  -0.017895
C   -1.191455  -0.139540  -0.423702
C   -2.274543   0.574547  -0.557188
C   -2.953892   1.278205   0.587726
H    0.469624  -2.825686  -0.345676
H   -1.151085  -2.622885   0.352916
H    0.300529  -2.376643   1.353551
H    4.209310   0.633922  -0.742669
H    4.044346   0.896542   0.998778
H    3.458482   2.118735  -0.139477
```

```
H    -1.117101   -0.996680   -2.340614
H    -2.724037    0.678600   -1.540870
H    -3.011046    2.353311    0.393669
H    -2.416779    1.122359    1.524020
H    -3.978233    0.912931    0.708062
```

Frequencies

-559.876	59.2324	102.7604
115.6323	127.129	150.1994
153.7791	180.828	204.5605
257.7116	304.8666	346.3962
413.5254	490.932	509.3978
564.0395	620.0303	666.6027
836.6709	879.7277	996.1451
1056.038	1057.966	1061.977
1064.527	1066.551	1109.024
1233.053	1300.388	1408.68
1412.822	1420.21	1432.344
1480.775	1488.404	1489.502
1493.158	1494.816	1508.723
2029.92	2369.786	3048.434
3049.522	3050.347	3112.022
3117.182	3120.854	3126.693
3146.55	3156.534	3165.823

i54 – p12b
```
C    -0.822484   -2.443536   -0.023055
C    -0.683721   -0.941169   -0.003383
C     3.200080    0.328293    0.009466
C     1.815396   -0.121847   -0.004577
C     0.659381   -0.459238   -0.010563
C    -1.765377   -0.137805    0.043866
C    -1.836733    1.317161    0.082113
C    -0.900981    2.202447   -0.289300
H    -0.362524   -2.858927   -0.924244
H    -1.871815   -2.742611    0.003076
H    -0.309639   -2.886270    0.835636
H     3.693988    0.095972   -0.937537
H     3.758658   -0.160574    0.811581
H     3.253473    1.408397    0.167352
H    -2.728463   -0.639662    0.093756
H    -2.782286    1.709188    0.450027
H    -1.101739    3.265702   -0.227051
H     0.042023    1.897747   -0.723883
H     0.414951    2.445208    1.623873
```

Frequencies

-289.489	54.8906	67.5592
83.9254	154.8187	160.9089
178.2617	210.7193	243.7018
272.4511	314.8119	349.45
370.2234	528.729	590.8954
634.0991	674.8159	716.4383
901.3527	961.7186	964.3436
1019.38	1038.87	1054.769
1056.984	1072.625	1073.194
1144.337	1244.646	1348.283
1414.02	1418.387	1427.015
1466.076	1479.313	1479.859
1488.02	1502.036	1661.019

1703.986	2365.431	3047.804
3050.291	3114.996	3122.163
3125.778	3138.919	3149.756
3171.932	3179.616	3274.48

i40 – p12a

C	-0.008758	2.472293	0.102070
C	-0.188253	0.980272	0.048807
C	1.000838	0.197551	0.020418
C	2.028820	-0.430658	0.000842
C	3.266329	-1.198507	-0.019352
C	-1.421033	0.408806	-0.023016
C	-2.889489	-1.559761	0.111504
C	-1.673809	-1.027732	-0.003221
H	0.599522	2.757217	0.964968
H	-0.971726	2.981641	0.165910
H	0.512133	2.823887	-0.793952
H	3.780204	-1.127554	0.942841
H	3.066885	-2.253577	-0.221008
H	3.943131	-0.825475	-0.792183
H	-1.714422	0.776940	-2.018838
H	-2.286285	1.057986	0.082576
H	-3.777112	-0.937661	0.179640
H	-3.036605	-2.632909	0.137079
H	-0.803592	-1.674082	-0.075337

Frequencies

-667.503	80.5817	105.8845
112.0831	118.9631	162.1249
190.1157	211.6824	289.3554
306.5873	330.3088	394.738
402.9932	459.6247	588.0375
619.7779	681.497	704.485
928.1377	947.0588	951.8282
1040.737	1043.209	1057.474
1061.027	1064.279	1067.629
1178.715	1246.829	1316.895
1377.835	1419.672	1425.467
1452.134	1478.084	1486.701
1489.89	1496.718	1613.222
1717.338	2353.197	3045.197
3050.469	3109.823	3122.023
3126.226	3143.135	3152.726
3176.196	3184.86	3247.376

i47 – p60

C	0.502343	0.948231	0.036135
C	-0.644266	0.219976	0.004603
C	4.232103	-0.718450	0.035565
C	2.901521	-0.125406	0.033789
C	1.800938	0.360533	0.023980
C	-1.954443	0.815207	0.125993
C	-3.129304	0.168881	0.089313
C	-3.356363	-1.299702	-0.084050
H	0.547951	1.653358	-1.887866
H	0.449597	2.010678	0.260202
H	-0.561332	-0.851659	-0.142645
H	4.321685	-1.472808	0.821485
H	4.996321	0.043617	0.206160
H	4.441565	-1.201203	-0.922513
H	-1.972793	1.894609	0.258994
H	-4.030464	0.767225	0.199406
H	-3.880212	-1.709597	0.785677
H	-2.433082	-1.863809	-0.217054
H	-3.994413	-1.486029	-0.953809

Frequencies

-736.313	61.4539	70.2686
97.9794	112.3534	123.3138
186.0452	223.5329	312.4785
323.3808	358.2276	372.9848
412.2363	498.3122	511.7121
627.3834	754.4902	815.4519
897.6473	940.2308	980.6314
1031.787	1048.417	1056.302
1062.461	1065.679	1172.52
1203.012	1261.15	1283.81
1318.854	1406.743	1423.71
1445.09	1482.891	1483.236
1489.379	1493.199	1612.876
1703.808	2375.746	3046.739
3047.929	3101.216	3119.862
3122.702	3147.481	3159.307
3167.464	3181.598	3199.326

i51 – p76'

C	-0.655922	1.618403	0.509680
C	0.204651	2.117481	-0.398534
C	-3.221670	-1.472317	-0.219313
C	-2.304216	-0.370488	0.039369
C	-1.548552	0.546112	0.243739
C	2.220651	0.642293	-0.229396
C	1.899452	-0.595095	0.053805
C	2.861906	-1.754785	0.120076
H	-0.654801	2.010215	1.522670
H	0.829923	2.966855	-0.153780
H	0.182611	1.790623	-1.430661
H	-2.690156	-2.427719	-0.234409
H	-3.716489	-1.346837	-1.185728
H	-3.992192	-1.526254	0.553589
H	3.147250	1.152278	-0.464821
H	0.852284	-0.825198	0.258181
H	2.831874	-2.219884	1.110137
H	3.887590	-1.441053	-0.083199
H	2.584310	-2.522649	-0.608533

Frequencies

-208.024	40.7744	64.2382
101.8548	108.8876	118.6484
152.0355	185.8778	212.9364
242.5187	332.6823	408.8738
412.4473	546.6623	675.0456
716.0864	730.5223	861.576
909.361	911.1668	947.651
976.1309	1051.248	1058.322
1064.511	1070.947	1108.147
1201.293	1303.331	1314.585
1402.865	1423.688	1439.867
1484.301	1488.005	1492.432
1492.921	1616.371	1702.698
2350.824	3043.706	3048.938
3109.159	3116.28	3119.095
3124.379	3139.105	3167.786

3181.288   3222.1   3266.822

i51 – p78

C	0.762456	-1.719519	-0.115331
C	-0.739712	-1.701614	0.014377
C	3.049818	1.420028	0.173272
C	2.278830	0.355724	0.084748
C	1.539865	-0.664034	-0.016495
C	-1.313901	-0.369595	0.391114
C	-2.212688	0.294052	-0.325075
C	-2.796711	1.622097	0.045716
H	1.223235	-2.687343	-0.303339
H	-1.016447	-2.454143	0.765485
H	-1.176912	-2.050543	-0.929094
H	2.630592	2.396037	0.392781
H	3.176462	2.201770	-2.012136
H	4.129051	1.336635	0.103163
H	-0.943895	0.064663	1.318727
H	-2.565713	-0.144016	-1.258383
H	-2.606159	2.364464	-0.735729
H	-2.374898	1.996229	0.981382
H	-3.883050	1.553411	0.163187

Frequencies

-388.068	44.1582	80.6433
113.2609	139.3633	173.5502
192.5583	210.3008	265.1828
280.0362	294.0545	390.5442
488.3508	522.5711	577.216
628.8706	786.4745	828.4697
856.5424	888.9298	936.6948
973.5045	1015.163	1032.906
1035.955	1076.156	1113.94
1140.247	1226.735	1299.165
1332.461	1347.226	1379.889
1420.693	1452.644	1470.627
1490.049	1498.502	1705.885
1779.987	2187.865	3022.302
3037.37	3060.11	3098.554
3121.931	3142.19	3148.954
3149.727	3151.795	3236.907

i51 – p58

C	-0.700270	1.605276	-0.147778
C	0.639892	1.404040	-0.032644
C	-3.527650	-1.326627	0.047162
C	-2.513602	-0.283621	-0.023191
C	-1.672561	0.578326	-0.077702
C	1.272434	0.092763	0.038931
C	2.589453	-0.094346	-0.059665
C	3.270178	-1.424366	-0.016382
H	-1.069706	2.618118	-0.271819
H	0.806873	1.922178	1.918801
H	1.294150	2.258021	-0.182484
H	-4.022236	-1.321913	1.022107
H	-3.081851	-2.312957	-0.102539
H	-4.291748	-1.178099	-0.720151
H	0.610462	-0.761058	0.163697
H	3.233313	0.776265	-0.179322
H	3.822856	-1.609645	-0.943376
H	2.552355	-2.235615	0.122430
H	3.998291	-1.463959	0.800275

Frequencies

-746.556	64.473	96.6387
114.6888	136.9246	181.0166
210.2182	212.3537	273.2793

288.768	363.5371	412.1458
431.4733	472.3743	539.4245
650.3003	785.414	798.0433
847.4776	953.6134	986.7315
1024.227	1056.389	1061.652
1071.251	1080.836	1139.561
1188.164	1246.914	1298.619
1333.057	1418.228	1420.753
1434.289	1483.543	1484.505
1490.746	1497.856	1591.893
1744.651	2349.805	3040.205
3046.926	3099.337	3119.22
3121.805	3129.358	3153.879
3174.68	3181.247	3196.911

i47 – p68
```
C    0.540954   1.589360   0.021063
C   -0.828564   0.978867  -0.129991
C    3.670128  -1.089320   0.083193
C    2.559774  -0.143627   0.059463
C    1.650378   0.639716   0.042284
C   -1.094780  -0.322646  -0.228621
C   -2.436115  -0.896952  -0.348133
C   -3.559291  -0.375821   0.165269
H    0.698839   2.311397  -0.789647
H    0.558069   2.181627   0.944850
H   -1.642920   1.699024  -0.168253
H    3.317206  -2.107164  -0.100028
H    4.172271  -1.075307   1.053567
H    4.407511  -0.843324  -0.684720
H   -0.262199  -1.022057  -0.244008
H   -2.500445  -1.848284  -0.870681
H   -4.523648  -0.835453  -0.014706
H   -3.553764   0.561351   0.712456
H   -3.685824  -1.299266   2.174012
```

Frequencies

-469.282	56.1227	74.9325
90.2922	145.7041	166.4958
198.9696	224.7347	242.5523
257.6873	305.0724	392.7192
399.3814	536.0896	640.8246
694.0204	763.0793	832.1932
963.9069	975.6048	982.6599
1006.177	1020.969	1038.38
1051.831	1064.023	1104.017
1177.694	1242.533	1302.394
1315.613	1351.481	1378.089
1416.375	1455.844	1467.361
1486.22	1490.795	1665.457
1741.735	2399.407	3031.732
3054.528	3059.161	3127.187
3128.215	3156.106	3165.265
3170.73	3179.359	3250.186

i47 – p71
```
C    0.495505   1.888677  -0.269725
C   -0.979318   1.584424  -0.141913
C    2.923993  -1.412261   0.125382
```

```
C    2.070424   -0.238839   -0.018232
C    1.366871    0.726052   -0.133432
C   -1.474000    0.469475    0.360396
C   -1.971479   -0.723211    0.549756
C   -2.239521   -1.689997   -0.571449
H    0.667537    2.364994   -1.241752
H    0.767351    2.639525    0.483512
H   -1.659094    2.396799   -0.387979
H    2.335419   -2.330136    0.052565
H    3.428444   -1.410276    1.094735
H    3.688406   -1.437250   -0.655108
H   -1.251547    1.035223    2.249700
H   -2.200159   -1.049728    1.559385
H   -1.691888   -2.622936   -0.408770
H   -1.935367   -1.272452   -1.531871
H   -3.303946   -1.939680   -0.619112
```

Frequencies

-747.176	28.4267	58.351
89.1878	93.6078	140.7065
157.4521	205.8575	225.5673
291.2073	320.1432	396.4524
468.0297	478.2203	586.929
648.0682	711.831	762.4254
885.2881	890.8304	956.1864
977.8888	1054.455	1062.268
1063.686	1107.638	1146.655
1188.456	1242.56	1299.579
1360.661	1411.241	1418.62
1447.383	1478.049	1483.413
1484.83	1492.552	1505.352
2029.372	2405.707	3031.067
3046.299	3053.539	3064.728
3109.26	3125.152	3127.237
3147.835	3164.955	3185.424

i47 – p61
```
C    0.458392    1.396454   -0.102886
C   -0.812153    0.910287   -0.104164
C    3.825852   -0.917023   -0.009684
C    2.622092   -0.097198   -0.043768
C    1.627537    0.579602   -0.062385
C   -1.152575   -0.482169    0.062867
C   -2.391787   -0.997174    0.083520
C   -3.690577   -0.268393   -0.060177
H    0.616368    2.448562   -0.315459
H    0.566086    2.091162    1.829186
H   -1.613388    1.633734   -0.209071
H    3.662272   -1.871392   -0.516289
H    4.120307   -1.126910    1.021985
H    4.657576   -0.407821   -0.502566
H   -0.314236   -1.162879    0.181230
H   -2.480020   -2.072394    0.219977
H   -4.254291   -0.661597   -0.912374
H   -3.568805    0.805355   -0.204178
H   -4.312555   -0.422135    0.827611
```

Frequencies

-722.306	43.5918	75.4675
116.2242	119.4627	170.751
210.5343	231.715	259.7892
322.04	370.2661	404.0998
411.0979	554.814	564.0046
680.0445	759.7968	784.4269
841.0199	942.1861	990.5533

1028.832	1031.301	1055.918
1062.465	1063.765	1146.144
1183.257	1258.808	1298.482
1381.916	1419.363	1421.502
1479.365	1486.022	1487.309
1490.744	1495.221	1593.561
1701.428	2372.662	3046.194
3048.714	3100.915	3120.446
3124.004	3144.321	3164.807
3184.945	3192.163	3206.694

i29 – p10a

```
C    0.608284   -0.732193   -0.511003
C   -0.479081   -0.414796    0.221016
C    4.376604    0.648289    0.226124
C    3.030323    0.157402   -0.035651
C    1.914281   -0.245051   -0.245010
C   -1.802245   -0.912213   -0.048934
C   -2.894269   -0.560753    0.670322
C   -3.793620    1.483661   -0.359048
H    0.500748   -1.403430   -1.360193
H   -0.361757    0.257102    1.068309
H    4.375443    1.732479    0.365451
H    5.045408    0.412620   -0.605269
H    4.787984    0.192576    1.130843
H   -1.918338   -1.573192   -0.904889
H   -2.793746    0.019083    1.581347
H   -3.855889   -1.024044    0.490874
H   -4.135757    1.062902   -1.295454
H   -2.868726    2.045104   -0.366355
H   -4.537033    1.732727    0.388444
```

Frequencies

-333.888	47.0606	81.9299
87.0642	91.0399	99.4784
146.1298	219.4466	243.5907
304.3812	350.6787	410.6322
443.7574	456.0347	476.3452
551.6218	716.9319	730.4918
823.4596	872.0199	909.3653
944.902	974.7312	1018.409
1050.618	1056.233	1194.188
1213.683	1279.538	1297.553
1328.488	1414.475	1415.846
1416.667	1451.325	1482.921
1488.368	1592.697	1647.773
2361.004	3050.116	3108.193
3120.059	3125.633	3161.082
3164.181	3169.213	3176.098
3258.439	3280.137	3285.481

i29 – p72

```
C    0.618262   -1.005676   -0.002995
C   -0.630875   -0.263243    0.013595
C    4.141748    0.660262    0.172820
C    2.951542    0.096359    0.122388
C    1.814656   -0.445246    0.061261
C   -1.827797   -0.855275   -0.051934
C   -3.161527   -0.171243   -0.042323
C   -3.125864    1.350815    0.029357
H    0.554689   -2.090205   -0.075107
H   -0.548879    0.817334    0.083235
```

```
H     4.248678    1.735075    0.270175
H     4.694920    1.044408   -2.155601
H     5.045293    0.060268    0.179714
H    -1.860533   -1.942162   -0.120114
H    -3.741543   -0.567803    0.800830
H    -3.711654   -0.485780   -0.938339
H    -2.595455    1.775542   -0.827194
H    -2.627297    1.694757    0.939529
H    -4.139083    1.758039    0.029861
```

Frequencies

-379.17	65.8514	69.292
107.9532	151.5603	175.4659
202.442	214.1207	269.6654
310.9262	319.9826	342.9316
492.4462	533.3157	591.6027
608.747	750.7108	864.335
881.9056	887.7854	903.3962
951.8497	1015.173	1032.841
1036.797	1107.32	1112.347
1180.609	1263.491	1294.971
1344.753	1351.467	1384.176
1424.998	1452.82	1476.623
1504.288	1516.561	1682.497
1730.678	2159.138	3030.257
3054.356	3055.621	3127.579
3135.149	3146.048	3147.487
3148.788	3189.163	3234.851

i29 – p74

```
C    -0.399049   -0.773228    0.743817
C     0.704237   -0.756682    0.026568
C    -4.099085    0.551279   -0.363194
C    -2.777994    0.078893    0.027803
C    -1.678593   -0.304379    0.328496
C     1.924774   -0.948742   -0.428230
C     3.007583    0.096607   -0.449514
C     2.715401    1.324469    0.403984
H    -0.329491   -1.178465    1.751670
H     0.129668    0.500924   -1.407397
H    -4.386467    0.138285   -1.333395
H    -4.112912    1.641381   -0.441735
H    -4.852053    0.253654    0.370593
H     2.137462   -1.895537   -0.921929
H     3.168916    0.395331   -1.493463
H     3.942541   -0.376719   -0.128877
H     2.576837    1.047981    1.452400
H     1.803099    1.824290    0.069181
H     3.538755    2.039576    0.344577
```

Frequencies

-769.773	30.67	48.9259
75.4657	106.7871	137.8708
187.0924	251.5717	272.4826
305.2016	376.6453	407.7848
452.4375	484.1413	505.0227
649.5698	723.6414	806.0388
816.3709	868.4215	897.4526
1007.789	1054.572	1058.619
1094.32	1103.85	1128.148
1211.774	1292.962	1302.204
1370.82	1416.836	1422.751

1461.763	1483.003	1484.18
1484.682	1501.45	1508.405
2004.891	2381.953	3029.186
3046.698	3049.575	3065.292
3119.433	3121.878	3126.197
3131.149	3143.028	3144.445

i49 – p77

C	0.626683	1.539442	-0.448938
C	-0.068969	0.653274	0.550741
C	-3.871329	-0.693774	-0.175036
C	-2.519723	-0.209695	0.080676
C	-1.406258	0.185146	0.299788
C	1.081036	0.109945	-0.295947
C	2.367824	-0.185716	0.352327
C	3.177856	-1.192429	0.005085
H	1.274951	2.316472	-0.061008
H	0.082839	1.797713	-1.348396
H	0.166951	0.832027	1.594849
H	-4.436283	0.017927	-0.782236
H	-4.410579	-0.840094	0.764154
H	-3.850153	-1.650059	-0.703799
H	0.783784	-0.572787	-1.084201
H	2.672901	0.493280	1.147132
H	2.886762	-1.913599	-0.751702
H	4.099077	-1.384737	0.541330
H	4.407033	-0.333304	-1.528290

Frequencies

-483.468	63.1984	97.883
107.8222	114.4762	181.8521
239.1563	266.6159	309.0964
327.0914	360.4201	443.1214
507.9107	528.4887	687.6039
752.8808	841.0294	883.9615
939.4604	955.4844	966.0728
1009.585	1023.529	1055.83
1061.478	1074.701	1110.41
1113.403	1198.94	1231.465
1240.074	1317.002	1335.812
1413.135	1424.088	1473.786
1487.668	1489.745	1504.686
1685.855	2393.717	3052.995
3124.636	3126.553	3151.518
3152.902	3164.136	3167.623
3190.297	3248.133	3254.338

i49 – p79

C	-0.739801	1.864668	0.178337
C	-0.106912	0.731807	-0.663652
C	3.622017	-0.716892	0.232247
C	2.298967	-0.194286	-0.086430
C	1.202413	0.228559	-0.335367
C	-1.288224	0.506905	0.205635
C	-2.369116	-0.257633	0.348002
C	-2.471973	-1.654556	-0.173428
H	-1.286944	2.634872	-0.355477
H	-0.156309	2.208825	1.024064
H	-0.321849	0.771720	-1.728536
H	4.183377	-0.010851	0.849300
H	4.195906	-0.898730	-0.679967
H	3.546587	-1.660370	0.778699
H	-0.334783	-0.152003	1.838404
H	-3.193559	0.120323	0.948512
H	-1.605208	-1.911655	-0.784879
H	-3.378199	-1.781221	-0.774153

H   -2.533246   -2.372337   0.651964

Frequencies

-765.091	65.5116	82.2901
93.7383	121.483	170.7249
198.1281	283.4134	296.4731
334.7871	397.6419	448.3587
473.1485	525.3088	542.2157
700.6182	745.2103	813.2487
917.4789	954.6503	971.3015
1045.805	1054.545	1055.811
1057.049	1063.298	1102.148
1121.144	1140.597	1215.277
1336.758	1383.871	1415.671
1418.286	1460.33	1479.669
1486.485	1487.689	1495.119
1805.449	2394.17	3038.354
3051.702	3098.109	3123.861
3124.855	3133.822	3136.19
3149.245	3166.797	3230.178

i49 – i50

```
C     0.606946   1.676759   0.024561
C     0.139972   0.317413   0.403840
C    -3.870102  -0.478984  -0.040730
C    -2.448127  -0.198923   0.121509
C    -1.277700   0.030703   0.259007
C     1.017572  -0.068079  -0.752333
C     2.305478  -0.537495  -0.672050
C     3.095898  -0.697106   0.587727
H     1.477530   2.096657   0.507016
H     0.025735   2.279200  -0.658730
H     0.521249  -0.019345   1.367398
H    -4.368375   0.334580  -0.573733
H    -4.355827  -0.593213   0.931538
H    -4.024246  -1.401386  -0.606035
H     0.531802  -0.030166  -1.720318
H     2.822939  -0.720231  -1.608387
H     2.469387  -0.965259   1.443028
H     3.625576   0.228833   0.851517
H     3.854606  -1.475395   0.477527
```

Frequencies

-612.645	57.6966	69.3084
94.9323	130.8484	159.1972
258.3995	283.0177	326.709
366.2595	488.1689	521.1382
547.5722	581.6779	656.2957
681.3974	768.0427	915.2776
943.1636	989.1783	1014.872
1032.05	1060.505	1065.335
1092.569	1157.991	1189.278
1222.386	1262.987	1347.924
1408.064	1425.292	1430.669
1462.439	1486.451	1486.764
1490.053	1502.886	1543.363
2397.5	3012.322	3049.459
3083.684	3117.274	3120.012

| 3124.818 | 3125.148 | 3181.75 |
| 3182.985 | 3213.899 | 3306.85 |

i29 – p60

C	-0.560134	-0.946603	-0.064451
C	0.577071	-0.228660	-0.027086
C	-4.312137	0.654147	0.051261
C	-2.972193	0.084252	0.013149
C	-1.860710	-0.378061	-0.019844
C	1.889028	-0.832935	-0.084410
C	3.068846	-0.179670	-0.063380
C	3.272254	1.306653	-0.070979
H	-0.503863	-2.030541	-0.137698
H	0.501345	0.851795	0.043407
H	-4.389676	1.412007	0.834941
H	-5.058768	-0.118676	0.249081
H	-4.558478	1.128302	-0.902542
H	1.912158	-1.918847	-0.138192
H	3.969583	-0.776927	-0.174557
H	3.500445	-0.509675	2.066802
H	2.406805	1.854665	0.303066
H	3.474325	1.652101	-1.090903
H	4.133978	1.581055	0.541040

Frequencies

-512.886	64.933	74.329
94.3254	105.6365	122.2715
194.7726	207.4705	272.6061
298.6348	322.838	358.2957
410.1959	500.058	510.2742
629.192	768.5853	817.9533
889.8514	939.6307	973.3032
1017.989	1047.996	1053.56
1057.968	1063.788	1170.315
1209.849	1263.909	1297.698
1336.294	1404.087	1421.467
1445.451	1481.842	1485.278
1491.806	1494.38	1658.736
1680.438	2368.196	3046.972
3049.483	3111.75	3121.241
3124.287	3146.056	3158.903
3163.02	3186.701	3193.799

i47 – i48

C	-0.112665	1.889546	-0.133648
C	-1.410110	1.168585	-0.377251
C	3.042366	-0.749513	0.174240
C	1.943077	0.202248	0.063358
C	1.031365	0.977933	-0.025057
H	0.071725	2.611278	-0.934549
H	-0.177387	2.473265	0.798339
H	-2.053212	1.518323	-1.178624
H	2.793516	-1.689026	-0.326339
H	3.260524	-0.971372	1.221908
H	3.951619	-0.353222	-0.284639
C	-1.907477	0.161441	0.570910
C	-1.729429	-1.155010	0.473586
C	-0.996533	-1.859615	-0.625584
H	-2.455464	0.539068	1.438165
H	-2.145758	-1.786215	1.255931
H	-0.147827	-2.420027	-0.220474
H	-0.612081	-1.154748	-1.364804
H	-1.649211	-2.581020	-1.128249

Frequencies

| -224.914 | 48.9385 | 63.5769 |
| 128.0855 | 153.0838 | 190.841 |

204.0287	235.7266	284.0927
361.462	393.4041	450.1594
556.1002	629.5601	720.8304
770.2634	859.7106	938.8198
992.4449	999.4694	1059.553
1064.869	1075.196	1087.87
1116.192	1175.9	1226.16
1261.987	1324.026	1347.238
1403.054	1421.459	1437.746
1463.9	1485.133	1488.925
1490.751	1492.82	1739.727
2396.505	2983.556	3041.62
3049.114	3086.028	3090.305
3100.917	3120.013	3123.054
3136.821	3167.547	3183.37

i50 – i52

```
C    0.484592    1.782203   -0.065402
C   -0.283132    0.512813   -0.296086
C    3.605155   -0.788844    0.027318
C    2.176952   -0.537244   -0.124992
C    1.093466    0.049021   -0.202416
C   -1.211651    0.064695    0.786047
C   -2.442441   -0.414525    0.632741
C   -3.193089   -0.631967   -0.646170
H    0.775988    2.395494   -0.906000
H    0.575275    2.174174    0.938572
H   -0.697354    0.426596   -1.299362
H    4.152177    0.135816    0.248378
H    4.024033   -1.219623   -0.886116
H    3.792794   -1.495786    0.840067
H   -0.804709    0.149700    1.791058
H   -2.980700   -0.691629    1.536601
H   -3.435836   -1.692089   -0.770536
H   -2.638111   -0.311480   -1.528747
H   -4.142669   -0.088086   -0.630150
```

Frequencies

-703.268	35.4715	88.2631
106.679	126.4738	133.5541
209.2924	250.5034	327.1187
364.1513	393.9482	496.8172
573.2426	619.9492	676.1589
720.2208	813.6582	871.6969
946.6307	1020.373	1034.554
1044.897	1060.363	1071.638
1084.865	1154.227	1194.453
1218.344	1292.424	1331.272
1414.027	1419.397	1439.218
1451.751	1479.941	1483.01
1486.24	1500.174	1767.024
2097.779	3021.788	3047.892
3092.736	3104.366	3116.112
3125.572	3140.607	3152.747
3168.654	3174.921	3290.999

i27 – i48

```
C    0.188131    0.983126    0.744336
```

```
C    -0.672128    1.254791   -0.464663
C     3.764288   -0.783541   -0.301171
C     2.501522   -0.157716    0.075109
C     1.462180    0.355576    0.388035
C    -1.888002    0.746833   -0.651493
H     0.391292    1.925220    1.267664
H    -0.357274    0.342054    1.444400
H    -0.239456    1.902678   -1.222164
H     4.612184   -0.158266   -0.010187
H     3.814622   -0.939514   -1.381716
H     3.878234   -1.755412    0.185548
H    -2.408112    1.007975   -1.577150
C    -2.583437   -0.169709    0.265311
C    -2.565550   -1.640262    0.021026
H    -3.261970    0.240185    1.007567
H    -3.029409   -2.193410    0.840175
H    -1.539153   -2.003228   -0.109718
H    -3.102980   -1.902869   -0.903357
```

Frequencies

-178.231	19.6333	95.5224
114.3204	117.1237	162.6159
218.0703	236.3231	305.5602
334.9739	398.6332	449.2813
548.0481	612.5233	712.9579
810.107	887.413	937.3992
980.8119	1008.243	1040.166
1057.297	1062.654	1106.146
1127.348	1172.363	1214.488
1269.359	1322.057	1344.172
1406.389	1418.71	1432.908
1473.717	1474.838	1488.161
1491.984	1493.012	1735.152
2395.773	2988.417	3040.491
3048.51	3056.066	3085.645
3090.258	3118.955	3122.472
3123.943	3171.612	3180.493

i50 – p76

```
C    -0.396773    1.911392    0.467377
C     0.033969    0.906122   -0.343566
C     3.795007   -0.679952   -0.029649
C     2.453780   -0.120148   -0.141578
C     1.350924    0.350503   -0.229911
C    -1.061712   -0.964649    0.399058
C    -2.355217   -1.128313    0.253582
C    -3.316059   -0.176822   -0.401775
H    -1.346464    2.399551    0.286266
H     0.161781    2.196071    1.350437
H    -0.470527    0.732042   -1.289035
H     4.540647    0.013433   -0.427189
H     3.873788   -1.618467   -0.583778
H     4.043840   -0.880758    1.015428
H    -0.301128   -1.575898    0.866635
H    -2.799781   -2.048030    0.647501
H    -2.808681    0.705408   -0.793492
H    -4.075418    0.154397    0.313218
H    -3.841577   -0.666547   -1.227226
```

Frequencies

-435.523	40.8068	73.8013
106.6717	123.8037	137.493
158.9874	189.1514	240.3327
296.2094	340.3913	416.7892
484.242	547.0047	605.3779
629.6065	725.8221	852.0767

875.5443	897.7655	944.1122
969.2286	1044.901	1058.549
1061.841	1071.305	1131.869
1194.927	1277.434	1289.002
1418.663	1420.79	1439.361
1487.514	1489.333	1491.185
1495.449	1567.875	1710.149
2382.02	3045.145	3048.538
3068.455	3103.503	3118.789
3124.492	3151.501	3162.483
3177.985	3238.659	3262.911

i47 – i52

```
C     0.802681   1.957717  -0.194482
C    -0.271317   0.921920  -0.383602
C     2.431695  -1.758704   0.099243
C     2.202500  -0.315071   0.029057
C     1.431376   0.658752  -0.101888
C    -1.153455   0.533049   0.690524
C    -2.198994  -0.308660   0.616356
C    -2.683332  -1.035809  -0.599648
H     1.054310   2.562589  -1.062827
H     0.754441   2.536616   0.726663
H    -0.516663   0.665370  -1.406177
H     3.103307  -2.089288  -0.697546
H     1.487763  -2.311376   0.006237
H     2.892810  -2.033548   1.051693
H    -0.921385   0.962930   1.663326
H    -2.756323  -0.494072   1.530734
H    -2.604461  -2.119162  -0.456425
H    -2.121119  -0.780105  -1.499049
H    -3.739607  -0.819118  -0.789997
```

Frequencies

-698.13	40.8029	84.9348
109.0757	120.8921	153.8513
204.1244	232.6301	357.231
378.3374	405.7441	486.8048
598.2084	703.8051	744.2799
823.0606	893.5626	950.0074
994.6094	1019.089	1031.912
1056.676	1058.896	1080.196
1102.575	1170.026	1191.348
1219.387	1290.591	1341.668
1407.264	1417.384	1465.429
1468.273	1475.232	1481.649
1490.101	1494.188	1670.85
2022.109	3014.863	3036.694
3089.267	3093.844	3094.514
3119.196	3133.6	3151.629
3169.839	3179.358	3210.94

i52 – p81

```
C     0.619656   1.865547  -0.108096
C    -0.265461   0.638375  -0.327124
C     3.212461  -1.118334   0.042505
C     2.218281  -0.261294  -0.048329
C     1.209472   0.520136  -0.153080
C    -1.148475   0.172546   0.764645
C    -2.325512  -0.436018   0.635757
C    -3.036093  -0.796822  -0.633205
H     0.784633   2.524129  -0.954274
```

```
H      0.561696    2.359511    0.857077
H     -0.621144    0.501643   -1.342962
H      3.821666   -1.356406   -0.822680
H      2.321063   -2.986680   -0.218258
H      3.544764   -1.483819    1.008101
H     -0.764604    0.350217    1.767052
H     -2.842551   -0.712165    1.551728
H     -3.208448   -1.876658   -0.681007
H     -2.484488   -0.508703   -1.529111
H     -4.018561   -0.315882   -0.674098
```

Frequencies

-527.084	35.6093	89.4425
148.7663	162.2336	179.7435
230.4862	267.1034	310.7255
341.7289	388.4891	488.994
558.5112	605.5175	650.0217
685.0291	777.1066	857.8285
900.6434	935.4767	941.8521
979.5652	1015.181	1024.035
1038.203	1057.22	1068.477
1093.943	1103.12	1178.717
1294.888	1310.111	1368.662
1418.008	1454.007	1461.359
1485.067	1504.505	1529.546
1762.02	2102.979	3046.704
3102.728	3130.234	3137.357
3146.973	3153.87	3175.79
3183.339	3222.054	3232.851

i48 – p69
```
C      0.101425   -0.342535   -0.478297
C     -0.599672    0.980112   -0.300409
C      4.136028   -0.061368    0.316843
C      2.709859   -0.164050    0.028223
C      1.535540   -0.254503   -0.203113
C     -1.862021    1.176705    0.095230
C     -2.879039    0.180712    0.426487
C     -3.018004   -1.045196   -0.100387
H     -0.351399   -1.099826    0.170918
H     -0.040750   -0.700996   -1.506484
H      0.011435    1.855996   -0.498037
H      4.338733   -0.297685    1.364348
H      4.500215    0.950522    0.122540
H      4.711192   -0.751950   -0.304788
H     -2.177921    2.209108    0.223369
H     -3.611445    0.499436    1.164875
H     -1.888246   -2.402204    1.274446
H     -2.387827   -1.402999   -0.906021
H     -3.848688   -1.678672    0.187376
```

Frequencies

-442.084	37.2752	78.7389
99.5511	121.6807	173.9429
214.9618	241.8854	253.6381
292.2818	354.173	395.9515
434.6302	509.6933	607.5843
701.3497	779.1675	833.5016
900.1831	941.3982	956.8688
1024.66	1038.182	1054.821
1064.306	1067.729	1102.403
1175.695	1233.984	1274.034

1324.013	1342.264	1421.311
1430.113	1457.819	1470.493
1489.078	1490.822	1666.398
1721.492	2399.477	3026.04
3051.485	3068.031	3122.832
3125.291	3156.21	3165.646
3172.895	3190.043	3258.103

i48 – p65

```
C     0.146101   -0.134726    0.122826
C    -0.600889    0.973347   -0.127605
C     4.230992   -0.128431    0.013028
C     2.774653   -0.123307    0.048030
C     1.571803   -0.121477    0.069127
C    -2.036473    1.131770    0.014266
C    -2.999383    0.198286    0.082907
C    -2.850027   -1.288915   -0.001860
H    -0.305790   -1.013143    0.568974
H    -0.083752   -1.172511   -1.647688
H    -0.063213    1.858422   -0.456375
H     4.634504   -0.779437    0.792535
H     4.629345    0.877043    0.169208
H     4.594749   -0.491394   -0.951947
H    -2.364826    2.167329    0.049563
H    -4.015572    0.564849    0.203997
H    -3.779021   -1.750350   -0.342036
H    -2.616151   -1.721343    0.978800
H    -2.050932   -1.578742   -0.689347
```

Frequencies

-682.275	51.8512	62.8686
82.4278	105.4068	172.2564
221.1933	248.5025	297.7449
342.8851	354.5955	376.0656
449.3436	505.6386	515.5368
689.2338	714.3873	859.6963
896.1324	916.4421	998.4454
1007.91	1051.595	1053.312
1058.522	1065.34	1102.143
1210.096	1280.238	1329.573
1337.829	1406.034	1417.958
1454.284	1482.131	1486.138
1489.466	1503.64	1613.941
1701.171	2375.193	3031.409
3049.202	3097.728	3119.208
3126.225	3131.181	3156.521
3175.034	3185.604	3208.01

i48 – p64

```
C     0.301889   -1.609811    0.329510
C     1.535988   -1.248621   -0.113522
C    -3.151176    0.464094   -0.345568
C    -1.919854   -0.272437   -0.095395
C    -0.895181   -0.868312    0.107855
C     1.937667    0.009002   -0.725296
C     1.602432    1.256452   -0.369972
C     0.779196    1.690010    0.799089
H     0.165755   -2.631068    0.671820
H     0.477056   -1.275672    2.306712
H     2.314148   -2.003908   -0.035459
H    -3.810451   -0.095055   -1.014360
H    -2.937738    1.430401   -0.809551
H    -3.691079    0.645616    0.587252
H     2.642796   -0.098644   -1.547157
H     2.014898    2.060304   -0.976095
```

```
H      1.257342    2.538106    1.297758
H      0.635577    0.888917    1.525139
H     -0.214071    2.018740    0.473743
```

Frequencies

-749.971	39.4935	78.0201
91.5068	178.5561	197.2304
248.3446	273.242	296.0652
338.9203	357.2981	399.6327
447.9223	545.3136	588.4502
691.8103	731.6247	815.25
856.2358	906.5394	999.3048
1005.343	1006.626	1054.411
1058.007	1069.904	1120.307
1165.675	1261.391	1291.113
1401.548	1417.777	1427.795
1464.241	1482.469	1482.968
1484.462	1505.764	1607.51
1714.349	2375.166	3037.416
3045.834	3097.681	3119.21
3119.795	3134.46	3143.809
3158.199	3166.793	3180.404

i42 – i30

```
C     2.517236   -1.093764    0.144940
C     1.336236   -0.395847   -0.069597
C    -0.008977   -1.022528   -0.056863
C    -1.184260   -0.311909    0.042604
C    -1.182057    1.192880    0.031201
C     0.198271    1.790855    0.029072
C     1.322159    1.081223   -0.041816
C    -2.517388   -0.987032    0.034272
H     2.525390   -2.171877    0.249762
H     3.466418   -0.575122    0.118267
H     0.728188   -0.785424   -1.214688
H    -0.027268   -2.107640   -0.001638
H    -1.752021    1.576601    0.891203
H    -1.736204    1.559490   -0.849790
H     0.260812    2.874279    0.075611
H     2.286320    1.578567   -0.047012
H    -2.423475   -2.074736    0.069027
H    -3.123969   -0.671997    0.892286
H    -3.091509   -0.725414   -0.865898
```

Frequencies

-1919.55	80.6795	126.0974
197.9696	280.912	322.2601
373.2019	415.1953	470.7905
517.3714	535.0952	586.2367
666.2859	696.2606	774.8879
868.3067	874.2448	924.2022
947.0274	951.8748	1003.129
1007.163	1039.597	1049.257
1096.625	1185.398	1206.768
1225.233	1305.986	1321.342
1378.83	1401.892	1421.155
1448.261	1473.2	1481.396
1488.412	1512.792	1567.199
1640.439	1745.725	2959.547

2993.392	3001.338	3052.967
3122.095	3168.38	3174.362
3177.892	3205.019	3268.068

i42 – i45

C	2.464681	-1.166654	0.129873
C	1.325179	-0.396407	-0.065356
C	-0.012044	-1.022246	-0.070614
C	-1.155838	-0.337594	-0.006136
C	-1.201733	1.173970	0.004730
C	0.151411	1.814065	0.082996
C	1.312596	1.084719	-0.009815
C	-2.489994	-1.019791	0.039229
H	2.404322	-2.245855	0.081954
H	3.440729	-0.711152	0.243799
H	1.447271	0.358089	-1.183582
H	-0.034104	-2.107961	-0.091775
H	-1.836653	1.507788	0.839103
H	-1.738233	1.509033	-0.899149
H	0.210280	2.894691	0.130083
H	2.278039	1.570391	0.090556
H	-2.394567	-2.105457	-0.018035
H	-3.017555	-0.766688	0.965731
H	-3.125069	-0.683260	-0.788133

Frequencies

-1892.67	83.7341	146.1719
209.0394	283.2629	330.9128
410.506	441.2843	477.9133
518.1904	526.5133	578.0278
649.6937	687.094	720.9781
858.5714	873.6787	896.3339
919.0303	954.2098	966.5895
1006.87	1043.912	1066.277
1113.295	1168.483	1190.388
1229.237	1311.755	1334.252
1361.506	1407.618	1424.411
1437.546	1479.849	1480.837
1493.952	1516.571	1559.684
1646.819	1760.263	2962.001
2999.349	3032.877	3089.855
3135.316	3164.351	3182.266
3184.609	3209.236	3265.412

i45 – p48

C	-2.412783	-1.183165	-0.127685
C	-1.309984	-0.447590	0.036482
C	0.018970	-1.056706	0.085895
C	1.149015	-0.340935	-0.026070
C	1.067961	1.116958	-0.225464
C	-0.115860	1.760924	-0.199568
C	-1.369257	1.054775	0.217140
C	2.514056	-0.959873	0.000521
H	-2.360128	-2.264349	-0.198441
H	-3.395180	-0.728108	-0.194164
H	0.070956	-2.138637	0.170237
H	1.961002	1.632058	-0.564904
H	1.779251	1.604616	1.606263
H	-0.166919	2.825428	-0.400386
H	-1.522855	1.264264	1.288032
H	-2.240287	1.470299	-0.296017
H	2.461679	-2.039699	0.148072
H	3.047728	-0.765044	-0.935808
H	3.112044	-0.527155	0.809614

Frequencies

-671.145	93.328	153.3833

203.1738	250.0975	297.9946
320.2681	382.8154	426.565
454.2759	527.4272	544.7807
595.4023	695.2897	709.1551
758.7911	870.1042	889.6824
907.6792	940.4672	958.4485
980.4469	1002.857	1024.015
1050.763	1072.115	1193.211
1197.555	1227.869	1316.347
1351.019	1367.213	1416.13
1440.897	1454.65	1462.538
1487.854	1495.774	1622.11
1700.831	1739.439	2990.76
3039.084	3098.728	3098.978
3141.171	3152.601	3176.101
3184.946	3207.348	3240.598

i45 – p46

```
C    -2.380338   -1.238558   -0.085514
C    -1.282565   -0.476057   -0.024614
C     0.065222   -1.046434    0.013050
C     1.178499   -0.307996    0.001888
C     1.123949    1.194538   -0.062808
C    -0.257188    1.759794   -0.124199
C    -1.363445    0.995526   -0.006969
C     2.550187   -0.912411    0.046242
H    -2.312915   -2.320451   -0.112101
H    -3.371427   -0.799315   -0.105115
H     0.140787   -2.130034    0.049079
H     1.705880    1.542191   -0.928768
H     1.650272    1.612783    0.809103
H    -0.354188    2.837658   -0.203706
H    -1.662434    1.183478    1.900604
H    -2.344570    1.443844   -0.124786
H     2.508458   -2.001479    0.101822
H     3.126433   -0.634243   -0.843306
H     3.107778   -0.544847    0.914715
```

Frequencies

-823.181	96.4694	136.514
197.3548	250.695	294.0311
349.8853	415.6681	431.1338
452.315	490.6196	537.9354
629.0765	701.4583	708.9316
789.05	879.6842	881.6547
907.5512	926.8194	955.6508
973.7252	1015.229	1027.357
1047.653	1066.556	1180.591
1199.204	1229.088	1323.091
1359.667	1402.181	1416.855
1439.804	1456.442	1466.441
1481.103	1493.702	1630.026
1701.428	1768.701	2999.962
3020.848	3032.255	3089.294
3137.117	3161.181	3172.312
3177.023	3196.597	3251.343

i45 – i43

C	-2.370600	-1.243386	0.173809
C	-1.277109	-0.479242	-0.019476
C	0.041200	-1.043835	-0.119118
C	1.195104	-0.271490	-0.088248
C	1.061906	1.195258	0.104078
C	-0.181867	1.791613	0.185933
C	-1.412291	1.026683	-0.201287
C	2.561346	-0.887205	0.065477
H	-2.294964	-2.322947	0.248179
H	-3.358184	-0.805212	0.265453
H	0.141154	-2.123167	-0.170719
H	1.272246	0.658814	-1.095588
H	1.967619	1.738672	0.350666
H	-0.259194	2.855312	0.372503
H	-2.284153	1.393164	0.348221
H	-1.632811	1.215335	-1.266216
H	2.624794	-1.841157	-0.461312
H	3.345579	-0.232005	-0.322570
H	2.771784	-1.067187	1.124366

Frequencies

-1954.5	97.9638	172.9498
210.5098	288.2917	332.5343
421.7754	448.4303	519.3976
532.9149	559.4028	656.668
669.7093	696.5729	780.5797
856.3222	865.0222	896.7521
934.7055	950.3112	975.5755
1019.783	1053.273	1076.271
1155.52	1176.45	1205.252
1233.788	1309.873	1337.611
1354.729	1401.874	1425.629
1443.294	1471.926	1492.877
1501.009	1530.893	1559.143
1627.804	1793.957	2955.012
3046.225	3081.017	3113.853
3137.878	3149.884	3186.472
3194.877	3218.949	3239.789

i51 – p62

C	-0.408226	-0.298107	0.197059
C	0.421483	0.762270	0.031292
C	-4.472132	-0.096129	-0.066085
C	-3.020439	-0.163706	0.030044
C	-1.819119	-0.213956	0.107801
C	1.881713	0.696982	0.176457
C	2.647578	-0.333967	-0.179601
C	4.129951	-0.401951	0.005442
H	0.014822	-1.279014	0.396412
H	-0.022690	1.751465	-0.028399
H	0.325441	0.955193	-1.994762
H	-4.828392	-0.647457	-0.940309
H	-4.807851	0.939461	-0.158875
H	-4.941446	-0.529408	0.820903
H	2.353977	1.582145	0.598412
H	2.180234	-1.192198	-0.659902
H	4.405539	-1.253847	0.635893
H	4.518778	0.506363	0.471069
H	4.636734	-0.541317	-0.954894

Frequencies

-731.056	35.911	64.4184
75.127	123.5405	163.3917
206.9619	214.3693	291.601
305.7877	345.205	366.8354
397.6975	477.2384	501.8334

632.5642	799.9764	857.2839
877.6876	925.0698	997.7588
1009.884	1050.982	1056.465
1065.126	1080.08	1136.81
1216.311	1305.47	1318.572
1346.56	1357.13	1416.136
1426.328	1483.062	1484.156
1487.129	1497.394	1631.716
1746.197	2356.554	3037.571
3051.356	3095.836	3121.23
3128.226	3128.665	3153.862
3159.402	3172.53	3185.708

i28 – p11b
```
C   -0.364582  -1.739754  -0.397369
C    3.118588   0.275576   0.273814
C    1.877260  -0.449649   0.041596
C    0.833535  -1.023373  -0.143989
H   -0.229961  -2.726803  -0.830185
H    2.932477   1.351238   0.332762
H    3.832270   0.097585  -0.534453
H    3.584401  -0.040026   1.211223
C   -1.629449  -1.319965  -0.173355
C   -2.105314  -0.070677   0.380920
C   -1.370456   0.905784   0.962755
C   -0.517133   2.334257  -0.883268
H   -2.410937  -2.015020  -0.467870
H   -3.176095   0.091299   0.288175
H   -0.323037   0.770377   1.194127
H   -1.865132   1.768181   1.392959
H   -1.458931   2.609246  -1.339090
H    0.069718   1.550045  -1.341910
H   -0.009466   3.070691  -0.272373
```

Frequencies

-305.423	35.5506	44.9286
68.6401	85.9689	107.9506
169.0137	236.2273	258.8583
337.5863	373.1292	404.1349
439.1992	468.0758	514.4129
671.8545	699.8346	704.9995
796.4899	817.4625	921.0227
953.9552	992.9498	1012.453
1052.17	1057.503	1108.624
1173.836	1276.311	1325.432
1409.66	1415.693	1419.112
1434.974	1472.821	1481.997
1483.997	1566.393	1666.094
2352.825	3043.804	3105.331
3115.529	3119.085	3154.032
3164.619	3174.716	3184.108
3272.64	3276.945	3290.882

i29 – p11a
```
C   -0.619889   1.475262   0.413848
C   -3.712029  -1.145039  -0.074035
C   -2.604104  -0.214654   0.096854
C   -1.686848   0.553641   0.236757
H   -0.866498   2.408381   0.910623
H   -3.879315  -1.360818  -1.132579
H   -4.635097  -0.729751   0.337620
```

```
H   -3.508525   -2.090674    0.435323
C    0.650684    1.263660    0.008868
C    1.124895    0.083003   -0.664064
C    2.420226   -0.103616   -1.011211
C    3.511339   -1.175653    0.910610
H    1.381146    2.045246    0.203391
H    0.398188   -0.700927   -0.858101
H    3.145131    0.696839   -0.907332
H    2.723797   -0.962364   -1.596169
H    2.928019   -2.086384    0.941633
H    3.287996   -0.410147    1.641939
H    4.519518   -1.229031    0.517887
```

Frequencies

-343.028	31.4755	42.7458
73.0591	80.9945	86.3373
183.4631	227.1429	250.2167
340.5355	353.1999	422.49
438.3186	456.1166	507.8987
661.8639	726.035	729.0027
792.9487	810.4835	908.7641
944.9257	981.9877	1025.223
1052.931	1057.681	1136.376
1200.706	1257.414	1302.32
1387.22	1411.961	1418.013
1418.622	1475.395	1483.6
1483.93	1592.148	1628.189
2358.91	3044.86	3104.198
3115.652	3120.759	3155.164
3161.518	3177.549	3185.231
3252.47	3275.327	3283.02

i8 – p1
```
C    2.514641   -1.009682   -0.068819
C    1.227413   -0.234940   -0.047447
C    0.000000   -0.922647   -0.023528
C   -1.227413   -0.234940   -0.047447
C   -1.207883    1.152327    0.002142
C    0.000000    1.841750    0.034607
C    1.207883    1.152327    0.002142
C   -2.514641   -1.009682   -0.068819
H    2.532029   -1.725835   -0.895077
H    2.631402   -1.577964    0.859921
H    3.377226   -0.349139   -0.172769
H    0.000000   -1.432869    1.820580
H    0.000000   -1.997229   -0.186404
H   -2.143603    1.701704    0.007195
H    0.000000    2.925495    0.070311
H    2.143603    1.701704    0.007195
H   -3.377226   -0.349139   -0.172770
H   -2.631403   -1.577963    0.859922
H   -2.532028   -1.725835   -0.895076
```

Frequencies

-723.097	71.8511	78.1466
181.7583	224.6108	275.5878
300.1297	358.9788	416.8444
489.8595	527.2639	543.0044
548.3253	726.9405	744.2945
792.0956	920.5589	927.324
969.7551	996.8228	1003.57
1026.68	1042.196	1063.988
1068.398	1130.236	1186.081

1200.327	1288.249	1324.52
1345.546	1417.023	1419.373
1448.115	1488.994	1489.519
1495.05	1509.196	1545.477
1657.922	1658.373	3038.807
3039.447	3103.54	3103.714
3134.663	3134.888	3165.047
3180.126	3188.257	3206.962

i8 – i32

```
C    -2.522478  -1.034962  -0.165265
C    -1.278559  -0.256939   0.143038
C     0.052978  -0.987059   0.139285
C     1.274185  -0.232739   0.009871
C     1.236743   1.123392  -0.029999
C    -0.032500   1.840949  -0.023103
C    -1.210023   1.173461   0.023298
C     2.561043  -1.001382  -0.080927
H    -2.532218  -1.997274   0.355777
H    -2.597786  -1.248742  -1.240042
H    -3.417760  -0.484971   0.135033
H     0.038673  -2.061508   0.002906
H    -0.636474  -0.654347   1.188052
H     2.159822   1.686989  -0.105479
H    -0.024076   2.922645  -0.085349
H    -2.147977   1.718444  -0.030897
H     3.421778  -0.333352  -0.139627
H     2.562833  -1.643736  -0.967633
H     2.684855  -1.652480   0.790076
```

Frequencies

-2570.45	126.8398	140.8083
180.8906	211.5815	265.3566
321.62	385.5976	485.5923
496.7639	516.1098	610.93
685.2722	716.9955	745.1167
830.8386	869.0689	940.5473
967.6035	981.0734	1021.812
1044.363	1061.603	1069.76
1152.375	1185.48	1221.558
1248.968	1298.453	1314.907
1390.063	1415.013	1425.467
1457.38	1482.751	1486.394
1497.16	1503.02	1601.065
1628.462	2206.181	3004.853
3036.822	3075.355	3098.188
3116.738	3136.318	3173.36
3190.34	3203.391	3210.394

i32 – p42

```
C     2.133354  -1.279218   0.889838
C     1.125594  -0.298720  -0.773935
C    -0.175710  -0.852309  -0.671862
C    -1.201506  -0.160924  -0.053226
C    -0.957753   1.144936   0.397984
C     0.277336   1.754343   0.181980
C     1.302310   1.064332  -0.436078
C    -2.562980  -0.780420   0.129223
H     2.022397  -2.333153   0.655094
H     1.529020  -0.910755   1.710877
H     3.144072  -0.887649   0.832446
H     1.838160  -0.769031  -1.442218
H    -0.350043  -1.858689  -1.039371
H    -1.754932   1.698774   0.883661
```

```
H    0.426728    2.784464    0.487183
H    2.258451    1.542389   -0.615656
H   -2.777945   -0.941320    1.189968
H   -2.632033   -1.745547   -0.376379
H   -3.347750   -0.131607   -0.269142
```

Frequencies

-577.333	37.9523	108.1316
138.741	145.4494	240.6212
349.5952	402.3133	477.2827
525.0235	571.6423	584.3113
644.5639	676.7589	766.104
807.6077	863.4974	885.9665
901.564	991.589	1000.768
1004.862	1008.644	1052.843
1066.2	1105.994	1180.941
1195.595	1234.774	1324.146
1352.261	1419.54	1425.971
1428.692	1463.105	1491.288
1504.086	1527.272	1612.018
1641.887	3043.443	3082.269
3108.559	3131.186	3174.399
3177.206	3188.245	3193.905
3208.863	3238.727	3251.007

i32 – p1

```
C   -2.497876   -1.017345   -0.145293
C   -1.205184   -0.264028    0.075813
C    0.028434   -0.947898    0.002204
C    1.239171   -0.274261   -0.017012
C    1.226243    1.124519   -0.022216
C    0.023460    1.822341   -0.036597
C   -1.181358    1.143190   -0.015163
C    2.545908   -1.023742   -0.019648
H   -2.460407   -2.010218    0.306243
H   -2.675777   -1.137928   -1.218526
H   -3.346707   -0.480275    0.281380
H   -1.353055   -0.327253    1.882242
H    0.020095   -2.034128    0.001246
H    2.165840    1.667551   -0.038071
H    0.030607    2.906120   -0.072702
H   -2.118959    1.688469   -0.029206
H    3.244405   -0.598490   -0.744626
H    2.399898   -2.077378   -0.265241
H    3.021274   -0.973120    0.964722
```

Frequencies

-981.233	42.6135	171.0109
192.9587	215.6632	275.6231
388.4217	439.4285	461.4139
481.6591	529.8271	554.4428
580.9013	701.1786	741.8312
793.4969	892.1052	915.0551
931.4845	1002.029	1006.167
1014.591	1038.645	1067.446
1067.701	1133.134	1187.259
1199.125	1279.678	1316.693
1347.448	1419.041	1421.877
1453.325	1491.972	1493.895
1496.158	1512.236	1530.313

1635.469	1663.594	3045.144
3047.235	3111.76	3119.727
3133.633	3143.384	3174.271
3179.438	3189.453	3206.769

i30 – p3

```
C    -2.536419   -0.883847   -0.015014
C    -1.209866   -0.199816    0.051250
C    -0.000543   -1.082243    0.199649
C     1.342630   -0.400258    0.025403
C     1.366333    1.057073    0.142046
C     0.239618    1.779048    0.110548
C    -1.072836    1.144098   -0.029004
C     2.457537   -1.097723   -0.209664
H    -2.666303   -1.569292    0.829979
H    -2.609788   -1.487142   -0.927711
H    -3.360318   -0.168455   -0.012799
H    -0.079825   -1.931842   -0.488128
H    -0.044952   -1.521829    1.207891
H     2.333777    1.544105    0.206116
H     0.280867    2.861368    0.157597
H    -1.955217    1.774534   -0.006900
H    -1.277784    1.381439   -1.995773
H     3.420006   -0.604854   -0.292812
H     2.440807   -2.176026   -0.328745
```

Frequencies

-680.825	39.581	121.2738
182.0176	271.9952	296.7835
312.1466	362.6369	419.0748
491.4592	495.9954	526.1404
573.7447	702.6141	733.448
814.7247	872.8831	887.7767
921.7883	929.0248	966.0124
979.4523	1002.27	1010.437
1059.993	1076.073	1183.681
1205.979	1235.157	1317.734
1341.669	1378.287	1417.203
1431.024	1448.795	1469.069
1482.025	1486.861	1638.111
1686.336	1730.457	3001.464
3030.626	3064.271	3086.852
3142.143	3153.317	3183.119
3190.026	3213.307	3241.02

i30 – i35

```
C    -2.511773   -0.957007    0.084021
C    -1.214750   -0.251029   -0.144964
C     0.044434   -1.050954   -0.130621
C     1.344735   -0.424316   -0.004616
C     1.360585    1.045409   -0.070154
C     0.254846    1.788734   -0.027867
C    -1.130116    1.222436    0.129640
C     2.490119   -1.121799    0.142911
H    -2.696717   -1.092790    1.160727
H    -2.515247   -1.951079   -0.372237
H    -3.354166   -0.394361   -0.328326
H    -0.516043   -0.708774   -1.212614
H    -0.049049   -2.122287    0.012641
H     2.331574    1.524918   -0.146254
H     0.338180    2.870728   -0.065458
H    -1.467195    1.412840    1.165379
H    -1.836563    1.772346   -0.504521
H     3.445684   -0.616037    0.216972
H     2.491061   -2.204338    0.203600
```

Frequencies

-1935.45	106.6649	154.842
218.8728	276.5805	318.9613
350.4168	404.3864	456.9397
508.6659	576.3534	643.6226
696.8945	776.5033	804.2774
852.4817	870.1872	911.9176
926.8199	961.1164	1006.937
1016.835	1036.21	1056.128
1159.8	1211.576	1213.716
1268.118	1299.019	1329.235
1366.257	1397.78	1422.063
1455.169	1469.305	1480.464
1487.602	1502.444	1633.412
1740.305	2197.671	2933.594
2988.236	3040.45	3077.388
3119.543	3159.629	3173.264
3188.57	3196.122	3250.381

i31 – i43

C	-2.578962	-0.849335	-0.101843
C	-1.250206	-0.187746	0.124968
C	-0.033901	-1.035692	0.170917
C	1.282745	-0.471896	0.025864
C	1.412609	1.031637	0.206917
C	0.160132	1.789246	-0.136548
C	-1.060063	1.218560	-0.119053
C	2.362859	-1.233463	-0.234722
H	-2.651147	-1.799606	0.434133
H	-2.722966	-1.062634	-1.168047
H	-3.400639	-0.210907	0.230479
H	-0.174853	-2.108620	0.102530
H	-0.691510	-0.585841	1.232890
H	2.258015	1.397853	-0.382783
H	1.673774	1.233674	1.257916
H	0.256692	2.851744	-0.332278
H	-1.947067	1.818508	-0.297246
H	3.346050	-0.792489	-0.352503
H	2.282377	-2.309547	-0.344082

Frequencies

-1888.36	83.5136	159.9186
219.6904	287.0987	309.8815
414.1763	442.3332	501.0148
528.33	554.5279	660.0897
696.5138	720.9859	796.5233
855.2651	863.2358	933.6855
945.3566	965.3899	974.0469
1022.986	1039.011	1057.474
1165.9	1188.178	1228.345
1257.135	1307.392	1339.048
1344.116	1404.071	1425.495
1450.463	1467.199	1477.624
1494.602	1508.317	1635.003
1641.316	2115.737	2980.217
3027.954	3081.237	3097.034
3129.837	3150.907	3181.181

3199.696	3203.572	3240.564

i31 – p3

C	-2.604639	-0.770752	-0.072005
C	-1.254328	-0.129032	-0.009456
C	-0.093002	-1.024238	0.345774
C	1.265701	-0.464470	-0.003421
C	1.378195	0.996315	0.038383
C	0.274187	1.767138	-0.092390
C	-1.052352	1.184631	-0.186455
C	2.302080	-1.241762	-0.322995
H	-2.830111	-1.285694	0.869029
H	-2.637939	-1.528060	-0.862824
H	-3.391623	-0.038547	-0.260794
H	-0.223511	-2.014841	-0.100785
H	-0.130108	-1.177909	1.436408
H	2.367632	1.438188	-0.004454
H	1.584318	1.151415	2.197972
H	0.373624	2.845449	-0.148700
H	-1.891123	1.840413	-0.397148
H	3.283035	-0.818596	-0.510862
H	2.200764	-2.318791	-0.402451

Frequencies

-537.547	100.4084	147.3914
206.8674	236.4631	276.496
300.6162	353.6639	418.338
477.8869	488.332	518.4463
587.6054	701.6079	741.7143
801.3142	876.14	879.781
914.0303	934.4336	957.3403
985.2648	989.1289	1015.58
1067.159	1084.166	1181.979
1202.708	1231.679	1319.957
1343.9	1381.935	1421.702
1434.834	1457.083	1473.385
1482.526	1500.615	1596.324
1707.948	1738.296	2992.513
3033.553	3076.407	3090.623
3135.246	3152.184	3184.478
3195.6	3212.697	3240.611

i30 – p43

C	-2.118465	-1.167348	-0.375152
C	-1.182121	-0.394194	0.185291
C	0.111916	-0.941053	0.722093
C	1.300914	-0.277745	0.057996
C	1.150418	1.154087	-0.218832
C	-0.016209	1.791394	-0.107275
C	-1.304067	1.103385	0.263038
C	2.421211	-0.940599	-0.229237
H	-2.019451	-2.247337	-0.392417
H	-1.498928	-1.188958	-2.424298
H	-3.053489	-0.750846	-0.734455
H	0.160227	-2.025416	0.606414
H	0.163733	-0.719202	1.797674
H	2.038289	1.697477	-0.528251
H	-0.068948	2.857717	-0.304595
H	-1.584556	1.397452	1.285466
H	-2.111995	1.451837	-0.386965
H	3.272494	-0.438330	-0.676606
H	2.521042	-2.001962	-0.029510

Frequencies

-460.676	92.3907	100.2039
189.6793	250.1643	305.3323
358.6606	411.7283	438.3215

273

470.5255	546.2872	571.1321
688.7834	726.1104	770.6119
813.825	860.5979	920.1302
933.3263	939.2083	947.2796
951.204	998.1782	1009.954
1015.483	1027.211	1173.992
1199.482	1231.239	1298.956
1316.861	1338.696	1353.294
1412.159	1450.352	1460.935
1470.329	1482.558	1697.29
1706.679	1751.249	3009.254
3019.245	3089.269	3117.068
3150.843	3155.354	3173.397
3196.94	3240.639	3242.786

i31 – p43

```
C   -2.400567  -0.764634  -0.377843
C   -1.228209  -0.201428  -0.057566
C   -0.102112  -0.985289   0.578525
C    1.239204  -0.494452   0.099394
C    1.451918   0.984501   0.293890
C    0.225826   1.777580  -0.073682
C   -0.977651   1.226617  -0.251151
C    2.139337  -1.287285  -0.468409
H   -3.517508  -0.593509   1.684854
H   -2.568198  -1.829345  -0.260604
H   -3.202828  -0.181524  -0.817112
H   -0.221898  -2.054440   0.393564
H   -0.164991  -0.829532   1.665275
H    2.309105   1.327355  -0.292666
H    1.700647   1.185345   1.346547
H    0.352483   2.847449  -0.208291
H   -1.819039   1.845326  -0.548846
H    3.092072  -0.902963  -0.818339
H    1.953689  -2.347816  -0.603322
```

Frequencies

-284.447	98.2215	119.4481
140.3261	181.5556	314.5786
358.1265	406.5297	439.0338
470.2843	546.8477	574.4974
697.7707	724.8166	744.0813
819.3186	864.1913	917.3324
932.5242	939.2216	945.4289
953.0611	998.9313	1012.758
1019.493	1029.798	1176.561
1206.739	1237.139	1301.485
1320.897	1340.468	1357.384
1414.14	1456.852	1463.935
1472.835	1486.096	1678.2
1725.006	1760.007	3008.467
3017.725	3087.142	3117.252
3147.291	3157.924	3170.925
3194.139	3233.703	3248.26

i8 – p3

```
C    2.572074  -0.934663  -0.064833
C    1.276412  -0.187397   0.000944
C    0.029602  -1.019943   0.165348
```

```
C    -1.277948   -0.297102   -0.079407
C    -1.252989    1.157511    0.029543
C    -0.093058    1.831130    0.057445
C     1.193070    1.147263   -0.020205
C    -2.409792   -0.962176   -0.350838
H     2.601104   -1.585465   -0.945805
H     2.690277   -1.582654    0.811276
H     3.426188   -0.256628   -0.108632
H     0.026610   -1.392612    1.201832
H     0.089625   -1.914691   -0.463212
H    -2.201878    1.683690    0.037232
H    -0.097014    2.914727    0.107132
H     2.094394    1.747189   -0.096508
H    -3.350978   -0.439144   -0.479615
H    -3.083170   -1.543657    1.993049
H    -2.419386   -2.038498   -0.484729
```

Frequencies

-264.732	53.19	110.6568
132.4853	148.2568	203.7069
292.893	336.5894	416.73
465.7359	491.6159	513.2424
578.8419	706.5367	737.1182
814.2171	874.1593	876.3841
909.5433	927.9238	950.801
979.7606	1001.924	1009.057
1066.721	1081.442	1181.454
1204.687	1234.233	1320.16
1341.339	1379.188	1416.321
1433.361	1445.442	1469.216
1483.31	1487.837	1662.682
1682.121	1751.466	2997.047
3031.529	3070.577	3087.373
3136.632	3156.305	3182.459
3191.888	3211.494	3245.15

i43 – p45

```
C     2.371065   -1.041157    0.986328
C     1.002388   -0.381641   -0.848989
C    -0.195207   -1.001998   -0.623196
C    -1.302885   -0.320356    0.008675
C    -1.034585    1.061124    0.579055
C     0.173222    1.745183    0.001214
C     1.126226    1.063928   -0.633843
C    -2.515566   -0.892065    0.104653
H     2.371136   -2.118361    0.873941
H     1.756211   -0.621564    1.772186
H     3.281678   -0.511373    0.731826
H     1.746391   -0.874072   -1.462920
H    -0.340955   -2.032327   -0.931378
H    -0.876388    0.959013    1.663104
H    -1.921940    1.691191    0.469882
H     0.270884    2.814184    0.158901
H     2.012898    1.565163   -1.006300
H    -3.358302   -0.370627    0.545570
H    -2.689554   -1.899328   -0.258195
```

Frequencies

-438.287	63.7536	73.0236
91.5879	149.4269	280.8033
386.4981	447.441	456.2346
475.0298	490.9479	533.9588
600.5418	660.7498	729.5824
775.4801	781.4026	822.7327
880.266	927.5389	945.6481

950.8801	965.7803	993.026
1010.962	1033.763	1174.535
1201.548	1230.119	1321.105
1338.208	1401.366	1412.256
1415.566	1435.119	1461.71
1470.592	1521.912	1648.287
1722.518	3003.962	3087.41
3103.125	3154.639	3185.269
3190.535	3207.254	3221.035
3243.798	3269.235	3280

i43 – p48

```
C   -2.549406  -0.847759  -0.080177
C   -1.172402  -0.253376   0.046070
C   -0.053626  -1.029039   0.070443
C    1.282595  -0.464829   0.011834
C    1.396964   1.028946   0.226940
C    0.158291   1.790642  -0.146409
C   -1.031063   1.193252  -0.190636
C    2.359043  -1.236272  -0.193109
H   -2.562255  -1.895649   0.223152
H   -2.882581  -0.785930  -1.122194
H   -3.272978  -0.302568   0.529956
H   -1.262732  -0.113673   2.069325
H   -0.149970  -2.110198   0.108175
H    2.273928   1.425081  -0.291340
H    1.574998   1.202155   1.300039
H    0.249270   2.857642  -0.319694
H   -1.931397   1.759362  -0.406918
H    3.353873  -0.812396  -0.276303
H    2.267468  -2.313217  -0.283933
```

Frequencies

-721.294	97.2153	150.2086
183.8703	288.6364	336.9192
362.1559	406.1769	437.9556
455.9379	532.319	545.4822
567.1099	686.7606	708.9024
753.3822	863.8459	873.4212
904.7625	939.9723	957.2309
984.1315	1011.704	1026.167
1047.886	1054.148	1190.19
1205.023	1235.502	1317.897
1350.387	1375.649	1409.741
1439.477	1454.071	1463.455
1482.114	1495.225	1594.297
1678.832	1730.976	2996.817
3043.092	3099.536	3114.053
3144.256	3152.41	3180.752
3181.525	3205.7	3242.025

i35 – p44

```
C   -2.065222  -1.270090   1.045752
C   -0.998447  -0.378634  -0.853794
C    0.244971  -0.917714  -0.736273
C    1.320035  -0.234570  -0.038468
C    1.006146   1.100337   0.488752
C   -0.161183   1.701659   0.259649
C   -1.249493   1.077953  -0.562187
C    2.533540  -0.790625   0.131759
H   -1.533178  -0.677183   1.779821
H   -1.813461  -2.321506   0.985968
```

```
H    -3.092832   -0.997350    0.831754
H    -1.738905   -0.889797   -1.459108
H     0.431972   -1.926498   -1.090801
H     1.771287    1.597890    1.076988
H    -0.344819    2.695286    0.656864
H    -2.219076    1.217438   -0.074013
H    -1.327735    1.617147   -1.518350
H     3.324671   -0.268817    0.658561
H     2.759988   -1.776502   -0.258828
```

Frequencies

-465.924	86.8318	94.7276
130.3904	207.3587	328.6946
367.3433	378.2031	477.9442
482.9017	520.2108	572.7417
609.2664	670.541	778.9565
794.2252	803.52	822.2718
891.2311	893.1538	940.0698
954.2695	969.0171	989.6774
1013.081	1032.204	1172.604
1209.375	1225.717	1334.155
1387.317	1388.379	1416.746
1422.435	1441.917	1468.847
1476.803	1566.192	1646.73
1741.845	3006.464	3071.132
3098.11	3155.658	3174.641
3183.154	3197.113	3205.009
3246.773	3262.001	3275.004

i35 – p46
```
C     2.488348   -0.940231   -0.075435
C     1.132176   -0.299943    0.032944
C    -0.009287   -1.024512   -0.018333
C    -1.334778   -0.419998   -0.019008
C    -1.380844    1.045222    0.032916
C    -0.276462    1.789091   -0.000439
C     1.096631    1.201249   -0.109029
C    -2.451642   -1.164266   -0.051922
H     2.889644   -0.793305   -1.084706
H     2.441312   -2.012283    0.122341
H     3.195426   -0.490323    0.626051
H     1.095259   -0.269303    2.044490
H     0.047734   -2.109418   -0.001464
H    -2.357234    1.514437    0.100982
H    -0.350516    2.871531    0.034871
H     1.529206    1.462300   -1.087309
H     1.764712    1.659557    0.629123
H    -3.434056   -0.705727   -0.048530
H    -2.406334   -2.247138   -0.086016
```

Frequencies

-718.547	112.7264	164.8934
219.5348	289.1501	337.3275
378.3345	410.987	470.0226
484.2458	497.817	546.7634
588.9342	684.1999	710.4336
793.4263	875.3562	882.9482
903.0589	928.5809	950.8266
977.9556	1010.293	1020.868
1045.345	1065.641	1177.748
1206.979	1228.821	1321.027
1366.818	1400.196	1418.526

1436.752	1464.999	1468.692
1489.868	1496.874	1650.384
1669.702	1751.146	3003.295
3039.244	3059.043	3105.321
3143.92	3162.234	3177.279
3178.308	3199.821	3253.284

i30 – p46

C	-2.501241	-0.924960	-0.096575
C	-1.150374	-0.284159	-0.056902
C	-0.012006	-1.010635	0.024946
C	1.325769	-0.398132	-0.026469
C	1.364714	1.065831	0.007515
C	0.256878	1.804954	0.025268
C	-1.119810	1.215038	-0.000286
C	2.438261	-1.136804	-0.108374
H	-3.063433	-0.687481	0.814608
H	-2.430761	-2.010652	-0.179829
H	-3.088146	-0.548861	-0.941306
H	-0.063715	-2.090161	-0.084095
H	-0.087481	-1.354697	1.955300
H	2.340699	1.540805	0.015696
H	0.328390	2.887856	0.053936
H	-1.681855	1.549240	0.885353
H	-1.681298	1.621718	-0.853781
H	3.417764	-0.674311	-0.154553
H	2.396690	-2.220253	-0.126072

Frequencies

-724.75	93.6802	114.2323
184.5505	267.2623	295.0597
321.6667	374.8245	420.039
485.7444	508.6162	542.6435
593.6542	708.4731	711.7194
795.3319	883.7707	904.4821
912.5915	931.3785	969.2915
973.2737	1008.826	1018.01
1045.246	1062.26	1182.593
1207.129	1228.726	1317.218
1361.647	1403.197	1417.292
1435.661	1455.99	1468.484
1481.718	1490.546	1653.113
1694.186	1762.391	2998.869
3023.621	3030.523	3089.687
3137.215	3161.13	3176.401
3179.363	3203.158	3250.894

i31 – p48

C	-2.573575	-0.802882	-0.041143
C	-1.185877	-0.237529	-0.047643
C	-0.084635	-1.014556	0.086133
C	1.266608	-0.454138	-0.006176
C	1.388092	1.024584	0.279217
C	0.155029	1.804401	-0.076026
C	-1.032529	1.207986	-0.207032
C	2.321233	-1.213946	-0.308445
H	-3.154151	-0.382889	0.787168
H	-2.564989	-1.888803	0.064255
H	-3.100602	-0.547680	-0.966419
H	-0.184408	-2.095765	0.099164
H	-0.209297	-1.161031	2.272777
H	2.269460	1.440089	-0.216379
H	1.559395	1.152621	1.359655
H	0.246461	2.880758	-0.177676
H	-1.920478	1.792958	-0.426597
H	3.313620	-0.789641	-0.416425

H   2.218918   -2.284152   -0.452827

Frequencies

-456.252	109.9989	137.4999
173.01	209.2957	250.6275
297.0099	337.3102	427.1846
453.0704	527.2979	552.0258
577.5938	701.6832	719.8991
760.7194	875.5035	885.4012
921.9987	944.4212	957.4426
984.5153	1008.891	1023.536
1047.393	1064.51	1197.475
1208.276	1229.032	1317.303
1352.807	1371.219	1413.681
1446.281	1454.073	1464.417
1484.621	1493.437	1619.398
1707.908	1737.704	2996.51
3040.409	3097.703	3100.359
3141.709	3151.307	3175.315
3184.019	3200.057	3239.761

Products
p10a + CH$_3$

```
C     0.140396    0.714961   -0.000252
C     1.171285   -0.142974   -0.000266
C    -3.792134   -0.380692    0.000509
C    -2.388279    0.008281   -0.000648
C    -1.225748    0.320450   -0.000679
C     2.563110    0.277710    0.000477
C     3.594658   -0.566652    0.000109
H     0.337088    1.784964    0.000273
H     0.973326   -1.211914   -0.000811
H    -4.071598   -0.822013    0.960803
H    -3.991138   -1.118909   -0.780598
H    -4.435912    0.484214   -0.176444
H     2.746918    1.350197    0.001444
H     3.443404   -1.641872   -0.000897
H     4.618185   -0.211175    0.000732
```

Frequencies

55.8267	82.3862	85.9817
156.637	236.3778	280.6826
348.406	437.057	458.8177
550.4739	663.0101	821.8724
883.8556	938.9782	964.7419
974.012	1037.238	1049.56
1052.265	1198.578	1211.095
1294.075	1329.123	1348.404
1410.822	1456.841	1479.869
1487.136	1685.689	1740.487
2375.703	3050.852	3120.865
3127.385	3153.868	3162.033
3166.537	3179.805	3249.487

p10b + CH$_3$

```
C     0.281635   -0.314982   -0.235168
C     1.156368    0.661154    0.044844
C     2.611403    0.524914   -0.055388
C     3.297710   -0.591617    0.182654
C    -3.772668    0.023251    0.110051
```

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```
C    -2.325545   -0.093552   -0.010469
C    -1.129045   -0.180493   -0.107999
H     0.647897   -1.272083   -0.599035
H     0.772133    1.631577    0.347521
H     3.154203    1.427580   -0.326682
H     2.806917   -1.501071    0.514680
H     4.374857   -0.624778    0.067891
H    -4.169301    0.711513   -0.641018
H    -4.051550    0.402544    1.096450
H    -4.254304   -0.947333   -0.030966
```

Frequencies

77.8812	83.2641	97.0024
184.8089	224.4364	271.9406
325.0407	448.2182	508.5483
566.4162	661.7907	835.1539
888.9466	959.1356	983.9538
1002.529	1037.578	1054.809
1063.082	1081.062	1213.673
1316.36	1323.341	1353.711
1421.91	1455.53	1485.217
1486.44	1707.02	1718.368
2377.095	3048.525	3119.399
3124.894	3154.534	3160.05
3165.48	3183.567	3249.061

p11a + CH₃

```
C     0.204006    1.377239    0.000018
C    -0.997706    0.613543   -0.001826
C    -2.026904   -0.011051   -0.002309
C    -3.270612   -0.769826    0.001240
C     1.441354    0.855479    0.001068
C     2.987802   -1.052748    0.000065
C     1.746685   -0.566081   -0.000338
H     0.085770    2.456518    0.001250
H    -3.081934   -1.828417   -0.192652
H    -3.772069   -0.686095    0.968966
H    -3.954606   -0.399746   -0.766705
H     2.285741    1.539695    0.003093
H     3.853132   -0.396273    0.001535
H     3.177877   -2.119543   -0.001192
H     0.898345   -1.245470   -0.001800
```

Frequencies

82.5915	119.2763	135.8382
176.2681	238.1967	344.1311
344.5192	450.0967	477.2245
661.2365	696.7473	790.8751
812.9387	945.6015	955.4388
1004.075	1058.221	1061.406
1065.908	1135.481	1199.5
1275.813	1321.121	1403.469
1426.216	1476.674	1488.591
1491.367	1671.261	1734.951
2372.411	3049.636	3120.37
3125.276	3150.35	3171.221
3181.579	3192.738	3246.307

p11b + CH₃

```
C     0.551239   -1.396577    0.032344
C    -0.696571   -0.718237    0.009289
C    -1.779890   -0.191980   -0.008553
C     1.374857    1.638889    0.066016
```

```
C     2.158777   0.566666  -0.067838
C     1.775775  -0.842866  -0.002517
C    -3.076980   0.469977  -0.028227
H     0.486236  -2.480068   0.077006
H     0.311531   1.559751   0.251381
H     1.799136   2.634178  -0.004362
H     3.219966   0.733335  -0.237027
H     2.608692  -1.540114   0.007191
H    -3.598709   0.325358   0.921374
H    -2.962407   1.544235  -0.193458
H    -3.707679   0.068094  -0.825184
```

Frequencies

74.4117	89.1857	105.909
171.1998	245.6838	335.167
355.7856	462.4921	478.7354
675.1284	690.6601	800.6214
810.0662	947.7782	974.3942
1012.18	1055.404	1057.849
1063.449	1108.655	1175.238
1279.206	1363.342	1420.404
1441.962	1472.601	1485.857
1488.756	1684.517	1718.672
2369.19	3051.141	3123.278
3126.001	3156.463	3167.357
3174.185	3192.216	3268.188

p12a + H

```
C     0.007721   2.482101  -0.000025
C     0.214547   0.989762   0.000040
C    -0.974672   0.193778  -0.000261
C    -1.999061  -0.438433  -0.000507
C    -3.231111  -1.216322   0.000049
C     1.439731   0.434171   0.000338
C     2.948454  -1.505461  -0.000343
C     1.717699  -0.992306   0.000399
H    -0.563799   2.790178   0.880309
H    -0.562879   2.790264  -0.880927
H     0.962808   3.010345   0.000472
H    -3.198805  -1.995209  -0.765900
H    -3.383998  -1.699882   0.968382
H    -4.094662  -0.577724  -0.200804
H     2.300699   1.099000   0.000521
H     3.828162  -0.868300  -0.001120
H     3.115382  -2.576103  -0.000239
H     0.857255  -1.656311   0.001165
```

Frequencies

79.2953	110.8606	118.3584
138.418	186.5459	203.8324
231.8406	302.409	368.8867
394.5467	460.7388	584.5067
619.8072	677.5559	698.4517
915.0286	950.3893	951.4787
1046.81	1050.745	1056.89
1061.221	1062.943	1072.977
1182.401	1252.885	1322.479
1379.121	1418.49	1422.233
1459.673	1478.567	1486.141
1491.156	1498.588	1681.833
1737.437	2370.741	3044.334
3050.008	3107.991	3120.579

3126.129	3142.809	3147.864
3163.57	3177.972	3244.541

p12b + H

C	-0.746664	2.418720	-0.086596
C	-0.651694	0.914730	-0.004045
C	0.679062	0.395720	0.016199
C	1.826501	0.031739	0.036019
C	-0.974035	-2.229033	-0.213270
C	-1.864988	-1.310010	0.161583
C	-1.753822	0.145233	0.065413
C	3.202573	-0.444792	0.060107
H	-0.269228	2.783914	-1.000355
H	-0.227277	2.881823	0.757389
H	-1.787161	2.748395	-0.081043
H	-0.024425	-1.965361	-0.661253
H	-1.189525	-3.283929	-0.085691
H	-2.810595	-1.658534	0.571740
H	-2.703875	0.673882	0.082923
H	3.810101	0.083638	-0.678828
H	3.651665	-0.283390	1.043519
H	3.248721	-1.514288	-0.160854

Frequencies

67.0218	73.8174	82.4834
152.3594	172.1845	223.8716
239.5117	312.4424	337.251
368.0144	528.1377	582.3303
632.8436	666.7151	708.3183
901.9226	961.2398	968.823
1019.006	1047.519	1054.643
1057.872	1070.853	1073.143
1138.338	1242.669	1347.768
1412.331	1415.722	1425.564
1459.875	1478.818	1481.551
1488.013	1501.432	1699.053
1718.761	2369.126	3046.702
3049.115	3113.23	3118.497
3126.072	3138.847	3147.655
3169.106	3176.192	3265.242

p13a + H

C	-0.276141	1.985094	0.000153
C	-0.106778	0.487159	-0.000218
C	1.250510	0.031336	-0.000665
C	2.405293	-0.308251	-0.000859
C	3.799051	-0.733337	0.000332
C	-1.106906	-0.414364	-0.000042
C	-3.465893	-1.087194	0.000055
C	-2.533506	-0.133191	0.000294
H	0.208489	2.416171	-0.880240
H	0.210101	2.415792	0.879839
H	-1.321387	2.291396	0.001167
H	4.246527	-0.596778	0.988395
H	3.884594	-1.789465	-0.266497
H	4.383818	-0.152396	-0.717343
H	-0.832698	-1.466113	-0.000202
H	-3.198404	-2.139671	-0.000409
H	-4.522566	-0.847308	0.000286
H	-2.852258	0.904864	0.000708

Frequencies

35.9513	85.4177	95.6391
117.7575	122.4787	227.2111
241.6528	313.2606	382.3446
390.7779	434.7124	558.3648

582.6458	675.8017	750.3193
918.1554	920.9346	946.4789
1011.146	1024.338	1055.248
1061.225	1066.017	1068.38
1199.456	1275.634	1326.524
1368.42	1422.45	1427.275
1457.869	1482.815	1483.78
1487.04	1498.437	1681.33
1737.444	2373.089	3049.043
3057.821	3117.634	3119.02
3126.968	3149.529	3159.179
3168.35	3183.904	3244.61

p13b + H
```
C    0.622467   1.643910  -0.203168
C    0.175969   0.206902  -0.110296
C   -1.239526   0.004058  -0.025284
C   -2.434185  -0.123288   0.046691
C    3.292968  -0.040036   0.417372
C    2.453424  -0.879644  -0.188885
C    0.991541  -0.864354  -0.122883
C   -3.878468  -0.295021   0.135942
H    0.642717   2.108780   0.787687
H   -0.080354   2.213648  -0.814388
H    1.620335   1.723095  -0.636979
H    2.943441   0.759819   1.060362
H    4.365701  -0.152474   0.308990
H    2.876977  -1.700334  -0.765015
H    0.516468  -1.841562  -0.117321
H   -4.392836   0.660138   0.005746
H   -4.236086  -0.982096  -0.635307
H   -4.161514  -0.704178   1.109282
```

Frequencies

68.0776	83.9259	95.5925
131.0123	187.277	253.403
265.2271	312.5115	337.9692
397.6439	550.0705	555.1689
570.3177	650.577	785.4403
903.8613	926.3536	966.2119
1024.877	1046.682	1053.101
1064.695	1066.992	1071.163
1112.914	1291.791	1338.302
1386.627	1421.391	1427.232
1461.982	1485.904	1487.306
1493.03	1501.492	1708.359
1715.25	2374.187	3050.411
3051.378	3118.992	3121.448
3125.894	3148.61	3151.817
3166.132	3183.22	3252.701

p39 + C₂H₃
```
C    1.132268   0.116939   0.000006
C    1.796695   1.274582  -0.000002
C    1.821464  -1.223775  -0.000002
C   -2.958892  -0.044793  -0.000003
C   -1.503105   0.019257   0.000003
C   -0.302028   0.087385   0.000004
H    2.881162   1.292559  -0.000003
H    1.275929   2.224319  -0.000006
H    1.530025  -1.803090   0.880591
H    2.906399  -1.105518   0.000068
```

```
H     1.530131   -1.803018   -0.880677
H    -3.303658   -1.081675    0.001438
H    -3.369142    0.448185   -0.885041
H    -3.369253    0.450666    0.883595
```

Frequencies

40.6061	114.1576	134.1695
169.315	310.0292	360.8824
383.2361	548.8619	579.0869
664.7475	742.5326	933.451
938.2265	1035.907	1056.124
1056.163	1072.148	1097.043
1331.673	1414.291	1420.324
1441.78	1477.039	1483.222
1486.848	1498.116	1717.304
2378.255	3045.836	3052.882
3112.028	3125.709	3125.819
3143.108	3165.867	3260.304

p49 + H
```
C    -0.565046    2.397133   -0.266931
C    -0.396549    1.124690    0.099045
C     0.886835    0.490308    0.042379
C     1.940522   -0.089111    0.017661
C     3.219089   -0.786404   -0.017930
C    -1.543456    0.257055    0.584000
C    -1.721098   -2.151228   -0.093073
C    -1.848829   -0.861916   -0.373279
H    -1.542297    2.864955   -0.217050
H     0.264938    2.997676   -0.618900
H     3.750224   -0.669659    0.930329
H     3.071116   -1.854496   -0.194770
H     3.856256   -0.393363   -0.813901
H    -2.428634    0.889304    0.707242
H    -1.291775   -0.158671    1.564760
H    -1.379591   -2.486625    0.882012
H    -1.949568   -2.916027   -0.826830
H    -2.179480   -0.556265   -1.364124
```

Frequencies

47.7174	55.1025	106.6987
118.5204	142.5331	237.5877
314.0665	347.5501	386.9941
439.7847	565.591	591.7442
637.658	729.8568	750.5923
917.9276	942.8178	949.2925
958.9372	976.8782	1034.023
1058.567	1063.013	1085.213
1129.717	1242.566	1304.926
1329.084	1338.197	1421.735
1447.102	1455.005	1481.335
1487.226	1490.128	1712.763
1739.63	2379.606	3052.573
3054.953	3104.893	3123.793
3128.458	3147.304	3163.401
3164.053	3240.559	3258.015

p50 + H
```
C    -0.021017    2.531991   -0.130472
C     0.098171    1.038726    0.014205
C    -0.957753    0.254950   -0.002612
C    -1.974508   -0.499282   -0.017039
```

```
C    -3.025495   -1.283112   -0.032045
C     1.502574    0.496723    0.171942
C     2.261224   -1.825696   -0.355468
C     1.592118   -0.979312    0.414240
H    -1.057651    2.839182   -0.264619
H     0.562173    2.877846   -0.990880
H     0.383381    3.033062    0.755677
H    -4.025316   -0.878803   -0.150338
H    -2.922538   -2.358022    0.072540
H     1.972750    1.034819    1.007511
H     2.080432    0.767874   -0.720709
H     2.790916   -1.488966   -1.242164
H     2.302243   -2.885602   -0.131285
H     1.061729   -1.351317    1.287760
```

Frequencies

51.0117	76.8526	104.5138
142.0657	176.113	228.1947
305.8039	374.7523	408.6384
424.3486	552.6636	562.0396
574.8347	632.9756	737.3653
886.6414	903.8324	933.448
964.1834	994.917	1033.887
1038.891	1047.956	1129.181
1160.049	1210.295	1261.003
1324.969	1355.652	1409.256
1445.345	1453.128	1473.301
1488.463	1489.849	1739.504
1744.917	2242.25	3013.304
3038.685	3054.398	3096.781
3144.921	3148.332	3160.142
3173.01	3230.085	3239.926

p51 + H

```
C    -0.172374    2.180949   -0.002382
C    -0.213531    0.675948   -0.315340
C     1.121468    0.077753   -0.197925
C     2.217270   -0.400189   -0.084679
C     3.545648   -0.987508    0.049839
C    -1.192266   -0.035705    0.602093
C    -3.364560   -1.199296   -0.236739
C    -2.281455   -0.616027    0.189563
H     0.532978    2.690393   -0.662233
H     0.145267    2.347624    1.030089
H    -1.163769    2.619534   -0.136412
H    -0.560111    0.542306   -1.344985
H     3.773434   -1.194283    1.098452
H     3.614165   -1.927545   -0.503120
H     4.311697   -0.309992   -0.335437
H    -0.952480   -0.038613    1.663169
H    -3.361174   -2.247580   -0.517753
H    -4.301209   -0.657385   -0.318348
```

Frequencies

38.5386	105.2215	110.0576
131.6338	178.334	255.9747
285.3965	302.4958	341.7172
353.6566	493.6793	519.1511
538.5121	637.9437	770.0315
889.0632	899.2516	906.4374
1020.631	1023.023	1058.607
1064.949	1094.751	1100.852
1155.645	1195.922	1270.294

1338.741	1383.799	1413.537
1421.665	1483.023	1488.823
1490.904	1498.522	1503.023
2089.698	2393.084	3050.322
3052.438	3072.881	3121.677
3124.563	3134.519	3141.377
3143.428	3158.382	3225.793

p52 + H

C	-0.522656	2.472459	0.054189
C	-1.216841	1.161831	-0.113807
C	0.793292	-0.201323	-0.049629
C	1.982146	-0.374714	0.016277
C	3.422518	-0.580393	0.099071
C	-0.630424	-0.045654	-0.137041
C	-2.581621	-1.533516	0.300375
C	-1.407142	-1.299173	-0.276308
H	-0.717869	3.125954	-0.802350
H	0.555777	2.346861	0.159747
H	-0.899834	2.992108	0.941486
H	-2.295900	1.193410	-0.241255
H	3.922319	-0.207842	-0.798753
H	3.840774	-0.056343	0.962165
H	3.655824	-1.642784	0.202934
H	-3.046416	-0.807678	0.960059
H	-3.107225	-2.467741	0.139958
H	-0.943082	-2.073046	-0.882755

Frequencies

41.663	79.8786	97.0884
127.9587	177.6211	192.0066
235.4168	292.2054	356.7278
397.6749	481.3827	565.7029
598.9224	687.7802	739.2482
879.3286	935.6188	959.1429
1016.766	1029.205	1057.808
1059.318	1067.268	1110.315
1151.178	1243.831	1322.357
1375.388	1417.755	1423.17
1458.882	1484.439	1486.972
1488.56	1489.327	1712.999
1724.217	2376.829	3040.785
3053.101	3097.134	3124.654
3127.887	3143.019	3155.249
3174.284	3178.385	3247.943

p53 + H

C	2.512688	-1.399444	-0.055474
C	1.032753	-1.213453	0.050108
C	-1.094102	-0.091519	-0.024551
C	-2.296195	-0.070971	0.017894
C	-3.752376	-0.059277	0.076908
C	0.340811	-0.069046	-0.085370
C	1.989398	1.772133	0.294851
C	0.933412	1.265052	-0.333754
H	2.966757	-1.512509	0.935709
H	2.999514	-0.557715	-0.550354
H	2.736833	-2.314601	-0.610491
H	0.451580	-2.113190	0.233100
H	-4.171500	-0.925772	-0.440751
H	-4.100108	-0.083338	1.113063
H	-4.152526	0.842778	-0.392430
H	2.506158	1.226073	1.076651
H	2.355303	2.765350	0.060431
H	0.409648	1.872069	-1.068597

SUPPORTING INFORMATION

Frequencies

32.4937	80.9077	100.6098
136.1829	197.3919	259.0988
282.8118	304.3612	337.93
424.9978	451.128	516.4342
569.6493	737.5833	760.038
874.66	935.6769	965.6173
998.9225	1034.341	1051.889
1059.613	1072.92	1113.992
1149.487	1267.153	1334.346
1366.733	1417.69	1431.265
1462.071	1483.771	1486.867
1498.691	1513.041	1713.631
1725.673	2377.979	3035.433
3051.416	3095.146	3121.193
3127.006	3138.914	3156.982
3172.81	3179.594	3249.095

p54 + C$_2$H$_3$

```
C   -2.058797   1.147399   0.000394
C   -1.990793  -0.344973  -0.001081
C    0.449857  -0.541397   0.001963
C    1.575634  -0.115635   0.001853
C    2.938469   0.400633  -0.001217
C   -0.872913  -1.077397   0.000033
H   -2.589248   1.509476  -0.886342
H   -1.063377   1.593910   0.015416
H   -2.614927   1.506535   0.872356
H   -2.939362  -0.875718  -0.003895
H    3.321924   0.498659   1.017837
H    3.605278  -0.268545  -0.550688
H    2.981373   1.384596  -0.474755
H   -0.950405  -2.160700  -0.001597
```

Frequencies

63.8301	85.4994	100.4738
171.3948	263.665	349.2574
413.9261	506.395	606.5902
748.1925	792.5268	939.8037
994.9002	1051.892	1059.062
1068.72	1104.323	1179.564
1276.746	1398.777	1417.868
1444.087	1481.953	1483.231
1487.156	1490.532	1727.104
2375.566	3043.156	3050.881
3100.227	3121.307	3125.261
3143.982	3168.883	3189.861

p55 + C$_2$H$_3$

```
C    3.138140  -0.113108   0.000019
C    1.670921  -0.399744  -0.000041
C   -0.679530   0.257845   0.000013
C   -1.865306   0.053267   0.000072
C   -3.300453  -0.200228   0.000028
C    0.719408   0.536157  -0.000055
H    3.620275  -0.552087   0.879492
H    3.337130   0.960932  -0.000461
H    3.620519  -0.552892  -0.878914
H    1.372354  -1.445362   0.000003
H   -3.620360  -0.633524  -0.951267
H   -3.573753  -0.896764   0.796798
H   -3.857073   0.727428   0.154238
```

H   1.001821   1.587137   -0.000106

Frequencies

55.8911	107.6327	114.6984
189.7898	275.8967	295.3903
394.9763	468.0742	517.1082
813.137	819.8098	953.36
988.7593	1052.353	1059.193
1073.354	1136.137	1206.699
1317.093	1333.851	1417.577
1425.695	1479.078	1483.64
1487.88	1498.798	1740.859
2378.269	3041.25	3051.205
3100.826	3120.79	3126.96
3130.028	3148.483	3167.943

p56 + H

```
C     1.895287    2.127907   -0.189177
C     1.126004    1.244354    0.428760
C    -0.902799   -0.001796   -0.155628
C    -2.101052   -0.002367   -0.080304
C    -3.557121   -0.001495   -0.000384
C     0.564770   -0.000225   -0.227592
C     1.901998   -2.124085   -0.189323
C     1.129196   -1.243494    0.428454
H     2.281944    2.999723    0.326027
H     2.164357    2.011343   -1.234866
H     0.862494    1.381472    1.475168
H    -3.910323    0.801128    0.651698
H    -3.999951    0.145754   -0.988537
H    -3.926610   -0.949530    0.398307
H     0.862470    0.000304   -1.282146
H     2.171730   -2.005895   -1.234660
H     2.291074   -2.994954    0.325661
H     0.865118   -1.382131    1.474518
```

Frequencies

64.1218	72.6807	77.6859
116.7028	130.06	273.5159
285.7509	289.2586	398.3834
435.5257	499.4591	500.2281
669.6413	683.9092	838.2402
926.7499	961.6875	965.2451
980.4386	1037.583	1042.795
1060.139	1063.305	1123.375
1161.939	1187.913	1273.136
1305.647	1323.386	1337.731
1423.704	1455.077	1457.01
1486.224	1489.963	1732.17
1742.374	2393.728	3048.891
3054.645	3119.502	3124.118
3153.164	3153.865	3171.989
3175.16	3245.918	3246.405

p57 + H

```
C    -0.377420    2.507647   -0.158838
C    -0.030602    1.185147    0.482179
C    -0.689924   -0.053144    0.043358
C    -1.734649   -0.797051   -0.016491
C    -2.794865   -1.554827   -0.080699
C     0.744098    0.125384   -0.309405
C     2.866077   -1.162595   -0.228352
```

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```
C    1.767863   -0.704012    0.359924
H   -1.262993    2.944034    0.309896
H   -0.591882    2.376003   -1.222256
H    0.448960    3.216473   -0.058236
H    0.216036    1.232475    1.541161
H   -3.500392   -1.464516   -0.899973
H   -2.999869   -2.297199    0.683382
H    0.947417    0.373577   -1.349027
H    3.080317   -0.952524   -1.271866
H    3.584572   -1.767352    0.312258
H    1.574365   -0.940265    1.404607
```

Frequencies

73.0693	110.2322	154.5482
209.5305	215.8254	256.2686
330.8523	375.4157	423.1113
485.1394	588.1631	603.5082
651.2663	759.3774	856.5526
872.8673	891.4819	953.1264
1006.991	1024.079	1024.948
1048.343	1055.938	1101.553
1129.364	1152.222	1209.084
1299.655	1320.441	1343.296
1414.551	1426.233	1466.427
1496.43	1506.523	1556.802
1735.869	2138.681	3050.334
3125.281	3127.043	3137.534
3144.314	3147.773	3150.288
3160.614	3230.19	3246.562

p42 + CH₃

```
C    1.195538    1.199818    0.002023
C   -0.193735    1.196971   -0.009046
C   -0.908973    0.000002   -0.012244
C   -0.193737   -1.196970   -0.009045
C    1.195536   -1.199819    0.002023
C    1.895986   -0.000001    0.008429
C   -2.415550    0.000000    0.009653
H    1.731705    2.142463    0.002303
H   -0.732363    2.139656   -0.017490
H   -0.732367   -2.139654   -0.017490
H    1.731700   -2.142466    0.002302
H    2.980100   -0.000002    0.014617
H   -2.820424   -0.884482   -0.487029
H   -2.820427    0.884525   -0.486952
H   -2.788313   -0.000044    1.038980
```

Frequencies

34.8642	207.7988	350.0785
417.0356	478.6255	533.5122
639.4238	717.9088	748.6522
808.5812	866.281	920.6975
995.496	1010.276	1013.52
1024.216	1064.215	1067.412
1121.635	1186.055	1217.239
1245.97	1332.672	1363.76
1419.204	1477.626	1499.92
1511.653	1547.483	1660.972
1684.996	3050.519	3116.919
3140.232	3183.009	3184.436
3198.008	3207.204	3220.419

p1 + H

C	2.514963	-1.033952	0.006534
C	1.218549	-0.265606	-0.006499
C	0.000002	-0.941214	-0.011637
C	-1.218547	-0.265611	-0.006540
C	-1.204417	1.127834	-0.000270
C	-0.000003	1.818600	0.002619
C	1.204416	1.127837	-0.000223
C	-2.514961	-1.033956	0.006561
H	2.510011	-1.829121	-0.743379
H	2.680066	-1.502609	0.981512
H	3.365844	-0.381223	-0.198287
H	0.000005	-2.028761	-0.022633
H	-2.142370	1.673914	-0.001767
H	-0.000004	2.903220	0.002943
H	2.142366	1.673921	-0.001681
H	-3.365733	-0.381447	-0.199415
H	-2.680609	-1.501586	0.981945
H	-2.509586	-1.829902	-0.742511

Frequencies

101.1151	101.8826	197.0954
229.1919	276.9222	409.5253
442.0371	525.766	539.3609
549.2396	717.6343	744.0453
787.8462	902.4466	918.2242
927.3635	996.9835	1003.002
1027.264	1040.423	1072.154
1074.803	1136.274	1182.911
1203.896	1291.103	1321.434
1349.55	1420.062	1422.737
1467.381	1494.587	1495.267
1500.325	1519.841	1541.364
1666.199	1686.82	3047.079
3047.695	3113.249	3113.402
3136.376	3136.643	3169.041
3183.593	3191.635	3211.684

p44 + CH₃

C	-1.042990	1.251076	-0.000004
C	0.289724	1.243525	-0.000006
C	1.068751	0.000000	-0.000001
C	0.289724	-1.243525	-0.000006
C	-1.042991	-1.251076	-0.000003
C	-1.868365	0.000000	0.000006
C	2.407902	0.000000	0.000006
H	-1.577451	2.196253	-0.000006
H	0.840985	2.179018	-0.000009
H	0.840984	-2.179020	-0.000011
H	-1.577451	-2.196253	-0.000006
H	-2.540333	0.000000	-0.869782
H	-2.540289	0.000001	0.869833
H	2.971511	-0.926496	0.000008
H	2.971511	0.926496	0.000010

Frequencies

116.4393	305.867	372.729
384.6247	510.2396	558.1417
601.2898	686.549	789.3702
802.7072	803.9673	896.1845
914.7541	960.7094	964.237
975.8652	1013.785	1023.656
1027.59	1185.131	1229.457
1230.296	1338.353	1395.328

1399.501	1449.145	1458.141
1475.877	1686.516	1711.33
1778.503	3014.857	3032.297
3156.411	3175.788	3176.547
3197.461	3200.398	3246.299

p45 + CH₃

```
C    1.831094   0.043797  -0.133275
C    1.227349  -1.144539  -0.085295
C   -0.243150  -1.272168   0.199734
C   -1.029444   0.013410   0.027950
C   -0.271722   1.262990   0.113557
C    1.066810   1.278335   0.038837
C   -2.350322   0.014089  -0.173146
H    2.899677   0.114201  -0.303620
H    1.796011  -2.060911  -0.204866
H   -0.683634  -2.067411  -0.408592
H   -0.350096  -1.605861   1.243053
H   -0.831321   2.190100   0.187448
H    1.602697   2.220656   0.071158
H   -2.906347   0.943072  -0.240169
H   -2.910672  -0.909329  -0.274580
```

Frequencies

63.8772	260.4228	383.5535
437.1575	482.1043	552.5186
596.8266	674.3314	760.124
775.535	826.3803	906.1617
937.4333	954.0288	966.3779
985.6579	1006.255	1017.25
1036.084	1190.576	1209.371
1229.833	1322.024	1350.695
1403.023	1440.465	1448.149
1474.563	1664.696	1705.32
1747.358	3004.996	3087.622
3154.335	3183.136	3189.162
3205.166	3216.2	3242.72

p46 + H

```
C   -2.502470  -0.950538   0.000011
C   -1.144409  -0.314249   0.000013
C   -0.014848  -1.027508   0.000090
C    1.319293  -0.421252   0.000019
C    1.362279   1.044575   0.000080
C    0.254372   1.783769   0.000040
C   -1.120699   1.190281  -0.000108
C    2.436827  -1.160190  -0.000093
H   -3.077106  -0.639834   0.879705
H   -2.436399  -2.039938   0.000790
H   -3.076526  -0.641052  -0.880491
H   -0.064925  -2.113388   0.000191
H    2.338819   1.518849   0.000155
H    0.325327   2.867304   0.000088
H   -1.682848   1.560380   0.869818
H   -1.682589   1.560248  -0.870270
H    3.417683  -0.697938  -0.000158
H    2.396497  -2.243956  -0.000141
```

Frequencies

98.0283	127.8892	194.6462
292.8185	335.9744	420.4396
440.1147	487.3031	538.7111
584.0904	694.3638	711.4303
793.4194	878.2767	883.3785
903.435	930.4697	953.1698

974.4961	1006.749	1017.487
1048.384	1066.788	1179.861
1207.216	1230.381	1320.846
1363.617	1403.028	1418.134
1440.274	1461.012	1468.752
1478.865	1493.691	1686.984
1721.792	1782.071	3006.279
3024.211	3030.212	3086.216
3136.578	3161.257	3172.764
3177.463	3201.525	3250.752

p3 + H

```
C    2.564604   -0.812764   -0.108497
C    1.231008   -0.140155   -0.005522
C    0.048116   -1.028167    0.294126
C   -1.307938   -0.407521    0.031775
C   -1.371903    1.052817    0.084945
C   -0.256682    1.794766    0.024932
C    1.063596    1.183393   -0.097202
C   -2.390865   -1.149356   -0.216954
H    2.578131   -1.526363   -0.939572
H    2.780795   -1.383484    0.802267
H    3.369022   -0.090732   -0.259857
H    0.108286   -1.287484    1.363040
H    0.140318   -1.977270   -0.243421
H   -2.350311    1.520954    0.115929
H   -0.324608    2.877414    0.027976
H    1.918811    1.830187   -0.266337
H   -3.365427   -0.691494   -0.348355
H   -2.334628   -2.229809   -0.297297
```

Frequencies

82.2211	162.4214	205.9829
295.7255	340.1813	419.2479
466.0654	490.25	513.3584
581.8149	691.4093	737.8093
804.0696	873.9876	876.123
911.138	931.8734	955.9367
983.1314	997.4677	1013.343
1068.066	1082.527	1182.964
1205.094	1235.625	1319.217
1343.136	1380.113	1420.412
1434.82	1455.162	1472.642
1483.017	1496.219	1669.455
1710.937	1755.922	2993.247
3031.747	3079.574	3088.759
3134.631	3148.666	3183.174
3192.637	3210.643	3236.482

p48 + H

```
C   -2.572178   -0.845121    0.039428
C   -1.186035   -0.270945    0.008721
C   -0.082253   -1.031035    0.100009
C    1.265214   -0.465512    0.028874
C    1.382334    1.030102    0.237160
C    0.128732    1.790525   -0.088491
C   -1.054072    1.181689   -0.168467
C    2.336822   -1.234813   -0.183789
H   -2.555456   -1.928554    0.169087
H   -3.105913   -0.617399   -0.889469
H   -3.153612   -0.409490    0.858807
H   -0.170551   -2.111415    0.174058
H    2.232621    1.426812   -0.324408
```

```
H     1.613517    1.214566    1.297481
H     0.207078    2.865956   -0.210291
H    -1.955397    1.753608   -0.367828
H     3.332094   -0.811914   -0.270105
H     2.244236   -2.311510   -0.278004
```

Frequencies

86.1886	149.7816	197.4024
293.3714	310.4419	425.0958
452.6088	524.9006	547.7813
564.2832	697.2429	710.6875
762.4669	869.77	885.5038
907.9335	941.9996	958.3021
979.7316	1011.462	1024.802
1050.874	1070.723	1194.574
1206.929	1233.519	1318.658
1353.367	1371.354	1415.437
1444.778	1453.045	1461.583
1487.503	1495.332	1679.042
1708.67	1757.524	3000.718
3039.048	3091.619	3098.039
3139.132	3150.206	3173.828
3175.524	3199.843	3238.053

p43 + H

```
C    -2.097858   -1.232195   -0.516646
C    -1.199512   -0.459379    0.081025
C     0.096804   -0.986202    0.639622
C     1.282905   -0.260390    0.040895
C     1.093620    1.176108   -0.185046
C    -0.095395    1.772278   -0.078891
C    -1.368433    1.030408    0.233720
C     2.433906   -0.873739   -0.235999
H    -1.943747   -2.301257   -0.620366
H    -3.016747   -0.822498   -0.923711
H     0.184823   -2.063313    0.485259
H     0.106811   -0.804887    1.723843
H     1.971424    1.758776   -0.448936
H    -0.176061    2.843715   -0.235638
H    -1.671245    1.262902    1.265410
H    -2.176772    1.389534   -0.409805
H     3.281020   -0.326351   -0.636064
H     2.564274   -1.937956   -0.072071
```

Frequencies

102.8299	121.9869	306.5873
354.9817	406.641	439.2356
469.0592	542.7892	572.2869
688.4891	717.5625	744.8351
813.2412	862.5536	917.9593
933.2465	940.0491	947.2836
955.1106	1000.079	1013.496
1019.165	1030.357	1174
1203.474	1235.402	1299.382
1319.737	1339.006	1355.851
1413.596	1455.653	1463.359
1473.28	1486.64	1699.911
1750.795	1760.651	3009.778
3022.523	3089.852	3116.202

3147.358	3155.64	3167.103
3192.603	3233.452	3242.854

p58 + H

C	0.685685	1.627587	0.000153
C	-0.641896	1.422664	-0.000499
C	3.534155	-1.300103	-0.000422
C	2.510549	-0.263244	0.000968
C	1.664489	0.593504	0.000802
C	-1.288446	0.122593	-0.000325
C	-2.613749	-0.040812	-0.000187
C	-3.314838	-1.361038	0.000270
H	1.063512	2.645355	0.000044
H	-1.292409	2.293591	-0.001127
H	3.562070	-1.818318	-0.962623
H	3.338972	-2.042359	0.777855
H	4.521928	-0.869316	0.180628
H	-0.636886	-0.748820	-0.000251
H	-3.248601	0.844743	-0.000293
H	-3.960061	-1.460503	0.879422
H	-2.604053	-2.190151	0.000521
H	-3.960165	-1.461135	-0.878731

Frequencies

63.0926	81.4329	90.8099
138.9581	182.1175	191.7206
229.3643	286.4884	374.5905
428.6395	471.0771	544.6058
647.8424	768.2988	793.0095
860.3915	951.2481	993.9411
1036.206	1057.768	1059.063
1070.339	1090.043	1141.937
1190.808	1255.781	1302.629
1335.298	1415.186	1419.721
1437.931	1483.752	1484.594
1488.528	1489.736	1683.183
1752.439	2373.538	3039.481
3047.949	3097.115	3119.769
3122.388	3128.473	3144.653
3160.36	3167.768	3191.067

p59 + H

C	0.588584	0.734144	0.001374
C	-0.452830	-0.111659	0.003391
C	4.507564	-0.411645	-0.002810
C	3.108168	-0.006056	0.000586
C	1.949694	0.321363	0.001781
C	-1.840584	0.316564	0.000703
C	-2.877270	-0.524936	0.000781
C	-4.315680	-0.117412	-0.002934
H	0.405486	1.806458	-0.001880
H	-0.262747	-1.182277	0.006660
H	4.629610	-1.382019	-0.490561
H	4.893001	-0.495628	1.016898
H	5.122384	0.316464	-0.537837
H	-2.023765	1.390345	-0.002204
H	-2.677052	-1.595581	0.003559
H	-4.831831	-0.516381	-0.882352
H	-4.425435	0.969338	-0.005375
H	-4.835520	-0.512905	0.875866

Frequencies

53.1973	64.5161	72.6551
127.8905	185.2636	192.7955
243.2009	305.3295	320.7334
396.3822	447.859	488.3711

587.8938	793.9654	816.2744
889.5093	954.0316	959.9027
1017.02	1052.799	1059.5
1068.385	1109.627	1189.845
1213.148	1264.223	1334.476
1349.987	1366.689	1419.63
1422.3	1478.043	1482.708
1488.717	1498.133	1702.302
1757.095	2374.968	3040.793
3049.209	3099.546	3118.51
3125.018	3128.849	3150.763
3155.212	3162.672	3176.883

p60 + H

```
C    0.505972  -0.948109  -0.001430
C   -0.630390  -0.233699  -0.000641
C    4.258094   0.661303   0.001886
C    2.918125   0.089464  -0.001689
C    1.807217  -0.374652  -0.002169
C   -1.948744  -0.844872   0.001377
C   -3.123865  -0.205290   0.001568
C   -3.359139   1.273134  -0.000736
H    0.453159  -2.034798  -0.000901
H   -0.555908   0.849246  -0.001203
H    4.363701   1.409962  -0.787540
H    5.012262  -0.112684  -0.160082
H    4.470123   1.146890   0.958147
H   -1.961873  -1.932663   0.003116
H   -4.023375  -0.816532   0.003513
H   -2.436638   1.854213  -0.003111
H   -3.941319   1.567959   0.878396
H   -3.943752   1.564733  -0.879332
```

Frequencies

71.0633	85.297	97.7501
112.1492	120.7265	185.3702
249.5173	315.4408	355.0123
396.4029	497.706	510.6392
627.5712	747.0897	816.6887
884.9354	941.3308	971.9514
1024.225	1045.195	1055.623
1065.129	1066.134	1170.867
1208.402	1264.615	1293.034
1334.899	1406.718	1423.181
1444.772	1483.471	1486.179
1489.854	1492.838	1690.999
1747.566	2373.539	3038.958
3046.826	3093.108	3118.416
3120.975	3139.44	3153.896
3161.142	3174.651	3194.204

p61 + H

```
C    0.458062   1.417502  -0.000083
C   -0.799635   0.943301  -0.001030
C    3.853480  -0.852839   0.000453
C    2.638606  -0.048564   0.000653
C    1.631650   0.611458   0.000299
C   -1.149211  -0.467032  -0.001652
C   -2.387180  -0.975005  -0.000617
C   -3.685125  -0.228725   0.001428
H    0.616149   2.491671   0.000533
H   -1.603105   1.672335  -0.000983
```

```
H     4.000897   -1.334174   -0.969954
H     3.801862   -1.635360    0.761772
H     4.729771   -0.234129    0.208753
H    -0.311100   -1.158417   -0.002764
H    -2.479860   -2.058690   -0.000568
H    -4.284778   -0.505346   -0.871882
H    -3.559058    0.854219   -0.007180
H    -4.274659   -0.492685    0.885564
```

Frequencies

49.1572	52.4023	73.1946
115.9931	178.9772	205.499
254.6138	314.987	398.622
402.5766	554.7639	559.772
679.5642	745.7116	784.8115
813.8496	943.6554	995.5354
1028.139	1034.785	1056.945
1062.416	1062.523	1146.431
1185.353	1265.115	1306.148
1385.602	1419.84	1424.56
1477.868	1481.384	1486.589
1491.33	1493.516	1676.699
1747.78	2370.738	3039.043
3047.982	3092.629	3118.179
3123.528	3143.086	3163.357
3180.204	3189.714	3209.219

p62 + H

```
C     0.396078   -0.232559   -0.257859
C    -0.429136    0.782537    0.036029
C    -1.888520    0.730476   -0.060085
C    -2.637776   -0.349875    0.167207
C    -4.127510   -0.398440    0.042801
C     4.459572   -0.110399    0.129741
C     3.009716   -0.148718   -0.009593
C     1.811153   -0.172401   -0.118666
H    -0.015362   -1.164017   -0.639336
H     0.007267    1.725387    0.355526
H    -2.384595    1.666434   -0.312102
H    -2.148063   -1.269405    0.483271
H    -4.431856   -1.147879   -0.695240
H    -4.536923    0.566682   -0.263961
H    -4.591537   -0.683286    0.992626
H     4.878910    0.747018   -0.403022
H     4.913727   -1.017464   -0.276425
H     4.746966   -0.027196    1.181216
```

Frequencies

43.3159	65.6979	77.7781
129.6249	166.0664	203.5178
226.6554	308.0745	329.8958
356.3313	484.6116	501.4075
627.6418	788.1359	859.2142
886.4911	931.5093	987.7603
1003.524	1052.666	1060.961
1073.493	1075.153	1136.682
1214.493	1320.412	1325.367
1345.966	1362.716	1419.47
1424.259	1480.659	1484.519
1485.638	1498.457	1711.303
1745.918	2374.56	3040.445

3050.8	3099.586	3121.201
3125.905	3128.414	3151.797
3160.002	3163.013	3178.195

p63 + H

C	0.424847	1.810526	0.039143
C	-0.918046	1.752136	-0.006999
C	-1.805177	0.594845	-0.081645
C	-1.492024	-0.693293	0.092217
C	-2.479056	-1.812600	-0.000719
C	3.113270	-1.259920	-0.037506
C	2.145734	-0.171272	-0.005955
C	1.332536	0.717308	0.015290
H	0.887105	2.791979	0.092306
H	-1.428707	2.711165	-0.000032
H	-2.846310	0.836163	-0.290531
H	-0.467017	-0.966537	0.321202
H	-2.180751	-2.530726	-0.771774
H	-3.481577	-1.449416	-0.238859
H	-2.529358	-2.366334	0.942870
H	3.225907	-1.710758	0.952153
H	4.093765	-0.900040	-0.358828
H	2.794435	-2.041870	-0.731471

Frequencies

57.037	59.6619	74.485
146.8731	187.289	201.243
229.4105	286.9953	376.9955
395.2003	505.5142	557.3356
678.2906	747.0934	842.7331
864.1253	907.1959	1002.225
1025.434	1044.87	1055.37
1059.245	1076.959	1138.248
1180.165	1285.148	1354.952
1366.007	1418.248	1421.069
1463.776	1482.827	1484.176
1486.19	1495.919	1692.016
1739.662	2367.107	3037.704
3047.509	3095.825	3117.16
3125.088	3128.82	3140.374
3168.949	3190.457	3200.498

p64 + H

C	0.288141	-1.621614	0.406028
C	1.527711	-1.276885	0.023208
C	-3.147176	0.460319	-0.323800
C	-1.919274	-0.277014	-0.057600
C	-0.897608	-0.878011	0.151196
C	1.934212	-0.064373	-0.690269
C	1.626450	1.200689	-0.389858
C	0.833121	1.688609	0.779724
H	0.150552	-2.569217	0.919342
H	2.317278	-2.000672	0.213182
H	-3.813669	-0.115748	-0.970892
H	-2.931382	1.410592	-0.818775
H	-3.680941	0.674209	0.605811
H	2.601744	-0.233545	-1.532913
H	2.022932	1.971964	-1.046655
H	1.311489	2.567832	1.220778
H	0.724358	0.922047	1.548295
H	-0.175822	1.982221	0.470050

Frequencies

78.6989	89.3834	129.6144
189.2154	209.7103	259.0353
319.9515	330.9655	382.4903

431.6498	525.349	593.8044
694.8148	731.7899	799.6599
862.3418	910.6633	1000.126
1003.236	1017.456	1056.597
1060.245	1073.643	1128.307
1170.681	1271.358	1284.484
1401.269	1419.195	1429.182
1467.133	1487.049	1490.236
1494.813	1524.252	1701.321
1735.033	2374.17	3044.811
3049.356	3104.97	3120.537
3123.521	3138.174	3148.396
3156.795	3173.189	3180.817

p65 + H

```
C   -0.145229   0.016205  -0.358438
C    0.635440   0.977883   0.156680
C   -4.191590  -0.215529   0.144265
C   -2.748132  -0.124430  -0.031200
C   -1.555324  -0.045309  -0.171783
C    2.085287   1.084423  -0.007653
C    2.983804   0.093793  -0.020276
C    2.731170  -1.370282   0.171203
H    0.291755  -0.759465  -0.980620
H    0.155830   1.777055   0.717033
H   -4.658682  -0.694775  -0.719688
H   -4.633083   0.777205   0.262169
H   -4.439305  -0.802691   1.032663
H    2.463236   2.100652  -0.093270
H    4.024579   0.376219  -0.160112
H    3.533362  -1.820365   0.761784
H    2.710261  -1.896955  -0.789686
H    1.779497  -1.557398   0.672929
```

Frequencies

71.824	77.5225	93.9907
123.4177	174.7135	237.3138
279.581	319.7619	371.8724
440.8061	504.3222	515.006
687.4783	728.4117	861.6314
890.2585	920.3735	998.7109
1018.944	1045.249	1057.686
1063.983	1074.841	1123.367
1211.48	1278.416	1329.073
1342.243	1415.046	1424.648
1449.177	1484.667	1489.347
1496.449	1529.167	1710.282
1731.838	2376.637	3042.514
3046.231	3102.945	3115.823
3122.828	3139.273	3152.941
3166.152	3180.273	3186.958

p66 + H

```
C   -0.648300   1.733156   0.000414
C    0.805508   1.336053  -0.000479
C   -3.323007  -1.400425  -0.000436
C   -2.373809  -0.292766   0.000305
C   -1.597104   0.622464   0.000401
C    1.278371   0.090973   0.000310
C    2.700451  -0.231829  -0.000530
C    3.184815  -1.472717   0.000336
```

```
H    -0.840291    2.369337    0.873460
H    -0.841175    2.370006   -0.871941
H     1.504850    2.170117   -0.001752
H    -3.340906   -1.899403    0.971541
H    -3.055961   -2.141294   -0.757892
H    -4.333381   -1.044652   -0.216615
H     0.578692   -0.742297    0.001799
H     3.390903    0.609639   -0.001936
H     2.524665   -2.334977    0.001775
H     4.251062   -1.665925   -0.000365
```

Frequencies

62.5932	68.0123	101.7721
160.263	179.2664	202.9892
254.3136	286.4714	396.6162
424.7499	472.3517	621.5597
644.6462	768.3163	835.1381
946.6429	958.6147	975.2431
1006.297	1011.148	1052.461
1060.925	1064.722	1174.836
1192.609	1240.371	1283.563
1325.713	1346.441	1374.726
1417.823	1456.633	1460.79
1485.969	1490.836	1701.044
1766.605	2399.594	3032.366
3054.755	3059.002	3127.648
3128.009	3149.197	3160.147
3162.672	3172.317	3245.782

p67 + H

```
C    -0.311354    0.735442   -0.798081
C     0.577594    0.989054    0.393494
C     1.793314    0.483577    0.613618
C     2.533828   -0.438591   -0.241633
C     3.760331   -0.873905    0.043844
C    -3.993401   -0.709254    0.368253
C    -2.695597   -0.193851   -0.053486
C    -1.624572    0.222543   -0.400329
H    -0.451968    1.678280   -1.340932
H     0.150404    0.040497   -1.503115
H     0.155560    1.658513    1.137917
H     2.303553    0.779646    1.527680
H     2.055556   -0.787734   -1.152295
H     4.277160   -0.553955    0.943895
H     4.285969   -1.560891   -0.608731
H    -3.921014   -1.184267    1.349704
H    -4.363955   -1.453616   -0.340968
H    -4.732118    0.093437    0.432764
```

Frequencies

22.6559	99.6604	118.8349
122.0496	179.4105	222.0025
271.4566	374.8978	377.9704
400.1575	514.6486	615.5969
651.6305	782.6419	833.101
915.4823	943.4925	956.4739
1011.343	1029.358	1047.902
1061.029	1068.168	1170.69
1174.052	1240.994	1300.309
1323.366	1342.081	1406.236
1424.471	1474.824	1476.009
1489.597	1493.386	1692.029

1760.597	2398.524	3043.361
3049.629	3105.18	3121.099
3123.798	3154.779	3158.393
3182.106	3186.166	3250.414

p68 + H

C	0.456677	1.576493	-0.037832
C	-0.907983	0.943154	-0.136835
C	3.622097	-1.056682	0.101331
C	2.498161	-0.128063	0.052129
C	1.578103	0.641957	0.012669
C	-1.161219	-0.362761	-0.166223
C	-2.505630	-0.949738	-0.236951
C	-3.594085	-0.459081	0.351688
H	0.593978	2.257452	-0.886862
H	0.481797	2.215524	0.853967
H	-1.733332	1.649235	-0.197996
H	3.285743	-2.083441	-0.062408
H	4.119405	-1.014644	1.073427
H	4.359717	-0.815901	-0.668089
H	-0.323547	-1.056696	-0.160733
H	-2.590344	-1.873503	-0.805611
H	-4.559882	-0.937910	0.238623
H	-3.550266	0.428211	0.975824

Frequencies

55.9729	75.795	100.1683
170.8728	189.7929	218.442
221.6092	264.8177	391.9325
400.2293	529.6692	615.1144
686.7543	762.8369	824.2879
953.0179	972.2027	983.0466
1004.931	1020.455	1044.014
1051.384	1064.611	1101.534
1177.185	1244.028	1301.046
1319.227	1352.884	1378.017
1415.989	1459.418	1462.058
1486.797	1491.508	1718.571
1751.106	2398.989	3031.804
3053.617	3060.296	3126.318
3126.645	3147.331	3159.358
3168.418	3174.46	3240.485

p69 + H

C	0.065866	-0.428004	-0.494164
C	-0.654155	0.896186	-0.439427
C	4.077079	-0.022183	0.367822
C	2.659302	-0.170559	0.058045
C	1.492022	-0.296288	-0.192198
C	-1.887968	1.116049	0.019839
C	-2.836041	0.128602	0.549974
C	-3.058856	-1.090355	0.061547
H	-0.396069	-1.135994	0.201314
H	-0.043720	-0.867833	-1.493791
H	-0.078899	1.748316	-0.790101
H	4.272860	-0.254707	1.417525
H	4.409690	1.002026	0.181524
H	4.683869	-0.691186	-0.247402
H	-2.232283	2.147457	0.043612
H	-3.423906	0.459167	1.404263
H	-2.550762	-1.454576	-0.824848
H	-3.784274	-1.753352	0.519275

Frequencies

47.3813	82.2429	116.7054
144.4019	188.8016	224.9966

280.9361	344.1863	401.328
422.9728	509.404	585.6847
706.1596	770.0486	831.5919
904.1684	946.2337	971.7772
1020.385	1035.851	1056.49
1064.518	1069.895	1096.02
1178.115	1249.559	1276.655
1331.557	1343.714	1422.965
1429.729	1462.571	1475.65
1490.504	1492.371	1716.931
1734.69	2397.817	3028.713
3050.122	3083.196	3121.454
3123.873	3146.312	3157.898
3166.312	3186.326	3250.045

p70 + H
```
C   -0.445116   1.010921  -0.207956
C    0.522217   0.250579   0.677237
C    1.648067  -0.251804   0.257053
C    2.776591  -0.745758  -0.168406
C    4.088097  -0.007565  -0.163757
C   -4.230977  -0.612088  -0.035803
C   -2.894951  -0.031311  -0.109160
C   -1.794243   0.444159  -0.167802
H   -0.490701   2.055962   0.120485
H   -0.071817   1.017143  -1.235436
H    0.234741   0.124716   1.718330
H    2.779092  -1.764799  -0.550928
H    4.829404  -0.544797   0.435497
H    3.972931   0.995819   0.248453
H    4.489512   0.077490  -1.178076
H   -4.198808  -1.597338   0.435933
H   -4.661903  -0.729109  -1.033237
H   -4.900555   0.022123   0.550543
```

Frequencies

36.9293	71.5131	120.1423
132.5536	163.7373	194.7237
223.2194	257.2421	339.9
399.355	498.1442	539.7644
578.0613	715.9504	786.7426
865.3909	919.4272	950.8657
1041.914	1060.634	1062.086
1066.551	1107.314	1163.341
1173.915	1219.803	1293.649
1337.884	1411.53	1423.515
1465.64	1466.475	1489.29
1489.777	1493.301	1514.275
2100.575	2398.174	3043.144
3045.56	3049.844	3101.685
3108.422	3120.222	3124.195
3138.521	3156.838	3168.554

p71 + H
```
C   -0.596043   1.898709  -0.195656
C    0.889123   1.678736   0.014632
C   -2.849459  -1.536153   0.081581
C   -2.060437  -0.313758  -0.018494
C   -1.407320   0.689321  -0.100513
C    1.447306   0.535390   0.292434
```

```
C     1.995046   -0.614813    0.561805
C     2.484817   -1.591777   -0.472052
H    -0.949991    2.633352    0.537366
H    -0.746139    2.361121   -1.178385
H     1.513772    2.564648   -0.076243
H    -2.734020   -1.993368    1.067469
H    -2.533014   -2.265328   -0.668322
H    -3.911376   -1.330141   -0.074001
H     2.105942   -0.896786    1.607147
H     3.554023   -1.786732   -0.344622
H     2.318470   -1.211857   -1.480801
H     1.964136   -2.548845   -0.372033
```

Frequencies

53.1186	79.9296	128.5912
135.5153	178.5096	211.4251
215.2594	282.2861	328.5864
401.5577	465.8781	564.7888
646.1371	707.203	763.8782
885.9648	903.2699	968.4615
975.3547	1065.918	1068.202
1071.481	1104.36	1151.311
1188.604	1249.927	1292.707
1364.515	1416.273	1429.014
1465.794	1485.884	1491.017
1492.572	1494.84	1517.206
2104.613	2404.647	3034.977
3045.613	3049.913	3063.959
3107.181	3119.993	3124.222
3142.11	3158.662	3159.204

p72 + H

```
C    -0.713410   -0.980062   -0.000042
C     0.547035   -0.252438   -0.000009
C    -4.212028    0.734059    0.000030
C    -3.033812    0.156387    0.000001
C    -1.900841   -0.403965   -0.000024
C     1.736377   -0.860954    0.000013
C     3.079154   -0.194172    0.000063
C     3.062888    1.329941   -0.000043
H    -0.661555   -2.067771   -0.000084
H     0.477369    0.831337    0.000007
H    -4.307055    1.814772    0.000082
H    -5.124344    0.146873    0.000009
H     1.756074   -1.950366    0.000003
H     3.639857   -0.557462   -0.870612
H     3.639730   -0.557344    0.870870
H     2.553109    1.721717    0.884267
H     2.553223    1.721589   -0.884476
H     4.081408    1.723869   -0.000003
```

Frequencies

67.3481	70.8119	131.687
195.9472	202.6748	253.4614
302.0015	319.3964	342.1523
491.8876	514.3469	571.8892
608.6653	750.1099	860.2545
879.4083	888.017	900.1741
956.0192	1008.7	1031.622
1036.01	1107.811	1112.484
1182.312	1263.46	1294.705
1345.693	1352.75	1383.241

1424.963	1453.41	1478.268
1504.7	1517.254	1701.225
1745.792	2232.173	3030.471
3055.313	3055.552	3128.995
3134.871	3146.643	3148.704
3150.766	3192.37	3231.631

p73 + H

C	0.495842	-0.248734	-0.259435
C	-0.370615	0.880943	0.047332
C	-1.702684	0.907024	-0.079686
C	-2.607379	-0.197323	-0.535992
C	-3.571147	-0.637565	0.571687
C	4.364303	-0.144683	0.193779
C	3.061585	-0.180694	0.040506
C	1.807053	-0.217941	-0.108132
H	0.047028	-1.166422	-0.630414
H	0.134213	1.771065	0.410702
H	-2.209747	1.829033	0.199213
H	-2.036517	-1.059022	-0.889399
H	-3.188961	0.160318	-1.393831
H	-4.171277	0.205157	0.926704
H	-3.021099	-1.038770	1.426438
H	-4.256267	-1.408905	0.211609
H	4.980442	-1.005611	-0.043486
H	4.860432	0.746994	0.562115

Frequencies

32.1209	68.5148	86.1916
199.4205	223.3875	249.9794
266.1653	307.3864	425.3394
493.5502	550.348	579.1076
609.8645	785.0231	808.7732
883.1672	886.6094	897.33
951.0385	1023.342	1031.982
1035.839	1078.842	1097.805
1175.652	1281.815	1293.645
1313.916	1344.086	1416.339
1429.896	1468.782	1490.695
1502.7	1511.732	1694.431
1740.288	2232.577	3046.722
3048.878	3102.343	3126.186
3132.845	3147.901	3156.519
3173.298	3192.98	3234.046

p74 + H

C	-0.364156	-0.965303	0.754369
C	0.742896	-0.908420	0.053822
C	-3.925203	0.671714	-0.406501
C	-2.653244	0.093890	0.007700
C	-1.598529	-0.382393	0.334264
C	1.845649	-0.846559	-0.632041
C	2.877860	0.249444	-0.519177
C	2.552319	1.318296	0.516044
H	-0.358265	-1.486131	1.709384
H	-4.092028	0.514071	-1.475037
H	-3.947085	1.747798	-0.215445
H	-4.755507	0.214105	0.137005
H	2.045468	-1.638701	-1.351841
H	2.994832	0.708022	-1.508067
H	3.844535	-0.214530	-0.291181
H	2.466801	0.882274	1.514689
H	1.602166	1.808031	0.288060
H	3.333526	2.081045	0.541550

Frequencies

49.9925	72.8182	95.2156
135.9368	152.1714	240.7514
263.4731	304.429	370.2804
399.9337	465.819	535.8745
655.7898	741.8485	806.6145
829.0632	865.7776	917.9524
1011.998	1055.69	1063.966
1096.867	1114.712	1134.33
1206.065	1299.566	1303.481
1377.612	1419.976	1427.961
1470.153	1485.984	1491.503
1495.52	1507.33	1510.936
2082.169	2385.028	3039.154
3050.459	3054.561	3069.828
3122.225	3123.914	3129.134
3136.868	3146.48	3156.303

p75 + H
```
C    -0.577757   1.099763   -0.202672
C     0.535497   0.578787    0.254442
C     1.645910   0.062529    0.690116
C     2.575008  -0.790894   -0.137818
C     3.957602  -0.153985   -0.291525
C    -4.243897  -0.696515   -0.001845
C    -2.934807  -0.060631   -0.076184
C    -1.849208   0.453995   -0.125282
H    -0.545076   2.082415   -0.668127
H     1.941393   0.264332    1.719365
H     2.126505  -0.963972   -1.118886
H     2.675658  -1.769102    0.345493
H     4.426790   0.009360    0.683068
H     3.883957   0.813556   -0.794266
H     4.618775  -0.795453   -0.879299
H    -4.166017  -1.686574    0.453889
H    -4.679485  -0.814099   -0.997415
H    -4.932589  -0.098766    0.600786
```

Frequencies

62.9624	80.3483	115.7544
126.5356	177.6451	239.7009
257.7531	297.3411	380.6915
400.9765	494.5501	523.2876
594.2206	774.4237	808.2518
817.0601	896.2972	919.0529
1021.205	1059.96	1064.182
1094.729	1112.472	1153.933
1206.423	1279.425	1315.245
1361.911	1422.143	1423.622
1476.916	1489.706	1490.223
1498.908	1507.905	1517.469
2083.78	2385.695	3044.863
3047.58	3048.089	3098.973
3118.104	3122.486	3123.02
3129.573	3140.639	3155.89

p76 + C₃H₅_b
```
C    -2.399426   0.473677    0.000001
C    -1.471392  -0.482327   -0.000012
```

```
C     2.564241    0.161451    0.000016
C     1.124440   -0.061610    0.000040
C    -0.065584   -0.237953   -0.000009
H    -2.129897    1.523631   -0.000017
H    -3.453698    0.223627    0.000029
H    -1.774515   -1.526164    0.000006
H     2.792614    1.229603    0.025236
H     3.022491   -0.263392   -0.896744
H     3.029335   -0.306731    0.871280
```

Frequencies

24.4431	140.0762	188.5809
332.0014	390.8488	545.7793
709.4461	726.7034	964.8887
1023.757	1054.747	1055.003
1058.66	1201.186	1328.813
1418.595	1451.104	1483.735
1484.151	1707.08	2378.718
3046.618	3118.232	3122.656
3157.391	3168.863	3255.855

p76' + C₃H₅_a

$p76' + C_3H_5\_a$

```
C    -2.399426    0.473677    0.000001
C    -1.471392   -0.482327   -0.000012
C     2.564241    0.161451    0.000016
C     1.124440   -0.061610    0.000040
C    -0.065584   -0.237953   -0.000009
H    -2.129897    1.523631   -0.000017
H    -3.453698    0.223627    0.000029
H    -1.774515   -1.526164    0.000006
H     2.792614    1.229603    0.025236
H     3.022491   -0.263392   -0.896744
H     3.029335   -0.306731    0.871280
```

Frequencies

24.4431	140.0762	188.5809
332.0014	390.8488	545.7793
709.4461	726.7034	964.8887
1023.757	1054.747	1055.003
1058.66	1201.186	1328.813
1418.595	1451.104	1483.735
1484.151	1707.08	2378.718
3046.618	3118.232	3122.656
3157.391	3168.863	3255.855

p77 + H

```
C     0.698924    1.541603   -0.458266
C     0.024389    0.630243    0.535960
C    -3.803798   -0.674066   -0.131234
C    -2.442767   -0.205953    0.103849
C    -1.321536    0.176088    0.305720
C     1.151496    0.109345   -0.351224
C     2.456014   -0.208085    0.260259
C     3.234651   -1.221467   -0.099979
H     1.356871    2.307623   -0.064260
H     0.131642    1.827012   -1.334844
H     0.285312    0.783071    1.578295
H    -4.372012    0.048293   -0.722714
H    -4.328120   -0.821866    0.816196
H    -3.802860   -1.626444   -0.667519
H     0.833675   -0.553866   -1.148323
H     2.779715    0.456535    1.060710
H     2.945299   -1.903659   -0.893560
H     4.186242   -1.402944    0.385511
```

Frequencies

67.2689	92.5346	116.1937
120.4699	242.4494	258.6953

319.4635	345.6374	437.4217
508.1655	527.8839	662.2775
744.8828	838.1725	889.3791
937.5238	950.4079	964.6729
1012.364	1032.834	1055.998
1062.637	1072.851	1107.62
1113.352	1199.803	1230.132
1238.469	1316.609	1344.906
1414.509	1425.333	1474.794
1488.035	1489.566	1505.584
1737.588	2393.455	3052.096
3123.718	3124.932	3143.37
3148.054	3158.996	3170.826
3186.57	3243.005	3245.072

p78 + H

```
C    -0.890077   1.648887  -0.089181
C     0.608870   1.695524   0.076099
C    -3.027915  -1.598812  -0.006278
C    -2.309618  -0.503239  -0.035311
C    -1.616453   0.556476  -0.064378
C     1.236662   0.376321   0.409580
C     2.169401  -0.221987  -0.320558
C     2.805366  -1.537494   0.007336
H    -1.390592   2.603412  -0.240955
H     0.833971   2.426654   0.864517
H     1.049577   2.103866  -0.841551
H    -2.564361  -2.568378   0.143160
H    -4.105164  -1.567187  -0.132847
H     0.876616  -0.107421   1.316414
H     2.511785   0.264460  -1.233636
H     2.648587  -2.260053  -0.799855
H     2.394689  -1.960024   0.927272
H     3.887478  -1.429384   0.133630
```

Frequencies

47.9241	98.904	116.9778
180.4462	216.2079	225.3755
282.5876	297.2478	391.2214
484.8013	498.7873	574.6453
629.6155	789.0545	831.6924
862.9862	900.6647	938.7772
976.3481	1016.379	1033.567
1036.912	1077.843	1115.261
1140.114	1229.007	1299.229
1332.69	1345.547	1380.9
1424.784	1454.232	1475.577
1491.168	1501.275	1728.957
1779.322	2245.341	3023.377
3038.217	3062.149	3098.635
3123.814	3143.29	3147.045
3150.364	3156.188	3228.362

p79 + H

```
C     0.871801   1.885463  -0.314635
C     0.174150   0.907495   0.663360
C    -3.475270  -0.715221  -0.269173
C    -2.180616  -0.130670   0.060575
C    -1.112269   0.346990   0.332682
C     1.372821   0.530903  -0.114776
```

```
C    2.209247   -0.438171   -0.418426
C    2.141817   -1.815698    0.168193
H    1.400138    2.721122    0.133482
H    0.345980    2.112390   -1.236327
H    0.324971    1.126008    1.717368
H   -4.058247   -0.045720   -0.906716
H   -4.054161   -0.905298    0.638206
H   -3.352652   -1.664987   -0.795965
H    2.995726   -0.238556   -1.143304
H    1.310392   -1.901808    0.870060
H    3.069601   -2.063547    0.693826
H    2.008171   -2.566150   -0.617424
```

Frequencies

59.1757	111.8581	114.9141
168.3769	174.8853	214.3262
269.5821	322.1599	378.5646
472.3485	518.4221	566.7156
699.3215	739.7736	834.8127
930.3506	957.7737	982.0024
1044.942	1056.888	1062.564
1065.016	1073.309	1103.539
1127.647	1138.116	1211.975
1334.811	1385.609	1420.124
1422.748	1466.932	1487.409
1488.444	1492.159	1499.762
1892.545	2394.159	3040.635
3049.754	3099.4	3120.854
3122.934	3129.227	3136.874
3149.099	3158.808	3218.79

p80 + H

```
C   -0.903293    1.743719   -0.362071
C   -0.011968    0.797113    0.446128
C   -3.216239   -1.416092   -0.004559
C   -2.296682   -0.490714    0.011796
C   -1.388109    0.416038    0.038926
C    1.144087    0.139515   -0.200655
C    2.279683   -0.164805    0.418656
C    3.452874   -0.836222   -0.225869
H   -1.306361    2.612456    0.147875
H   -0.653480    1.899108   -1.407416
H    0.120498    1.053070    1.494200
H   -3.968739   -1.472561    0.774958
H   -3.253441   -2.155265   -0.797854
H    1.020478   -0.106376   -1.254960
H    2.381963    0.079341    1.475214
H    4.352741   -0.217529   -0.148030
H    3.266817   -1.035200   -1.283836
H    3.677413   -1.788365    0.265742
```

Frequencies

58.6233	116.4886	176.0509
188.8268	209.9529	219.9969
341.5814	396.011	435.3816
463.4109	579.9786	621.0697
670.0416	828.302	880.8872
881.6427	952.4417	959.6089
991.871	1005.857	1027.156
1040.433	1062.98	1074.755
1109.085	1126.129	1201.118
1277.445	1340.793	1352.661

1407.176	1426.269	1468.872
1490.882	1500.012	1554.882
1772.305	2140.864	3038.886
3098.364	3124.757	3129.623
3148.109	3149.678	3152.786
3160.169	3220.04	3232.544

p81 + H
```
C     0.722063    1.779940   -0.067818
C    -0.206491    0.587413   -0.317620
C     3.247227   -1.234395    0.005790
C     2.248569   -0.398317   -0.069783
C     1.259952    0.416537   -0.152961
C    -1.103617    0.127010    0.765519
C    -2.307272   -0.424966    0.627883
C    -3.040718   -0.714344   -0.646692
H     0.903170    2.456779   -0.896253
H     0.680702    2.250267    0.910031
H    -0.574272    0.494910   -1.334345
H     3.815814   -1.509691   -0.876342
H     3.535520   -1.678758    0.952668
H    -0.705711    0.257023    1.769904
H    -2.829895   -0.707734    1.538715
H    -3.239199   -1.786889   -0.739773
H    -2.492488   -0.399608   -1.535693
H    -4.011919   -0.209570   -0.654815
```

Frequencies

42.8326	94.1345	141.3965
175.9962	201.2369	279.5261
318.5867	389.5484	487.6775
548.3369	587.2281	618.9209
659.226	777.2761	857.2757
872.2178	940.1642	954.5991
984.2854	1017.453	1021.368
1035.83	1054.504	1068.844
1085.241	1103.402	1177.66
1293.588	1305.306	1377.446
1412.466	1454.499	1465.147
1485.337	1499.94	1551.58
1761.257	2141.691	3046.377
3102.413	3129.43	3136.292
3145.594	3150.652	3172.459
3177.588	3219.599	3229.253

p82 + H
```
C     0.076255    2.485399    0.000709
C    -0.064552    1.152348   -0.000409
C     3.227653   -1.283545    0.000873
C     2.051302   -0.423407   -0.001560
C     1.091502    0.300798   -0.001411
C    -1.396717    0.526711   -0.000065
C    -1.631483   -0.783956   -0.000244
C    -2.992487   -1.403635    0.000357
H     1.053714    2.950427    0.000760
H    -0.793545    3.133228    0.001691
H     3.728697   -1.250489    0.971687
H     3.943309   -0.963365   -0.760412
H     2.954304   -2.321276   -0.204581
H    -2.233154    1.222860    0.000600
H    -0.782799   -1.464896   -0.000692
H    -3.130363   -2.040828   -0.879268
H    -3.780345   -0.647078    0.001958
H    -3.128655   -2.042864    0.878760
```

Frequencies

308

75.8223	79.8335	103.3179
141.157	190.046	204.0626
209.0405	313.1813	384.2392
396.3173	454.3461	616.4362
646.1392	675.406	734.728
855.3075	925.2936	932.9498
1011.688	1012.239	1056.461
1063.916	1072.067	1086.04
1134.28	1302.498	1337.26
1364.455	1417.583	1421.105
1444.799	1483.301	1487.141
1489.829	1490.788	1683.354
1758.789	2382.758	3041.582
3051.811	3100.724	3124.627
3125.356	3130.257	3162.591
3165.409	3169.278	3265.685

p83 + H

```
C    0.200998   2.079424  -0.013950
C   -0.000187   0.759427  -0.112150
C   -3.736862  -0.902749   0.098867
C   -2.411571  -0.302223   0.019489
C   -1.321503   0.203123  -0.035247
C    1.096928  -0.213044  -0.315816
C    2.295395  -0.128911   0.256914
C    3.411468  -1.102113   0.041489
H   -0.621969   2.760583   0.163644
H    1.194297   2.498470  -0.124977
H   -4.494146  -0.232494  -0.315094
H   -4.002284  -1.114755   1.137853
H   -3.771664  -1.842587  -0.457517
H    0.865838  -1.060297  -0.958130
H    2.489078   0.690510   0.946882
H    4.295371  -0.598040  -0.362787
H    3.123257  -1.893786  -0.653472
H    3.714223  -1.565218   0.986021
```

Frequencies

67.05	84.6413	89.7886
159.3052	185.6795	210.9873
225.4249	313.3562	379.7932
392.9749	431.868	583.5121
610.7154	743.3203	758.6871
844.7305	923.0083	943.1659
996.2113	1013.45	1054.576
1060.901	1074.614	1083.681
1134.357	1277.524	1336.361
1364.201	1418.575	1420.786
1442.259	1484.291	1486.533
1487.686	1496.464	1692.761
1752.611	2381.161	3042.691
3049.724	3102.27	3120.358
3126.181	3131.988	3158.669
3163.224	3167.06	3263.348

p84 + H

```
C   -0.733542   2.416035   0.086120
C   -0.597970   1.083011   0.006092
```

```
C    3.199342   -0.448657   -0.041854
C    1.849581    0.098800   -0.019345
C    0.724777    0.523423   -0.000639
C   -1.801060    0.236823   -0.103929
C   -1.946169   -1.090623   -0.068063
C   -0.926054   -2.171592    0.117334
H   -1.715601    2.875863    0.078836
H    0.128914    3.066361    0.159274
H    3.713893   -0.253756    0.902448
H    3.787148   -0.001475   -0.847329
H    3.174981   -1.530196   -0.199053
H   -2.709874    0.819566   -0.232750
H   -2.965302   -1.452107   -0.191578
H   -1.287506   -2.898046    0.851305
H    0.038494   -1.793556    0.446559
H   -0.778582   -2.715974   -0.822012
```

Frequencies

44.3646	73.7145	79.7085
117.6012	151.3934	250.5158
306.8164	324.9928	352.5683
405.989	533.2493	614.8005
639.7361	714.838	720.5568
802.7828	902.4671	934.3368
979.6291	1021.307	1051.887
1058.739	1077.152	1081.02
1121.383	1294.048	1363.103
1409.819	1415.135	1430.891
1463.277	1482.113	1487.466
1491.8	1498.446	1668.769
1752.255	2381.062	3044.738
3051.01	3097.541	3123.785
3124.943	3147.54	3168.962
3176.203	3186.802	3266.027

p85 + H

```
C    0.616124    1.746498   -0.218939
C    0.161663    0.491224   -0.322893
C   -3.770123   -0.449591    0.330167
C   -2.373425   -0.107894    0.094413
C   -1.222076    0.186218   -0.091455
C    1.014429   -0.656093   -0.710494
C    2.227124   -0.944774   -0.236138
C    2.997263   -0.211522    0.819140
H    1.650694    1.981756   -0.437189
H   -0.043138    2.557819    0.064782
H   -4.429572    0.146440   -0.305666
H   -4.042114   -0.260975    1.371882
H   -3.953342   -1.505629    0.117992
H    0.566645   -1.336193   -1.430293
H    2.711832   -1.830525   -0.640492
H    2.364551    0.473002    1.386452
H    3.812640    0.371607    0.376956
H    3.455933   -0.921700    1.512774
```

Frequencies

40.9345	99.0548	134.1789
139.8908	175.768	263.8655
270.3995	331.462	366.2481
431.1129	535.5172	564.8916
616.3166	749.0003	784.4281
800.062	909.2014	956.0361
972.1489	1019.395	1059.748
1068.697	1072.702	1083.835

1120.792	1281.287	1299.085
1408.163	1424.362	1440.241
1451.075	1489.903	1491.045
1491.418	1502.94	1693.262
1743.397	2380.285	3042.008
3049.571	3099.537	3121.162
3125.451	3141.802	3158.77
3168.424	3180.821	3264.916

p86 + H

```
C     0.327317    2.459880    0.000091
C     0.118214    0.966311   -0.000033
C     3.153440   -1.481151   -0.000028
C     2.130807   -0.656532   -0.000019
C     1.150040    0.139376   -0.000012
C    -1.275598    0.496252   -0.000177
C    -1.669134   -0.778385    0.000145
C    -3.093152   -1.230120    0.000000
H     1.386682    2.713829    0.000210
H    -0.141932    2.907680    0.882252
H    -0.141755    2.907792   -0.882107
H     3.007027   -2.555952   -0.000183
H     4.172567   -1.109331    0.000105
H    -2.030616    1.280802   -0.000546
H    -0.907638   -1.556307    0.000554
H    -3.304806   -1.848752   -0.878443
H    -3.785905   -0.385571   -0.000539
H    -3.305222   -1.847971    0.878894
```

Frequencies

41.5727	75.9387	131.079
159.5209	173.6486	197.5654
222.9281	303.6169	376.6893
435.4777	466.2639	521.2823
599.5731	622.8023	737.2856
831.0735	855.466	933.689
1011.566	1020.056	1032.312
1055.054	1073.243	1102.474
1174.809	1242.149	1337.659
1362.963	1413.34	1416.193
1448.267	1484.289	1485.594
1489.761	1494.893	1713.607
1742.34	2225.024	3036.435
3042.033	3094.224	3103.757
3128.246	3150.037	3154.899
3157.999	3166.116	3235.274

p87 + H

```
C     0.724452    2.404327    0.256561
C     0.479343    0.944134   -0.038540
C    -3.163677   -0.443613   -0.108607
C    -1.939659    0.029980   -0.073517
C    -0.751305    0.458421   -0.042076
C     1.664876    0.134122   -0.344720
C     1.823093   -1.184756   -0.185760
C     0.827340   -2.157086    0.364035
H     1.217131    2.882339   -0.596681
H     1.389249    2.511320    1.119414
H    -0.207294    2.930510    0.461221
H    -3.354780   -1.480204   -0.366263
H    -4.017423    0.185758    0.119216
H     2.514301    0.702956   -0.716851
H     2.784468   -1.599340   -0.478876
H     0.191574   -2.557878   -0.433415
H     0.162231   -1.687018    1.091360
```

H   1.333769   -3.001614   0.836616

Frequencies

59.2578	78.7365	129.8182
149.1037	163.9917	263.0031
300.2524	313.8846	369.2284
495.1235	517.7791	545.4281
590.0499	653.6445	732.8365
752.0774	873.9628	935.3862
996.5717	1006.354	1032.632
1052.336	1063.87	1091.214
1164.192	1223.65	1294.179
1404.043	1410.5	1447.519
1451.262	1484.507	1486.12
1493.048	1505.303	1709.858
1728.732	2227.913	3042.436
3045.158	3104.952	3107.396
3138.352	3144.656	3155.32
3159.437	3180.331	3229.179

p88 + H

C	0.084623	2.263230	0.187337
C	0.085063	0.772230	-0.074373
C	-3.574131	-1.057599	0.057518
C	-2.267327	-0.414228	0.009806
C	-1.180815	0.099605	-0.034765
C	1.188639	0.108755	-0.329074
C	2.293052	-0.535361	-0.569660
C	3.162576	-1.168280	0.484175
H	-0.545117	2.774785	-0.545634
H	1.095712	2.667214	0.128922
H	-0.325686	2.471086	1.179244
H	-4.103182	-0.934854	-0.891155
H	-4.192645	-0.626684	0.848805
H	-3.470634	-2.127980	0.251655
H	2.617121	-0.633026	-1.604900
H	3.273727	-2.240467	0.297761
H	2.736350	-1.031843	1.478756
H	4.164278	-0.728343	0.470763

Frequencies

66.3666	93.6556	100.2556
142.5663	159.8071	182.5443
189.6929	257.4974	299.7643
352.6606	486.8338	487.8224
559.6722	613.2403	671.21
813.7854	876.5916	995.8838
1056.236	1058.538	1059.299
1062.666	1068.249	1107.122
1223.254	1288.098	1407.058
1413.366	1419.098	1447.869
1481.845	1486.891	1488.602
1491.345	1497.879	1518.627
2087.623	2381.522	3046.744
3051.708	3052.665	3111.211
3121.416	3122.67	3126.802
3136.305	3150.881	3153.829

SUPPORTING INFORMATION

p89 + H

C	1.952357	-0.693339	0.000072
C	1.952360	0.693334	-0.000055
C	0.743540	1.378304	-0.000126
C	-0.473624	0.702229	-0.000074
C	-1.770304	1.468066	0.000157
C	-1.770303	-1.468065	-0.000140
C	-0.473627	-0.702221	0.000035
C	0.743533	-1.378304	0.000106
H	2.887458	-1.242047	0.000136
H	2.887465	1.242036	-0.000089
H	0.743486	2.464057	-0.000206
H	-2.374792	1.227939	0.880783
H	-2.376432	1.226199	-0.878872
H	-1.591519	2.544553	-0.001201
H	-2.376218	-1.226444	0.879102
H	-1.591511	-2.544552	0.000859
H	-2.375007	-1.227708	-0.880553
H	0.743472	-2.464056	0.000185

Frequencies

73.9748	161.4469	175.5241
266.2542	326.9478	418.6681
446.6175	516.3771	526.1988
595.4907	735.4075	757.8958
760.0258	843.1808	880.8254
954.9303	1006.778	1019.243
1023.904	1050.379	1075.708
1085.499	1152.092	1192.156
1217.129	1260.204	1319.008
1331.72	1420.375	1430.508
1474.972	1482.184	1501.75
1502.198	1514.269	1541.2
1655.823	1686.359	3038.089
3038.573	3093.765	3097.064
3136.834	3138.288	3182.447
3187.226	3201.507	3217.117

p90 + H

C	-1.937986	0.597729	-0.000025
C	-1.855141	-0.895101	0.000041
C	-0.449751	-1.409298	0.000010
C	0.642961	-0.638529	-0.000003
C	2.020549	-1.238970	-0.000033
C	1.565266	1.662880	0.000045
C	0.511124	0.834674	0.000006
C	-0.855168	1.372377	-0.000045
H	-2.926896	1.045637	-0.000059
H	-2.393673	-1.296429	0.870225
H	-2.393750	-1.296519	-0.870051
H	-0.331515	-2.490005	-0.000007
H	2.587156	-0.922753	0.881439
H	2.587118	-0.922735	-0.881524
H	1.969160	-2.328906	-0.000048
H	1.422641	2.738024	0.000052
H	2.587383	1.305716	0.000085
H	-0.958753	2.453391	-0.000086

Frequencies

85.5407	212.6982	260.5215
311.6728	352.8072	402.9461
422.658	490.1881	569.9931
601.1285	717.6419	721.5123
793.6231	835.4378	837.2834
903.0597	918.0553	971.6949
973.226	1009.128	1015.819

1067.99	1089.617	1177.399
1203.528	1218.737	1311.924
1384.226	1400.324	1416.339
1449.167	1463.669	1472.264
1484.283	1509.23	1683.678
1721.005	1776.983	3015.051
3032.32	3040.972	3101.666
3139.425	3167.365	3169.429
3176.147	3200.38	3255.782

p91 + H

```
C   -2.048039   0.248789   -0.050343
C   -1.722583   -1.039426   -0.159209
C   -0.335882   -1.474118   -0.020938
C    0.692919   -0.610228    0.050249
C    2.115660   -1.086717    0.107919
C    1.378544    1.740526   -0.239592
C    0.420387    0.839771   -0.001244
C   -1.005491    1.279326    0.268602
H   -3.079062    0.575228   -0.136531
H   -2.482697   -1.789201   -0.349384
H   -0.135818   -2.541362   -0.013808
H    2.650066   -0.631445    0.947316
H    2.657247   -0.818559   -0.805185
H    2.158843   -2.171546    0.217363
H    1.147003    2.798308   -0.307973
H    2.416647    1.461137   -0.371814
H   -1.092799    1.512625    1.341328
H   -1.212513    2.217273   -0.253983
```

Frequencies

80.1349	180.5634	235.6187
317.4718	347.4911	427.7778
478.0148	496.9244	523.543
599.6542	699.9832	721.3854
765.5393	832.2531	892.0069
915.6713	941.3085	962.2621
988.4637	1004.511	1023.716
1071.869	1089.562	1170.7
1198.035	1228.861	1306.582
1349.062	1402.979	1421.45
1441.151	1454.894	1465.165
1488.522	1505.111	1680.512
1703.544	1746.757	2996.976
3041.409	3090.63	3101.799
3137.318	3165.586	3178.989
3189.55	3208.759	3253.867

p92 + H

```
C   -1.510052   -1.115264    0.345482
C   -1.925832    0.165263   -0.221271
C   -1.020368    1.071184   -0.596324
C    0.455567    0.863230   -0.376907
C    0.896511    1.699672    0.843438
C    2.055106   -1.050102   -0.413098
C    0.823438   -0.595634   -0.163038
C   -0.217774   -1.472609    0.371367
H   -2.271440   -1.793365    0.715129
H   -2.985756    0.362407   -0.338577
H   -1.330701    2.025842   -1.010273
H    1.001918    1.235841   -1.249574
H    1.974095    1.601096    0.997146
H    0.385055    1.350984    1.744307
H    0.656435    2.756610    0.698277
```

```
H    2.331298  -2.076509  -0.196122
H    2.818760  -0.410801  -0.844361
H    0.080764  -2.446540   0.746153
```

Frequencies

77.9368	193.0692	258.9895
279.0033	375.4522	398.5227
481.5418	532.9296	592.7384
686.2387	699.9271	749.4104
777.8238	837.349	876.9512
923.7747	946.4181	962.7763
1006.786	1008.701	1018.512
1034.652	1089.704	1120.152
1190.21	1210.997	1310.134
1322.817	1349.347	1396.154
1416.178	1439.742	1472.576
1496.378	1504.189	1660.406
1701.033	1744.64	3045.465
3062.886	3127.537	3133.913
3150.533	3179.349	3185.278
3201.641	3212.879	3238.801

p93 + H

```
C    1.604746  -1.029465  -0.236247
C    1.915734   0.436687  -0.126331
C    0.794952   1.193458   0.597581
C   -0.551946   0.802096   0.044494
C   -1.405544   1.684226  -0.470313
C   -2.030386  -1.183758   0.244556
C   -0.813708  -0.660949   0.059985
C    0.366672  -1.516329  -0.131466
H    2.433213  -1.710097  -0.408539
H    2.864883   0.577570   0.399734
H    2.057080   0.854478  -1.131585
H    0.942865   2.272686   0.517493
H    0.830962   0.930598   1.661689
H   -2.342738   1.373911  -0.918762
H   -1.182452   2.746176  -0.468115
H   -2.185717  -2.257292   0.225349
H   -2.895110  -0.557587   0.430881
H    0.193889  -2.586241  -0.201699
```

Frequencies

102.0691	180.7724	288.4418
338.6294	374.0542	430.5281
476.1036	556.863	631.746
688.9755	732.6397	768.4871
770.5723	816.659	879.6195
898.7484	927.3136	944.2461
973.3199	986.7463	1008.187
1049.712	1058.238	1188.155
1197.426	1235.617	1279.405
1342.51	1352.769	1372.404
1421.437	1448.577	1466.879
1486.413	1496.577	1687.995
1729.498	1747.437	3030.365
3041.543	3086.91	3112.014
3154.762	3160.772	3174.049

3196.863	3243.714	3251.629

p94 + H

C	1.826254	0.628569	0.213239
C	1.826154	-0.628782	-0.213353
C	0.573581	-1.420388	-0.475575
C	-0.667477	-0.739697	0.054934
C	-1.680946	-1.411951	0.595055
C	-1.680592	1.412236	-0.595178
C	-0.667334	0.739790	-0.054899
C	0.573779	1.420227	0.475783
H	2.770874	1.133841	0.392499
H	2.770708	-1.134086	-0.392879
H	0.666228	-2.420784	-0.041668
H	0.466298	-1.565518	-1.559597
H	-1.662962	-2.494614	0.671724
H	-2.551333	-0.896886	0.985856
H	-1.662361	2.494894	-0.671848
H	-2.551008	0.897340	-0.986137
H	0.666482	2.420743	0.042164
H	0.466550	1.565040	1.559852

Frequencies

105.098	111.3272	265.0585
319.9615	393.4076	429.0506
470.2685	557.8958	614.8211
667.4989	725.3501	725.9052
788.575	843.993	921.6108
936.8191	938.8146	945.8685
982.6226	987.4221	993.1301
1030.14	1037.452	1195.317
1209.943	1230.678	1248.259
1338.072	1350.531	1359.909
1426.669	1443.821	1458.551
1478.416	1480.461	1727.671
1734.595	1760.703	3018.391
3019.012	3078.817	3078.843
3153.171	3153.935	3167.193
3191.298	3244.544	3245.166

Fragments

CH₃

C	-0.000134	-0.000001	0.000023
H	-1.080503	0.038158	-0.000046
H	0.507588	-0.954443	-0.000046
H	0.573721	0.916289	-0.000046

Frequencies

470.9451	1399.8856	1409.5749
3117.6199	3301.0861	3304.8947

C₂H₃

C	0.705692	-0.145170	0.000001
C	-0.586151	0.030184	0.000004
H	1.596113	0.468363	-0.000011
H	-1.031552	1.027946	-0.000006
H	-1.281806	-0.806397	-0.000015

Frequencies

714.0578	840.5185	933.8993
1052.7836	1393.8374	1668.5191
3080.5313	3173.8401	3244.2107

C₃H₅_a

C	1.360710	-0.154448	-0.000002
C	0.212046	0.468550	0.000003
C	-1.144382	-0.198036	-0.000001
H	1.712354	-1.177916	0.000006
H	0.205954	1.559708	0.000001
H	-1.716533	0.103752	0.882327
H	-1.055489	-1.285695	0.000001

H   -1.716526   0.103757   -0.882332

Frequencies

168.9855	385.3664	647.3666
840.5820	851.0793	933.7929
1054.3478	1100.1094	1271.3097
1401.6285	1481.6880	1487.2425
1697.5024	3041.1762	3107.3980
3119.5989	3142.8723	3240.2883

$C_3H_5\_b$

C	-1.309507	-0.319898	-0.000002
C	-0.212496	0.389802	0.000004
C	1.190894	-0.152769	-0.000003
H	-2.374484	-0.136085	0.000000
H	-0.304052	1.482050	-0.000004
H	1.192372	-1.243371	-0.000111
H	1.736365	0.197200	0.881404
H	1.736452	0.197396	-0.881279

Frequencies

179.5659	408.1387	600.9251
805.6738	822.0556	937.9675
1062.3207	1115.0819	1277.4664
1403.5440	1483.2804	1487.1065
1707.6747	3046.7708	3056.3888
3110.6582	3150.5075	3256.8466