

Supplementary Information for

**Gas-Phase Synthesis of Naphthalene Through an Unconventional Thermal
Alkyne–Alkene [2+2] Cycloaddition Mechanism**

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Table of Contents

1. Experimental Methods
2. Computational Methods
3. Comparison of H vs D Loss
4. Precursor Synthesis and Characterization
5. Figs. S1–S14
6. Tables S1–S11
7. Molecular Cartesian Coordinates
8. Supplementary References

Experimental Methods

The reactions of the phenylethynyl radical ($\text{C}_6\text{H}_5\text{CC}\cdot$, X^2A_1) with ethylene- d_4 (C_2D_4 , 99.7 % D atom, CDN Isotopes) and propylene (C_3H_6 , ≥ 99 % purity, Sigma-Aldrich) were conducted under single-collision conditions using a crossed molecular beams machine.¹ A (2-iodoethynyl)benzene ($\text{C}_6\text{H}_5\text{CCI}$) precursor was purified by multiple freeze–pump–thaw cycles in a stainless steel bubbler and seeded at a fraction of 0.5 % in neon (Ne, 99.9999 %, Matheson) at a backing pressure of 500 Torr before exiting a Proch-Trickl² pulsed valve with a 120 Hz repetition rate, -450 V amplitude, and open time of $80\ \mu\text{s}$. The precursor gas mixture was interrogated by an excimer laser (Coherent, COMPex 110) operating at 193 nm, 60 Hz, and 20 mJ per pulse, thus generating phenylethynyl radicals *in situ* via photodissociation of (2-iodoethynyl)benzene.³ The molecular beam was then skimmed, and a chopper wheel selected a portion of the beam with a velocity (v_p) of $863 \pm 12\ \text{m s}^{-1}$ and speed ratio (S) of 19.7 ± 2.4 . The phenylethynyl beam crossed perpendicularly with pulsed ethylene- d_4 ($v_p = 880 \pm 15\ \text{m s}^{-1}$, $S = 15.7 \pm 0.2$) and propylene ($v_p = 840 \pm 10\ \text{m s}^{-1}$, $S = 11.0 \pm 0.2$) beams with backing pressures of 550 Torr and pulsed valve parameters of -350 V and 120 Hz. This resulted in collision energies (E_c) of 18.5 ± 0.5 and $21.5 \pm 0.6\ \text{kJ mol}^{-1}$, as well as center-of-mass (CM) angles (θ_{CM}) of 18.7 ± 0.5 and $22.8 \pm 0.5^\circ$ for the phenylethynyl/ethylene- d_4 and phenylethynyl/propylene systems, respectively.

Products formed through reactive scattering were received by a triply differentially pumped mass spectrometric detector, which is rotatable in the plane of the reactant beams. Collected products were ionized by electron impact ionization at 80 eV and filtered by a quadrupole mass spectrometer (150QC, Extrel) operating in the time-of-flight (TOF) mode. Up to 2.9×10^7 TOFs were taken at each angle in either 5° or 2.5° steps in the $8.5^\circ \leq \theta \leq 30.5^\circ$ angular range with 0° defined by the phenylethynyl beam. A laboratory angular distribution (LAD) was derived by integrating the TOFs at different angles and normalizing to θ_{CM} . To obtain additional chemical dynamics information on the system, the laboratory data were fit using a forward convolution routine, in which user-defined CM translational energy ($P(E_{\text{T}})$) and angular ($T(\theta)$) flux distributions were refined iteratively until a reasonable fit of the data was achieved.^{4,5} The functions developed a flux contour map as an image of the outcome of the reaction, given as $I(u, \theta) \approx P(u) \times T(\theta)$.⁶

Computational Methods

Geometries of the reactants, intermediates, transition states, and products partaking in the reactions of the phenylethynyl radical with ethylene and propylene were optimized at the hybrid density functional ω B97X-D level of theory⁷ with the 6-311G(d,p) basis set. Vibrational frequencies and zero-point vibrational energies (ZPE) were calculated using the same ω B97X-D/6-311G(d,p) method. Single-point energies at the optimized geometries of all structures were then improved within the G3(MP2,CC)//DFT modification^{8,9} of the original G3 scheme,¹⁰ where the final energies at 0 K were evaluated according to the following formula:

$$E_0[\text{G3(MP2,CC)}] = E[\text{CCSD(T)/6-311G(d,p)}] + \Delta E_{\text{MP2}} + E(\text{ZPE})$$

with $\Delta E_{\text{MP2}} = E[\text{MP2/G3large}] - E[\text{MP2/6-311G(d,p)}]$ being the basis set correction and $E(\text{ZPE})$ the zero-point energy obtained at the ω B97X-D/6-311G(d,p) level. Restricted open-shell calculations for the radical species were carried out both at the MP2 (ROMP2) and CCSD(T) (ROCCSD(T)) levels using the initial ROHF wavefunctions, in order to minimize spin contamination. For the most important reaction pathways of the $\text{C}_6\text{H}_5\text{CC} + \text{C}_2\text{H}_4$ reaction (Fig. S7), additional refinement of the single-point energies was carried out using the explicitly correlated CCSD(T)-F12 method with the cc-pVTZ-f12 basis set.^{11,12} The results showed a very close agreement between the G3(MP2,CC) and CCSD(T)-F12/cc-pVTZ-f12 relative energies with the average unsigned and maximal deviations being only 1.7 and 6.0 kJ mol⁻¹. For comparison, for critical transition states we have also recomputed their single-point energies within the G3(MP2,CC) scheme with unrestricted UMP2 and UCCSD(T) and also at the multireference CASPT2(13,12)/cc-pVTZ level with active space including the entire π -system and the unpaired electron. The differences between the restricted and unrestricted G3(MP2,CC) energies appeared to be within 1–2 kJ mol⁻¹, whereas the CASPT2(13,12)/cc-pVTZ values are 1–13 kJ mol⁻¹ lower than the G3(MP2,CC) and CCSD(T)-F12 values (see Fig. S7). However, these minor differences practically did not affect the computed product branching ratios. The electronic structure calculations were carried out employing the Gaussian 09¹³ and MOLPRO 2015¹⁴ quantum chemistry packages.

The energetic and molecular parameters from the electronic structure calculations were utilized to evaluate energy-dependent rate constants for all unimolecular reaction steps occurring on the $\text{C}_{10}\text{H}_{11}$ and $\text{C}_{11}\text{H}_{13}$ PESs following the initial $\text{C}_6\text{H}_5\text{CC} + \text{C}_2\text{H}_4/\text{C}_3\text{H}_6$ addition steps using the

Rice–Ramsperger–Kassel–Marcus (RRKM) theory.¹⁵ Here, the internal energy for each C₁₀H₉ or C₁₁H₁₁ intermediate or transition state was taken as a sum of the collision and chemical activation energies, with the chemical activation energy being a negative of the relative energy of the species with respect to the initial reactants. The rate constants were computed at the zero-pressure limit in order to reproduce the crossed molecular beams conditions. The RRKM-computed rate constants were used in calculations of reaction product branching ratios within the steady-state approximation.¹⁶ In order to assess the sensitivity of the predicted branching ratios of different products including naphthalene and methylnaphthalenes, the heights of critical barriers were varied within $\pm 4\text{--}5\text{ kJ mol}^{-1}$, which is the anticipated error margins of the electronic structure methods employed in this study. The branching ratios were then recomputed using different variations as shown in Tables S5, S10, and S11.

Atomic Deuterium Loss for the $\text{C}_6\text{H}_5\text{CC}-\text{C}_2\text{D}_4$ System

In the bimolecular reaction of the phenylethynyl radical ($\text{C}_6\text{H}_5\text{CC}\bullet$, 101 amu) with ethylene- d_4 (C_2D_4 , 32 amu), reactive scattering signal was observed at mass-to-charge ratios (m/z) of 132 ($\text{C}_{10}\text{H}_4\text{D}_4^+$, $^{13}\text{C}_{10}\text{H}_5\text{D}_3^+$) and 131 ($\text{C}_{10}\text{H}_5\text{D}_3^+$, $\text{C}_{10}\text{H}_3\text{D}_4^+$, $^{13}\text{C}_{10}\text{H}_4\text{D}_3^+$). In addition to the data at $m/z = 132$ shown in the manuscript, time-of-flight (TOF) spectra and a laboratory angular distribution (LAD) were obtained at $m/z = 131$ (Fig. S1). Products at $m/z = 131$ can originate from atomic deuterium loss, molecular hydrogen loss, or from fragmentation in the electron impact ionizer of products formed through atomic hydrogen loss. First, the laboratory data could not be fit using H_2 loss as this produces a much broader LAD with faster TOFs. Second, a reasonable fit of the data was achieved with a reaction channel corresponding to H loss, shown as the blue curves in Fig. S1. Third, the D loss channel could also replicate the data (red curves) and the fit is nearly identical to the H loss fit. The best-fit center-of-mass (CM) functions, i.e. the product translational energy ($P(E_{\text{T}})$) and angular ($T(\theta)$) flux distributions, are compiled in Fig. S2. For both the H loss and D loss cases, the $T(\theta)$ is isotropic and thus provides no differing points for comparison. The $P(E_{\text{T}})$ s are slightly different in the lower energy regime but end with E_{max} values that are nearly identical, with well-overlapping error bars. Altogether this shows that reactive scattering signal at $m/z = 131$ could be attributed to both H loss and/or D loss. Therefore, since the data shown in the manuscript at $m/z = 132$ reveal the formation of H loss products, at least the atomic hydrogen loss channel is open, while it cannot be concluded whether atomic deuterium loss is present.

Precursor Synthesis and Characterization

The synthesis of the (2-iodoethynyl)benzene precursor was performed analogously to a reported procedure^[39] with an increase in the concentration of the starting materials due to the large scale of precursor needed. Regarding the purification, badges performed with less than 10 g of phenylacetylene could be purified by either column chromatography or distillation whereas larger badges (20–50 g) decomposed before affording the desired product and, thus, had to be purified by column chromatography. A solution of phenylacetylene (26.0 mL, 24.2 g, 0.16 mol) in MeOH (300 mL) was cooled to 0 °C and KOH (32.5 g, 0.41 mol) was added. After 20 min of stirring at 0 °C, N-iodosuccinimide (63.1 g, 0.27 mol) was added to the mixture in portions and stirred at 0 °C for 15 min. The cold bath was replaced by a rt water bath and the mixture was stirred for 30 min. Then, Et₂O (1 L) was added and the mixture was extracted with brine (5 x 150 mL), dried over MgSO₄, filtered and evaporated to afford a brown oil/liquid. This liquid was purified by column chromatography (SiO₂; hexane) to afford the product as a light-yellow oil (32.5 g, 60%). ¹H NMR (200 MHz, CDCl₃): δ = 7.44 (dd, 2H), 7.34 (m, 3H) ppm. ¹³C NMR (50 MHz, CDCl₃): δ = 132.43, 128.92, 128.36, 123.46, 94.26 and 6.48 ppm. GC-MS: m/z 228.1 [M⁺] 101.1 [M⁺–I]. The characteristic C≡C stretching vibration was found at 2172 cm^{–1} whereas for the starting material it is observed at 2110 cm^{–1}. The provided characterization is in accordance with the literature^[39]. ¹H and ¹³C NMR data were recorded with a Bruker DPX-200 NMR spectrometer referenced towards CDCl₃ (7.26 ppm for ¹H NMR and 77.16 ppm for ¹³C NMR). The GC-MS data were recorded with an Agilent 7820A GC spectrometer. IR data were recorded with a Bruker Equinox 55 FT-IR spectrometer.

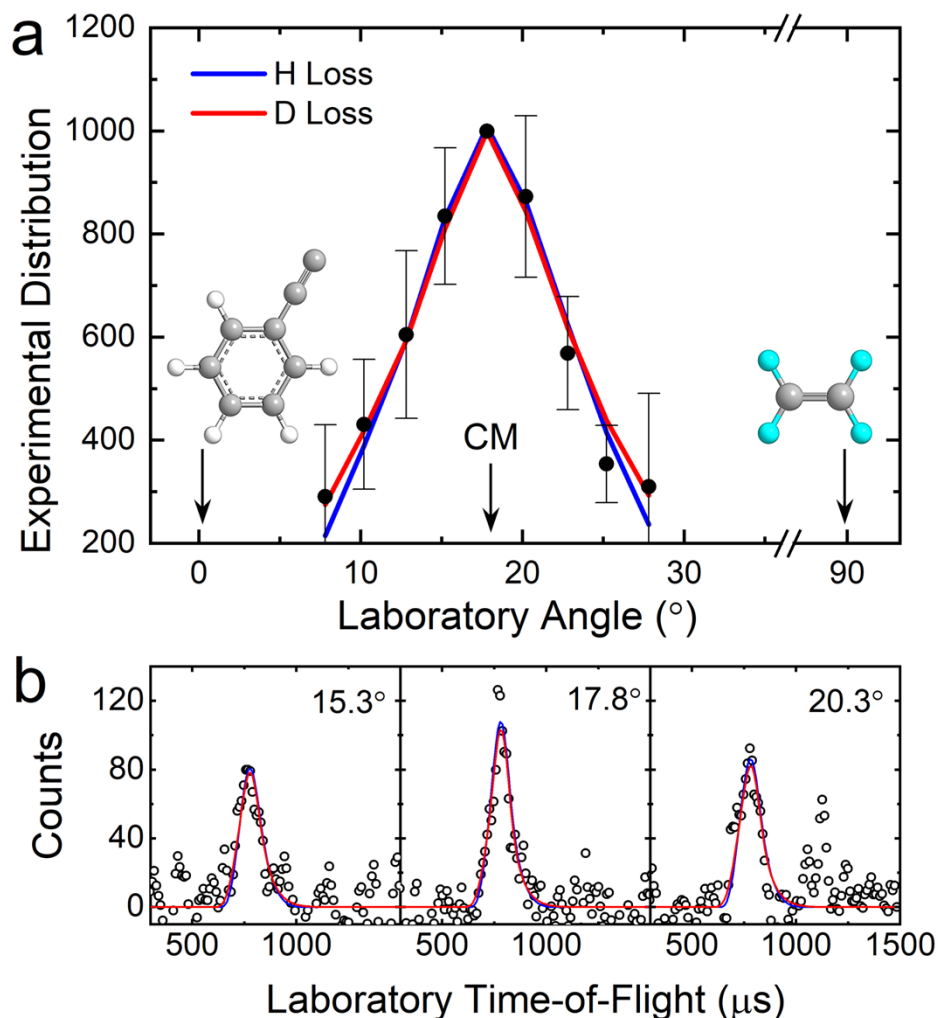


Fig. S1 Laboratory angular distribution (a) and time-of-flight (TOF) spectra (b) recorded at mass-to-charge (m/z) = 131 for the reaction of phenylethynyl (C_6H_5CC) with ethylene- d_4 (C_2D_4). The black circles depict the data, which are fit with fragmentation from the H loss products (blue) and with the D loss channel (red). CM represents the center-of-mass angle, and 0° and 90° define the directions of the phenylethynyl and ethylene- d_4 beams, respectively. Carbon atoms are colored gray, hydrogens are white, and deuteriums are light blue.

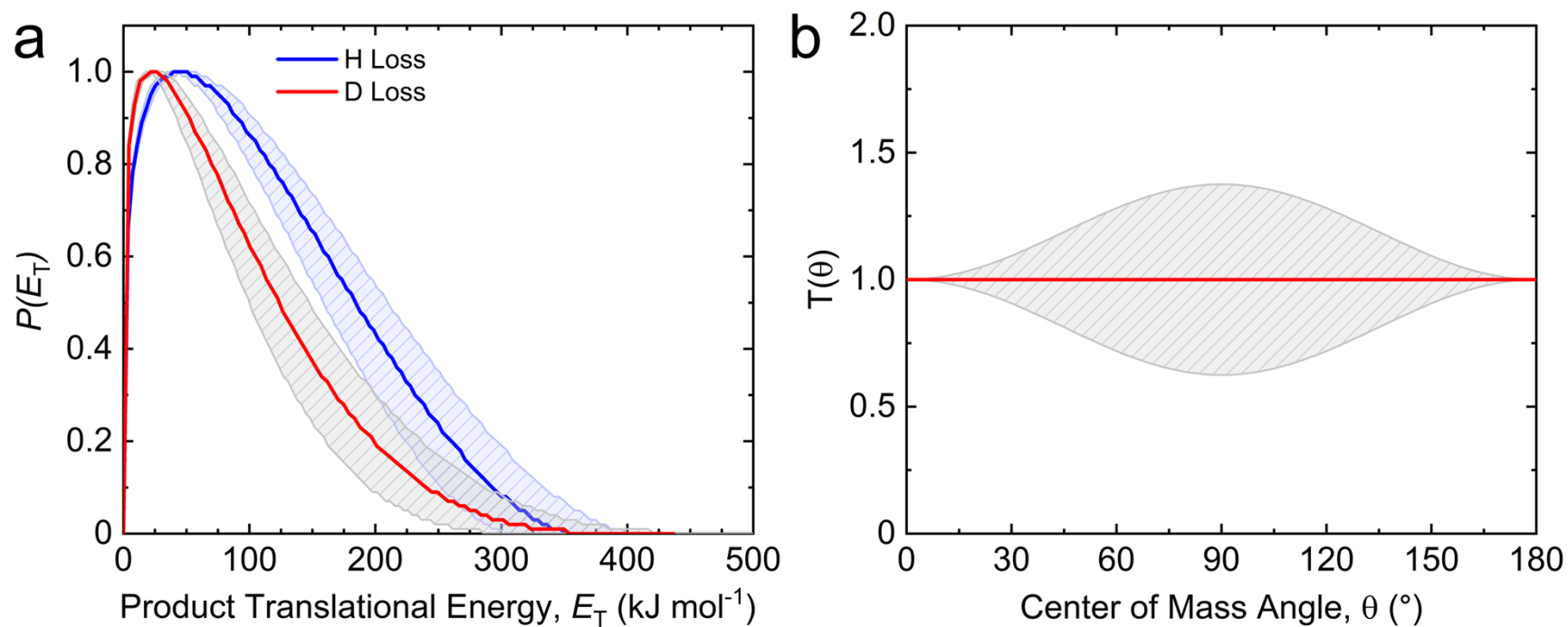


Fig. S2 CM product translational energy (a) and angular (b) flux distributions leading to the formation of $C_{10}H_4D_4$ isomers in the reaction of phenylethynyl (C_6H_5CC) with ethylene- d_4 (C_2D_4). Blue and red lines define the H loss and D loss best-fit functions, respectively, while shaded areas provide the error limits.

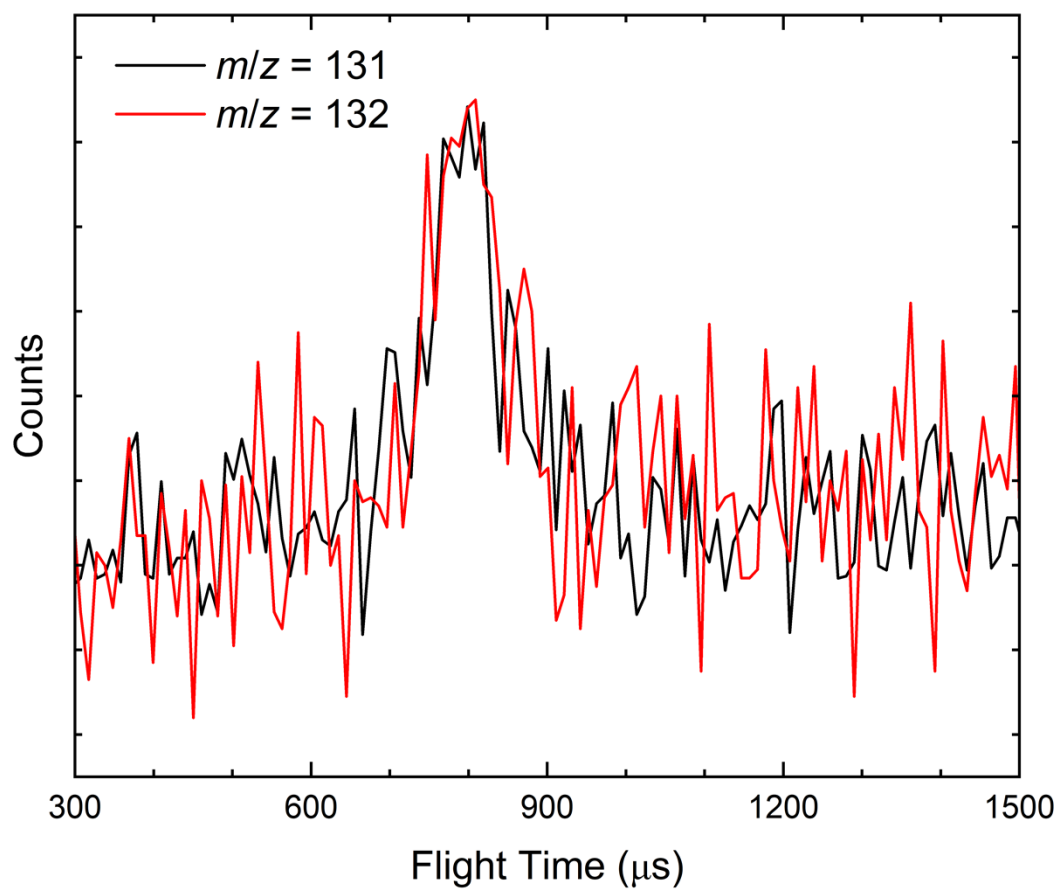


Fig. S3 Normalized time-of-flight (TOF) mass spectra for the reaction of phenylethynyl radicals ($\text{C}_6\text{H}_5\text{CC}$) with ethylene- d_4 (C_2D_4) at $m/z = 131$ and 132.

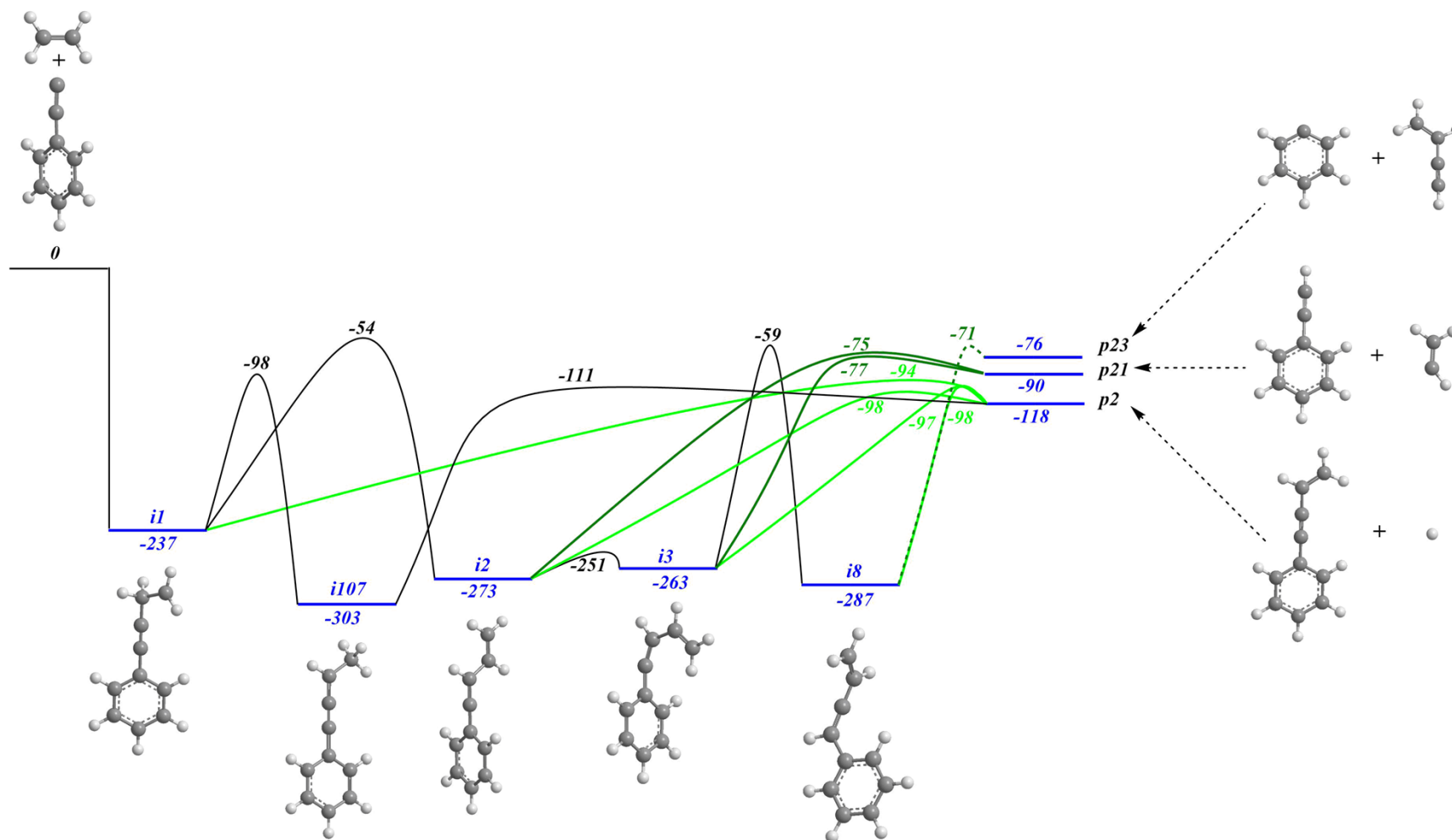


Fig. S4 Potential energy surface for the reaction of the phenylethynyl radical with ethylene leading to products **p2**, **p21** and **p23**. The level of electronic structure calculations used to generate PES in Figs. S4–S12 is G3(MP2,CC)// ω B97X-D/6-311G(d,p) unless mentioned otherwise.

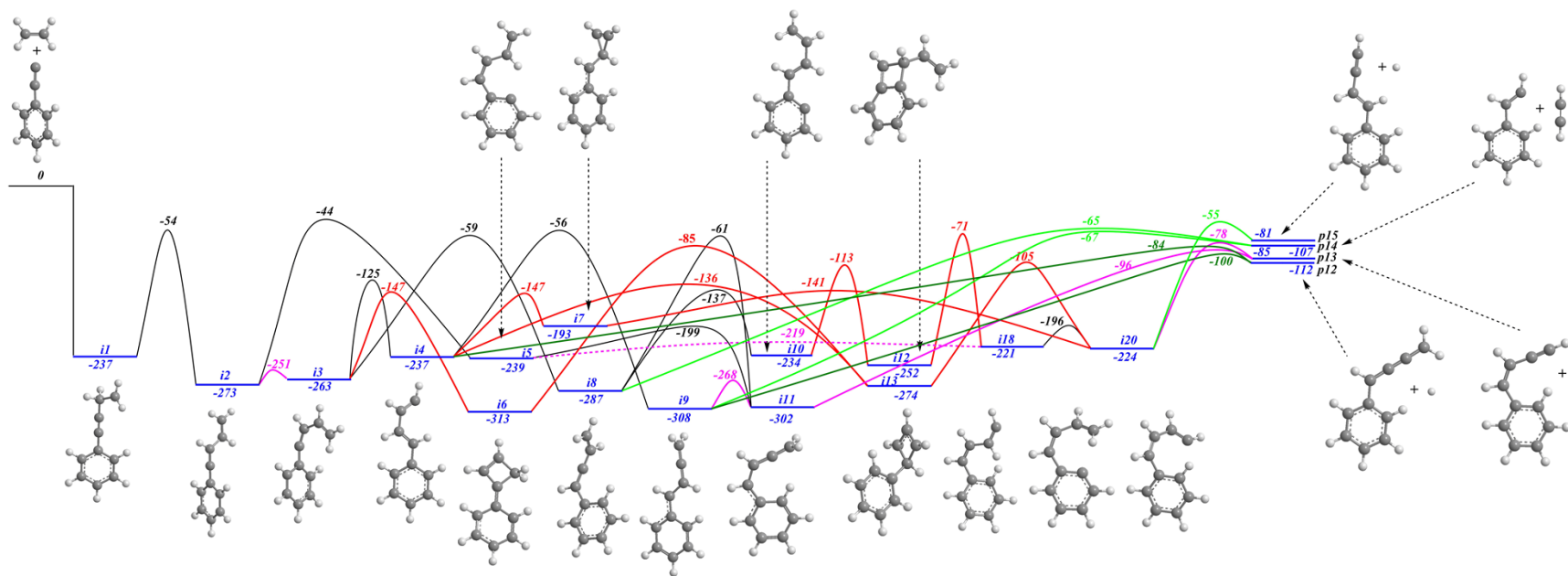


Fig. S5 Potential energy surface for the reaction of the phenylethynyl radical with ethylene leading to products **p12–p15**.

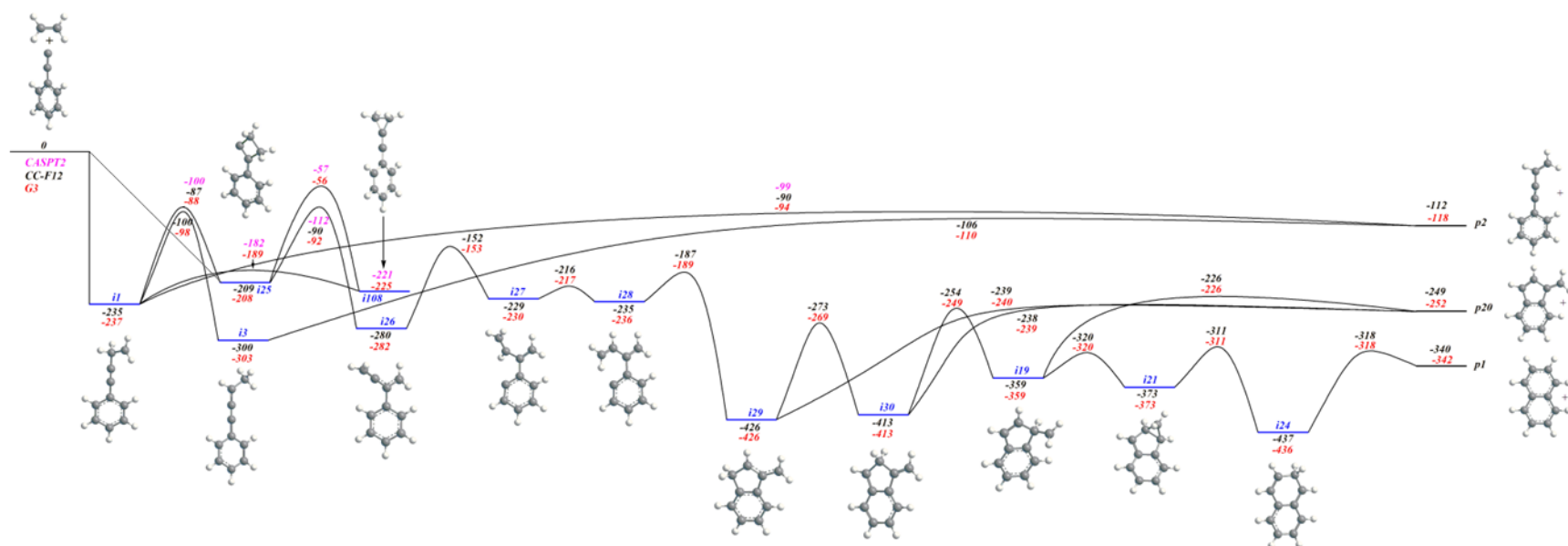


Fig. S7 Potential energy surface for the reaction of the phenylethynyl radical with ethylene leading to products **p1**, **p2**, and **p20**. Relative energies shown in black, red, and magenta were computed at the CCSD(T)-F12/cc-pVTZ-f12// ω B97X-D/6-311G(d,p), G3(MP2,CC)// ω B97X-D/6-311G(d,p), and CASPT2(13,12)/cc-pVTZ levels of theory, respectively.

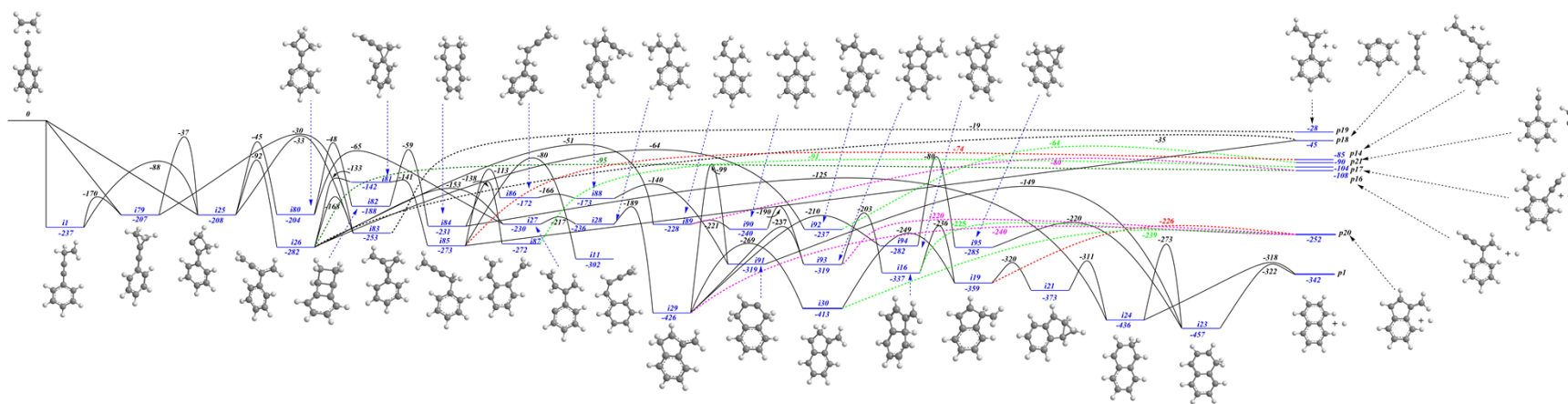


Fig. S8 Potential energy surface for the reaction of the phenylethynyl radical with ethylene leading to products **p1**, **p14**, and **p16–p21**.

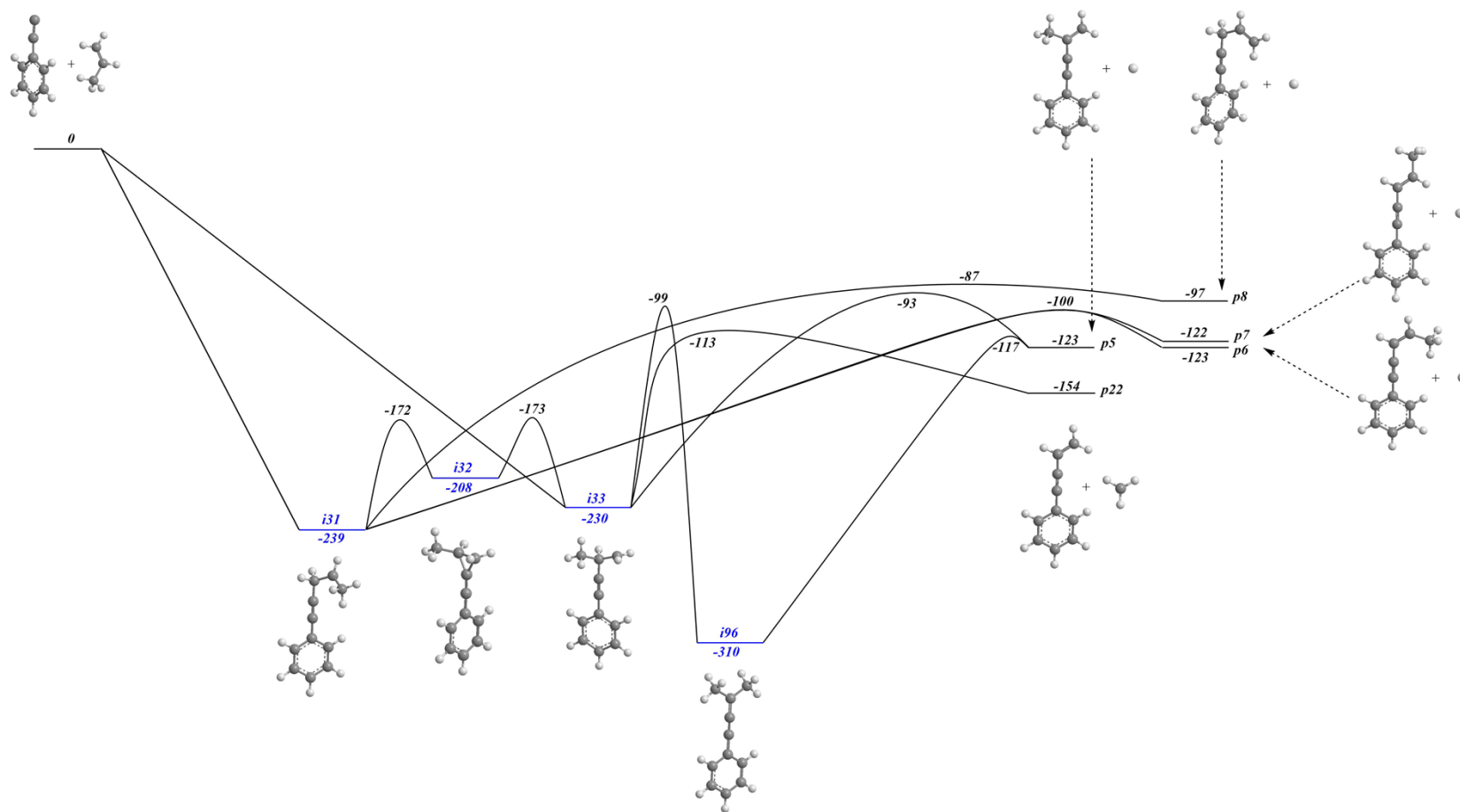


Fig. S9 Potential energy surface for the reaction of the phenylethynyl radical with propylene leading to products **p5–p8** and **p22**.

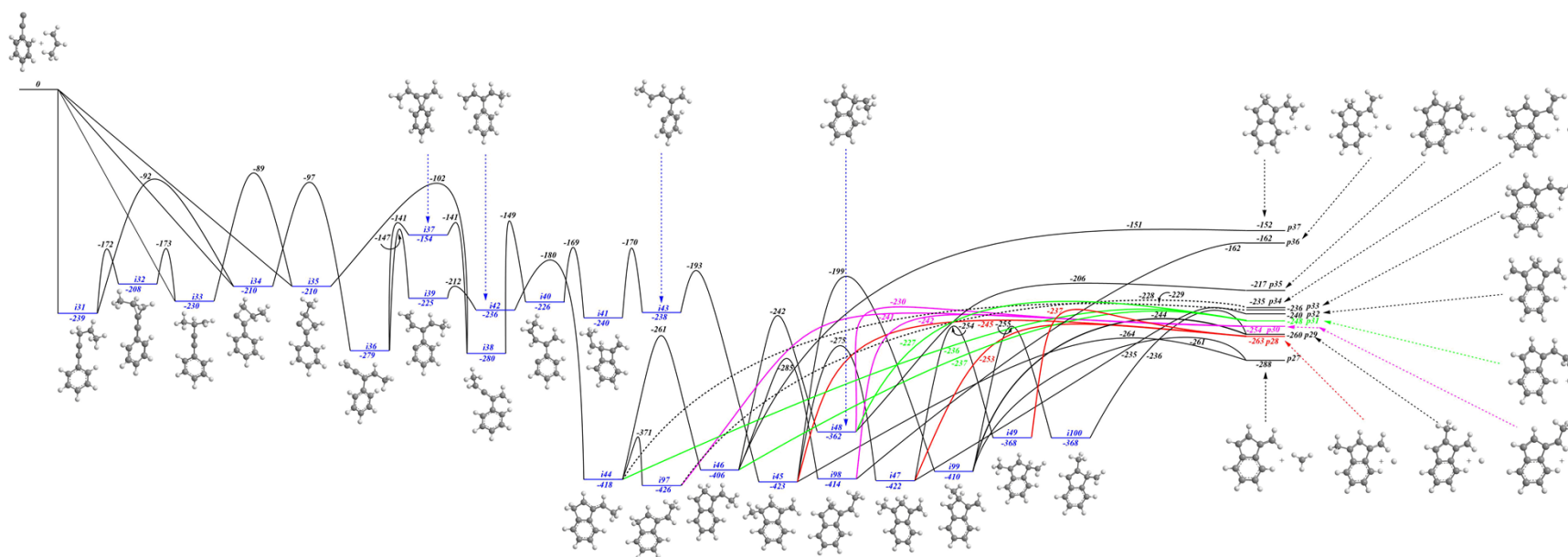


Fig. S10 Potential energy surface for the reaction of the phenylethynyl radical with propylene leading to products **p27–p37**.

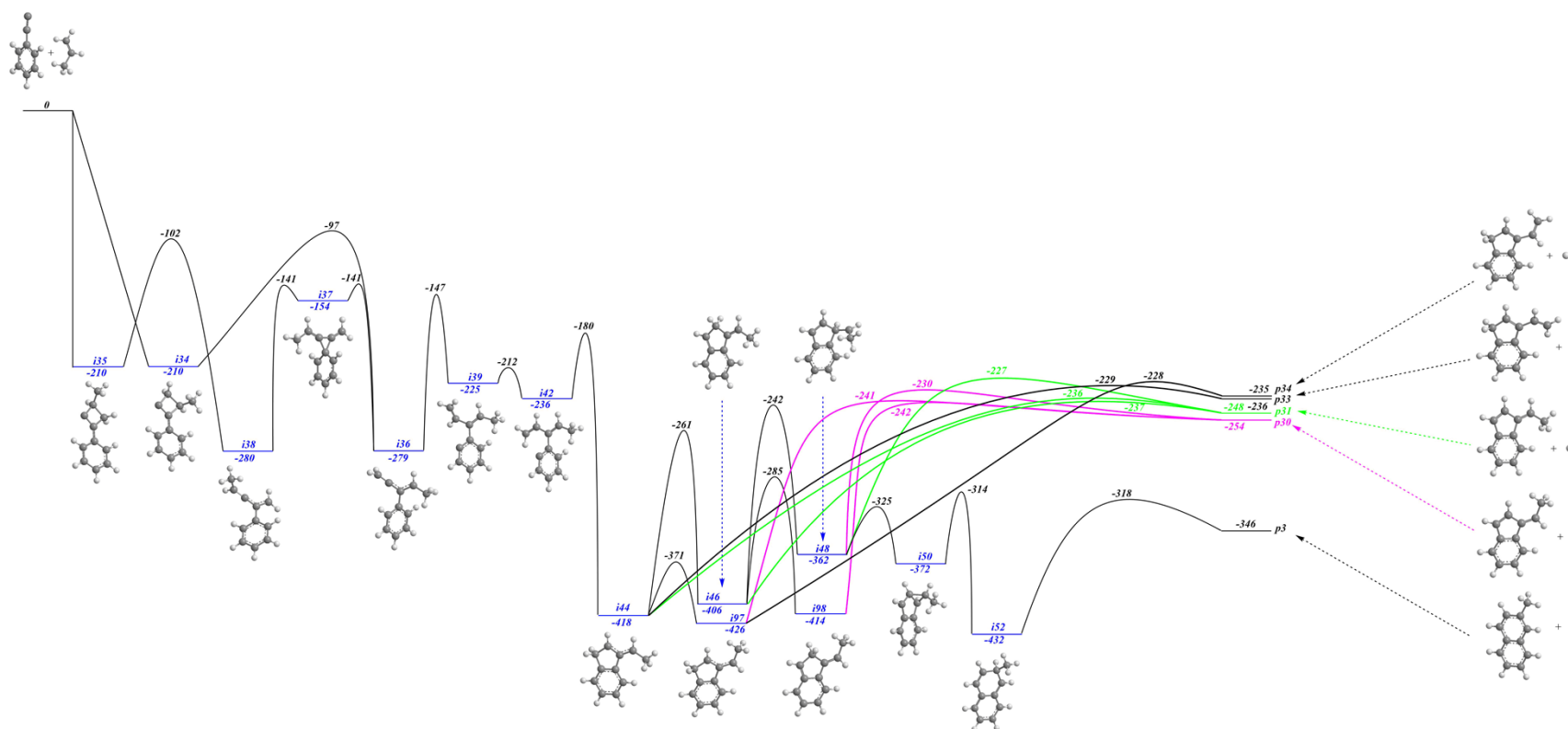


Fig. S11 Potential energy surface for the reaction of the phenylethynyl radical with propylene leading to products **p3**, **p30**, **p31**, **p33**, and **p34**.

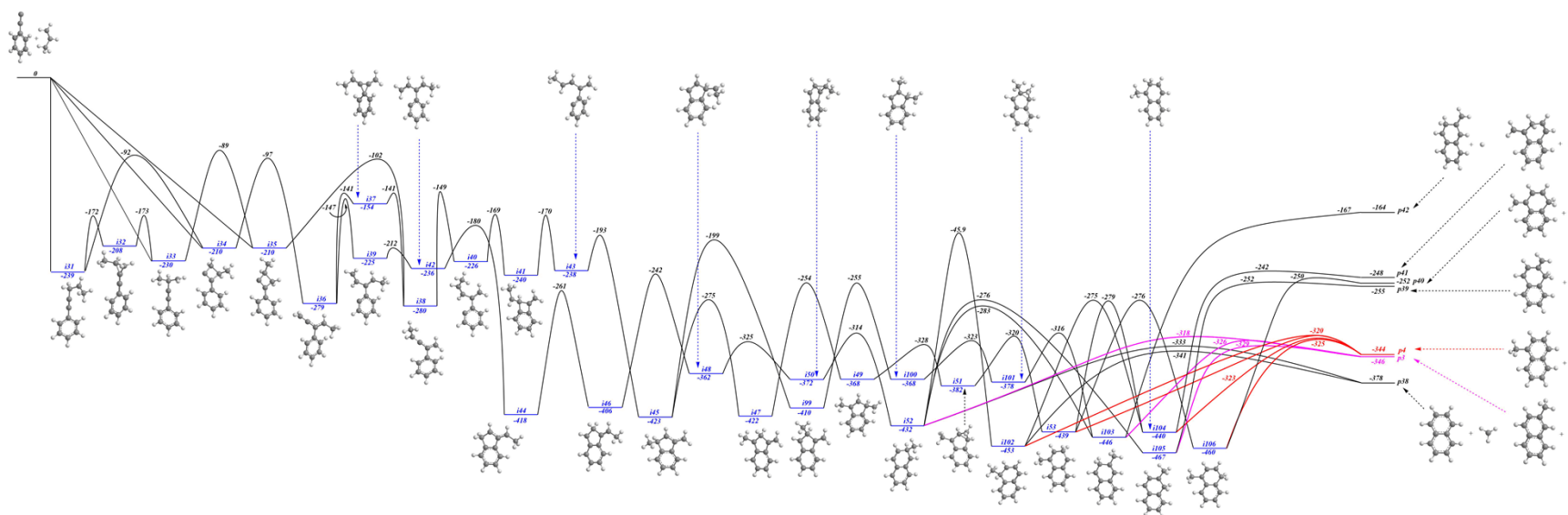


Fig. S12 Potential energy surface for the reaction of the phenylethynyl radical with propylene leading to products **p3**, **p4**, and **p39–p42**.

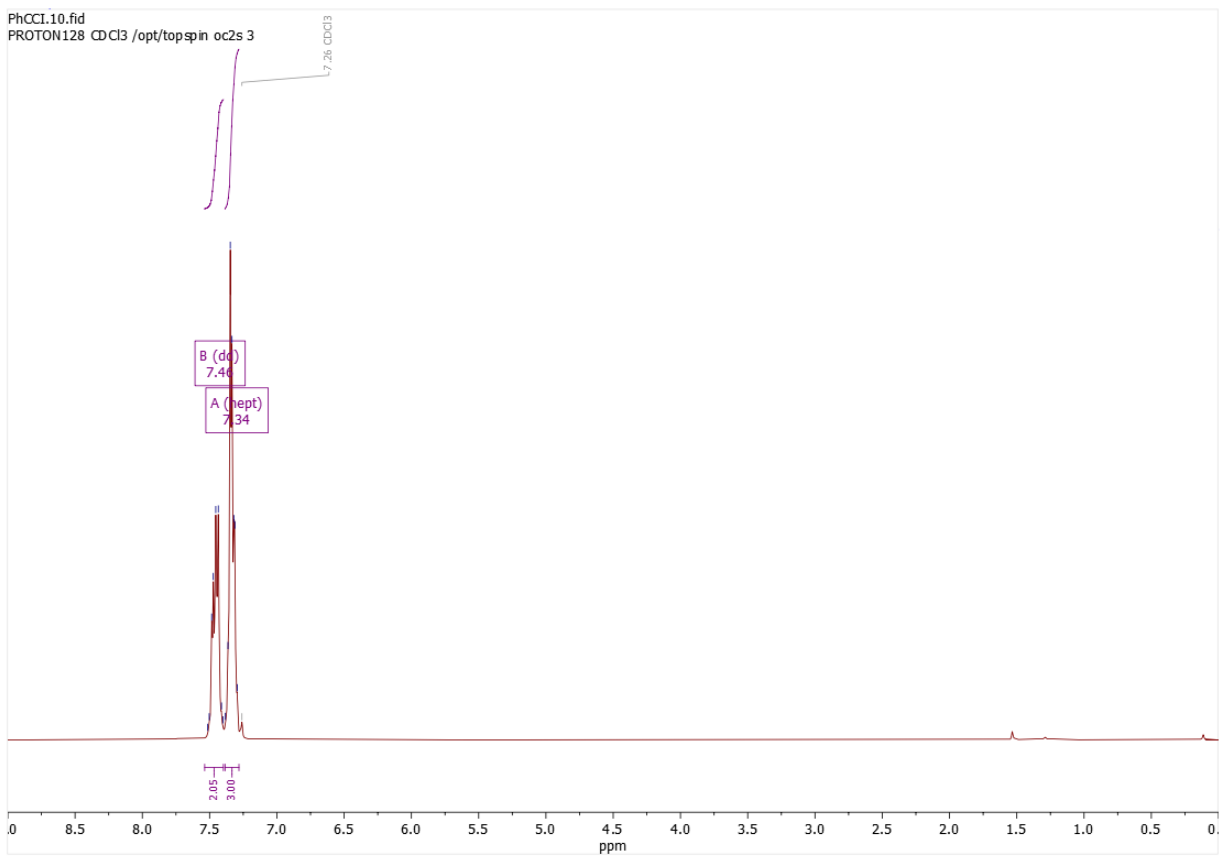


Fig. S13 ^1H NMR spectrum of (2-iodoethynyl)benzene.

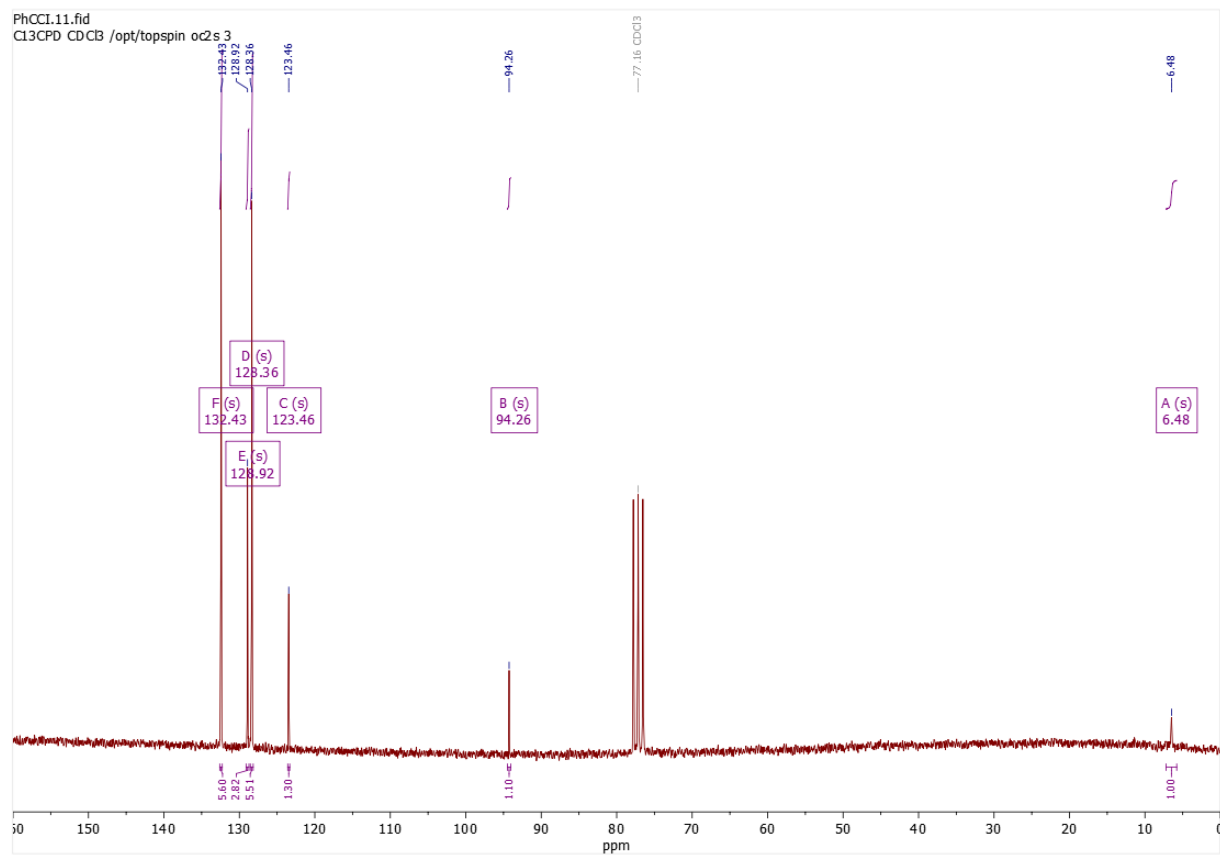


Fig. S14 ^{13}C NMR spectrum of (2-iodoethynyl)benzene.

Table S1 RRKM calculated rate constants ($k(E)$, s^{-1}) of the reaction of the phenylethynyl radical with ethylene for unimolecular reaction steps at different collision energies (E_C , $kJ \cdot mol^{-1}$).

E_C	0	5	10	15	20	25	30	35	40
Reaction step	$k(E)$								
<i>i20 – i22</i>	7.57E+10	7.74E+10	7.91E+10	8.07E+10	8.24E+10	8.40E+10	8.57E+10	8.73E+10	8.88E+10
<i>i22 – i20</i>	5.73E+07	6.69E+07	7.78E+07	9.01E+07	1.04E+08	1.20E+08	1.37E+08	1.57E+08	1.78E+08
<i>i22 – p1</i>	1.19E+11	1.25E+11	1.32E+11	1.39E+11	1.46E+11	1.54E+11	1.61E+11	1.69E+11	1.77E+11
<i>i23 – p1</i>	2.89E+09	3.16E+09	3.45E+09	3.76E+09	4.09E+09	4.45E+09	4.83E+09	5.24E+09	5.67E+09
<i>i18 – i23</i>	6.74E+11	6.80E+11	6.86E+11	6.92E+11	6.97E+11	7.03E+11	7.08E+11	7.14E+11	7.19E+11
<i>i23 – i18</i>	1.53E+05	1.86E+05	2.26E+05	2.73E+05	3.29E+05	3.94E+05	4.71E+05	5.60E+05	6.64E+05
<i>i1 – p2</i>	1.55E+05	2.24E+05	3.20E+05	4.48E+05	6.19E+05	8.45E+05	1.14E+06	1.51E+06	1.99E+06
<i>i20 – i66</i>	1.20E+11	1.24E+11	1.29E+11	1.34E+11	1.39E+11	1.44E+11	1.49E+11	1.54E+11	1.59E+11
<i>i66 – i20</i>	1.32E+09	1.50E+09	1.70E+09	1.92E+09	2.17E+09	2.43E+09	2.73E+09	3.04E+09	3.39E+09
<i>i1 – i2</i>	1.47E+02	2.47E+02	4.03E+02	6.41E+02	1.00E+03	1.53E+03	2.29E+03	3.38E+03	4.90E+03
<i>i2 – i1</i>	3.76E+00	6.60E+00	1.13E+01	1.88E+01	3.05E+01	4.87E+01	7.60E+01	1.17E+02	1.76E+02
<i>i23 – i68</i>	3.56E+01	4.81E+01	6.45E+01	8.58E+01	1.13E+02	1.49E+02	1.94E+02	2.51E+02	3.24E+02
<i>i68 – i23</i>	1.21E+06	1.52E+06	1.90E+06	2.36E+06	2.90E+06	3.56E+06	4.33E+06	5.25E+06	6.33E+06
<i>i2 – p2</i>	1.07E+05	1.58E+05	2.29E+05	3.25E+05	4.57E+05	6.33E+05	8.67E+05	1.17E+06	1.57E+06
<i>i3 – i4</i>	3.21E+05	4.05E+05	5.06E+05	6.27E+05	7.72E+05	9.45E+05	1.15E+06	1.39E+06	1.67E+06
<i>i4 – i3</i>	8.21E+06	1.00E+07	1.22E+07	1.47E+07	1.76E+07	2.09E+07	2.48E+07	2.92E+07	3.42E+07
<i>i3 – i18</i>	2.49E-01	4.52E-01	8.01E-01	1.39E+00	2.35E+00	3.89E+00	6.31E+00	1.00E+01	1.57E+01
<i>i18 – i3</i>	6.39E+01	1.11E+02	1.87E+02	3.10E+02	5.02E+02	7.97E+02	1.24E+03	1.90E+03	2.85E+03
<i>i69 – i71</i>	5.30E+12	5.42E+12	5.53E+12	5.65E+12	5.76E+12	5.87E+12	5.98E+12	6.09E+12	6.20E+12
<i>i71 – i69</i>	1.52E+10	1.61E+10	1.71E+10	1.80E+10	1.90E+10	2.00E+10	2.11E+10	2.21E+10	2.32E+10
<i>i66 – i69</i>	7.99E+05	9.88E+05	1.21E+06	1.48E+06	1.79E+06	2.16E+06	2.59E+06	3.09E+06	3.67E+06
<i>i69 – i66</i>	4.97E+08	5.79E+08	6.71E+08	7.74E+08	8.88E+08	1.01E+09	1.16E+09	1.31E+09	1.48E+09
<i>i71 – i73</i>	2.36E+09	2.64E+09	2.94E+09	3.27E+09	3.63E+09	4.01E+09	4.42E+09	4.86E+09	5.33E+09
<i>i73 – i71</i>	7.17E+07	8.41E+07	9.82E+07	1.14E+08	1.32E+08	1.53E+08	1.75E+08	2.01E+08	2.30E+08
<i>i71 – i72</i>	3.42E+06	4.01E+06	4.68E+06	5.43E+06	6.28E+06	7.22E+06	8.28E+06	9.45E+06	1.08E+07
<i>i72 – i71</i>	8.93E+11	9.39E+11	9.86E+11	1.03E+12	1.08E+12	1.13E+12	1.18E+12	1.23E+12	1.28E+12
<i>i72 – i76</i>	1.52E+08	1.88E+08	2.31E+08	2.82E+08	3.40E+08	4.07E+08	4.84E+08	5.72E+08	6.71E+08
<i>i76 – i72</i>	1.41E+02	2.04E+02	2.90E+02	4.08E+02	5.68E+02	7.80E+02	1.06E+03	1.43E+03	1.90E+03
<i>i76 – p24</i>	1.16E+07	1.41E+07	1.71E+07	2.06E+07	2.47E+07	2.95E+07	3.51E+07	4.15E+07	4.88E+07
<i>i73 – p26</i>	2.25E+03	3.32E+03	4.84E+03	6.95E+03	9.86E+03	1.38E+04	1.92E+04	2.63E+04	3.57E+04
<i>i22 – i67</i>	3.96E+07	4.54E+07	5.18E+07	5.89E+07	6.68E+07	7.56E+07	8.52E+07	9.59E+07	1.08E+08
<i>i67 – i22</i>	6.33E+10	6.76E+10	7.21E+10	7.67E+10	8.14E+10	8.64E+10	9.15E+10	9.67E+10	1.02E+11
<i>i67 – i76</i>	5.67E+12	5.71E+12	5.75E+12	5.78E+12	5.82E+12	5.86E+12	5.89E+12	5.93E+12	5.96E+12
<i>i76 – i67</i>	2.23E+10	2.36E+10	2.49E+10	2.63E+10	2.77E+10	2.92E+10	3.07E+10	3.23E+10	3.39E+10
<i>i2 – i5</i>	9.31E-01	1.61E+00	2.73E+00	4.52E+00	7.34E+00	1.17E+01	1.83E+01	2.81E+01	4.26E+01
<i>i5 – i2</i>	5.70E+01	9.53E+01	1.56E+02	2.50E+02	3.94E+02	6.09E+02	9.25E+02	1.38E+03	2.03E+03
<i>i20 – i18</i>	6.93E+10	7.22E+10	7.51E+10	7.81E+10	8.11E+10	8.42E+10	8.72E+10	9.03E+10	9.34E+10

<i>i18 – i20</i>	2.20E+11	2.29E+11	2.38E+11	2.47E+11	2.57E+11	2.66E+11	2.75E+11	2.85E+11	2.94E+11
<i>i5 – i11</i>	4.92E+10	5.21E+10	5.51E+10	5.81E+10	6.13E+10	6.45E+10	6.78E+10	7.12E+10	7.47E+10
<i>i11 – i5</i>	1.09E+08	1.23E+08	1.38E+08	1.54E+08	1.73E+08	1.92E+08	2.13E+08	2.36E+08	2.61E+08
<i>i8 – p14</i>	2.01E+01	3.62E+01	6.31E+01	1.07E+02	1.78E+02	2.87E+02	4.55E+02	7.06E+02	1.08E+03
<i>i9 – p12</i>	1.15E+04	1.75E+04	2.60E+04	3.81E+04	5.50E+04	7.83E+04	1.10E+05	1.53E+05	2.10E+05
<i>i8 – i10</i>	5.51E+05	6.89E+05	8.55E+05	1.05E+06	1.29E+06	1.57E+06	1.90E+06	2.29E+06	2.74E+06
<i>i10 – i8</i>	7.41E+07	8.76E+07	1.03E+08	1.20E+08	1.40E+08	1.62E+08	1.87E+08	2.15E+08	2.46E+08
<i>i8 – i11</i>	3.38E+00	5.87E+00	9.93E+00	1.64E+01	2.64E+01	4.17E+01	6.46E+01	9.83E+01	1.47E+02
<i>i11 – i8</i>	1.59E+00	2.81E+00	4.82E+00	8.06E+00	1.32E+01	2.11E+01	3.31E+01	5.09E+01	7.71E+01
<i>i11 – p13</i>	8.78E+03	1.34E+04	2.01E+04	2.97E+04	4.32E+04	6.20E+04	8.77E+04	1.23E+05	1.69E+05
<i>i4 – p12</i>	1.70E+05	2.56E+05	3.78E+05	5.49E+05	7.84E+05	1.10E+06	1.53E+06	2.09E+06	2.82E+06
<i>i107 – p2</i>	7.60E+04	1.11E+05	1.59E+05	2.24E+05	3.13E+05	4.30E+05	5.84E+05	7.85E+05	1.04E+06
<i>i8 – p2</i>	1.27E+04	1.89E+04	2.78E+04	4.01E+04	5.71E+04	8.01E+04	1.11E+05	1.52E+05	2.06E+05
<i>i9 – p14</i>	6.95E+00	1.26E+01	2.21E+01	3.78E+01	6.30E+01	1.02E+02	1.63E+02	2.56E+02	3.93E+02
<i>i75 – p26</i>	8.82E+03	1.29E+04	1.85E+04	2.62E+04	3.67E+04	5.08E+04	6.97E+04	9.45E+04	1.27E+05
<i>i2 – i3</i>	7.55E+11	7.74E+11	7.93E+11	8.13E+11	8.32E+11	8.51E+11	8.71E+11	8.90E+11	9.09E+11
<i>i3 – i2</i>	1.64E+12	1.67E+12	1.70E+12	1.72E+12	1.75E+12	1.77E+12	1.80E+12	1.82E+12	1.85E+12
<i>i71 – p26</i>	2.01E+04	2.87E+04	4.05E+04	5.64E+04	7.75E+04	1.05E+05	1.42E+05	1.88E+05	2.48E+05
<i>i20 – p13</i>	2.15E+05	3.28E+05	4.91E+05	7.21E+05	1.04E+06	1.48E+06	2.06E+06	2.84E+06	3.87E+06
<i>i66 – i67</i>	1.78E+10	1.90E+10	2.01E+10	2.13E+10	2.26E+10	2.39E+10	2.52E+10	2.66E+10	2.80E+10
<i>i67 – i66</i>	9.81E+11	1.01E+12	1.05E+12	1.08E+12	1.11E+12	1.15E+12	1.18E+12	1.21E+12	1.25E+12
<i>i68 – i21</i>	1.54E+04	2.04E+04	2.69E+04	3.50E+04	4.53E+04	5.81E+04	7.39E+04	9.35E+04	1.17E+05
<i>i21 – i68</i>	7.67E+02	1.05E+03	1.42E+03	1.90E+03	2.52E+03	3.32E+03	4.33E+03	5.62E+03	7.24E+03
<i>i73 – i75</i>	2.33E+08	2.66E+08	3.03E+08	3.45E+08	3.91E+08	4.41E+08	4.97E+08	5.58E+08	6.25E+08
<i>i75 – i73</i>	6.40E+08	7.24E+08	8.15E+08	9.16E+08	1.03E+09	1.15E+09	1.28E+09	1.42E+09	1.57E+09
<i>i76 – i77</i>	1.84E+09	2.03E+09	2.23E+09	2.45E+09	2.69E+09	2.94E+09	3.21E+09	3.49E+09	3.80E+09
<i>i77 – i76</i>	9.49E+07	1.07E+08	1.20E+08	1.34E+08	1.50E+08	1.67E+08	1.85E+08	2.05E+08	2.27E+08
<i>i77 – i78</i>	2.85E+08	3.19E+08	3.57E+08	3.98E+08	4.43E+08	4.91E+08	5.44E+08	6.01E+08	6.62E+08
<i>i78 – i77</i>	1.59E+09	1.78E+09	1.99E+09	2.21E+09	2.45E+09	2.72E+09	3.00E+09	3.31E+09	3.64E+09
<i>i2 – p21</i>	4.21E+03	7.10E+03	1.17E+04	1.87E+04	2.92E+04	4.49E+04	6.76E+04	1.00E+05	1.46E+05
<i>i78 – p24</i>	9.43E+06	1.16E+07	1.42E+07	1.72E+07	2.08E+07	2.51E+07	3.00E+07	3.58E+07	4.25E+07
<i>i20 – p15</i>	3.23E+03	5.95E+03	1.05E+04	1.81E+04	3.00E+04	4.85E+04	7.65E+04	1.18E+05	1.78E+05
<i>i23 – i24</i>	2.48E+07	2.82E+07	3.18E+07	3.59E+07	4.05E+07	4.54E+07	5.09E+07	5.70E+07	6.36E+07
<i>i24 – i23</i>	1.01E+08	1.14E+08	1.28E+08	1.43E+08	1.59E+08	1.77E+08	1.97E+08	2.18E+08	2.41E+08
<i>i8 – p23</i>	6.22E+02	1.08E+03	1.81E+03	2.96E+03	4.73E+03	7.40E+03	1.14E+04	1.71E+04	2.53E+04
<i>i24 – i21</i>	5.14E+08	5.58E+08	6.04E+08	6.54E+08	7.07E+08	7.62E+08	8.21E+08	8.83E+08	9.49E+08
<i>i21 – i24</i>	1.07E+11	1.12E+11	1.17E+11	1.22E+11	1.28E+11	1.33E+11	1.39E+11	1.45E+11	1.51E+11
<i>i24 – p1</i>	8.33E+09	9.05E+09	9.82E+09	1.06E+10	1.15E+10	1.24E+10	1.34E+10	1.44E+10	1.55E+10
<i>i18 – i5</i>	6.84E+12	6.87E+12	6.89E+12	6.93E+12	6.95E+12	6.98E+12	7.00E+12	7.03E+12	7.05E+12
<i>i5 – i18</i>	7.50E+11	7.70E+11	7.90E+11	8.11E+11	8.30E+11	8.50E+11	8.70E+11	8.90E+11	9.10E+11
<i>i5 – i19</i>	7.59E+10	7.88E+10	8.17E+10	8.47E+10	8.77E+10	9.07E+10	9.37E+10	9.67E+10	9.98E+10

<i>i19 – i5</i>	2.59E+07	3.00E+07	3.46E+07	3.98E+07	4.56E+07	5.21E+07	5.92E+07	6.72E+07	7.61E+07
<i>i10 – i12</i>	7.30E+05	9.39E+05	1.19E+06	1.50E+06	1.88E+06	2.33E+06	2.86E+06	3.49E+06	4.22E+06
<i>i12 – i10</i>	1.14E+06	1.50E+06	1.95E+06	2.51E+06	3.20E+06	4.04E+06	5.07E+06	6.30E+06	7.77E+06
<i>i13 – i6</i>	3.75E+03	5.41E+03	7.68E+03	1.08E+04	1.49E+04	2.04E+04	2.77E+04	3.71E+04	4.92E+04
<i>i6 – i13</i>	2.32E+02	3.46E+02	5.09E+02	7.39E+02	1.06E+03	1.50E+03	2.09E+03	2.89E+03	3.95E+03
<i>i13 – i65</i>	4.18E+03	5.64E+03	7.51E+03	9.91E+03	1.29E+04	1.67E+04	2.15E+04	2.73E+04	3.44E+04
<i>i65 – i13</i>	1.20E+11	1.33E+11	1.46E+11	1.60E+11	1.74E+11	1.89E+11	2.05E+11	2.21E+11	2.38E+11
<i>i4 – i13</i>	6.05E+06	7.27E+06	8.66E+06	1.03E+07	1.21E+07	1.41E+07	1.65E+07	1.91E+07	2.20E+07
<i>i13 – i4</i>	4.07E+06	5.11E+06	6.36E+06	7.86E+06	9.66E+06	1.18E+07	1.43E+07	1.72E+07	2.06E+07
<i>i64 – i13</i>	1.03E+13	1.04E+13	1.05E+13	1.06E+13	1.07E+13	1.08E+13	1.08E+13	1.09E+13	1.10E+13
<i>i13 – i64</i>	1.02E+06	1.27E+06	1.57E+06	1.92E+06	2.34E+06	2.82E+06	3.39E+06	4.04E+06	4.80E+06
<i>i65 – p9</i>	3.53E+03	7.77E+03	1.58E+04	3.02E+04	5.48E+04	9.46E+04	1.57E+05	2.53E+05	3.95E+05
<i>i22 – i65</i>	2.68E-01	4.56E-01	7.55E-01	1.22E+00	1.95E+00	3.04E+00	4.66E+00	7.05E+00	1.05E+01
<i>i65 – i22</i>	5.42E+08	7.01E+08	8.94E+08	1.12E+09	1.40E+09	1.71E+09	2.09E+09	2.51E+09	3.00E+09
<i>i19 – p20</i>	6.24E+07	7.19E+07	8.25E+07	9.45E+07	1.08E+08	1.23E+08	1.39E+08	1.57E+08	1.77E+08
<i>i12 – p10</i>	1.22E-01	3.14E-01	7.48E-01	1.67E+00	3.50E+00	7.02E+00	1.35E+01	2.49E+01	4.44E+01
<i>i11 – i9</i>	1.98E+11	2.05E+11	2.12E+11	2.19E+11	2.26E+11	2.33E+11	2.40E+11	2.47E+11	2.54E+11
<i>i9 – i11</i>	1.10E+11	1.14E+11	1.18E+11	1.23E+11	1.27E+11	1.32E+11	1.36E+11	1.41E+11	1.45E+11
<i>i11 – i15</i>	5.68E-01	1.05E+00	1.87E+00	3.27E+00	5.56E+00	9.23E+00	1.50E+01	2.39E+01	3.74E+01
<i>i15 – i11</i>	2.67E+02	4.59E+02	7.70E+02	1.26E+03	2.01E+03	3.13E+03	4.80E+03	7.21E+03	1.07E+04
<i>i9 – i4</i>	3.30E+00	5.83E+00	1.01E+01	1.70E+01	2.80E+01	4.52E+01	7.16E+01	1.12E+02	1.71E+02
<i>i4 – i9</i>	6.13E+02	1.01E+03	1.62E+03	2.55E+03	3.93E+03	5.95E+03	8.85E+03	1.30E+04	1.87E+04
<i>i11 – i17</i>	1.10E+04	1.39E+04	1.75E+04	2.18E+04	2.69E+04	3.31E+04	4.04E+04	4.90E+04	5.92E+04
<i>i17 – i11</i>	8.13E+09	9.32E+09	1.06E+10	1.21E+10	1.36E+10	1.54E+10	1.72E+10	1.92E+10	2.14E+10
<i>i64 – i66</i>	1.65E+03	4.28E+03	9.94E+03	2.12E+04	4.21E+04	7.88E+04	1.41E+05	2.40E+05	3.96E+05
<i>i66 – i64</i>	3.39E-05	1.11E-04	3.25E-04	8.66E-04	2.13E-03	4.93E-03	1.08E-02	2.24E-02	4.46E-02
<i>i21 – i19</i>	5.68E+11	5.90E+11	6.12E+11	6.35E+11	6.58E+11	6.81E+11	7.04E+11	7.28E+11	7.53E+11
<i>i19 – i21</i>	1.10E+11	1.13E+11	1.16E+11	1.19E+11	1.22E+11	1.24E+11	1.27E+11	1.30E+11	1.33E+11
<i>i21 – i70</i>	4.17E+09	4.61E+09	5.09E+09	5.60E+09	6.14E+09	6.73E+09	7.36E+09	8.03E+09	8.75E+09
<i>i70 – i21</i>	1.13E+12	1.14E+12	1.15E+12	1.16E+12	1.17E+12	1.18E+12	1.19E+12	1.20E+12	1.21E+12
<i>i12 – p11</i>	1.03E-02	3.35E-02	9.60E-02	2.50E-01	6.00E-01	1.35E+00	2.86E+00	5.79E+00	1.12E+01
<i>i68 – i74</i>	4.10E-01	7.53E-01	1.34E+00	2.32E+00	3.90E+00	6.43E+00	1.04E+01	1.63E+01	2.53E+01
<i>i74 – i68</i>	3.79E-05	7.43E-05	1.41E-04	2.60E-04	4.66E-04	8.15E-04	1.39E-03	2.33E-03	3.83E-03
<i>i3 – i6</i>	2.67E+06	3.21E+06	3.84E+06	4.57E+06	5.40E+06	6.34E+06	7.42E+06	8.64E+06	1.00E+07
<i>i6 – i3</i>	1.42E+06	1.79E+06	2.25E+06	2.81E+06	3.48E+06	4.28E+06	5.24E+06	6.37E+06	7.70E+06
<i>i20 – i15</i>	1.32E+12	1.34E+12	1.35E+12	1.36E+12	1.38E+12	1.39E+12	1.40E+12	1.41E+12	1.42E+12
<i>i15 – i20</i>	9.58E+11	9.83E+11	1.01E+12	1.03E+12	1.06E+12	1.08E+12	1.11E+12	1.13E+12	1.15E+12
<i>i22 – i17</i>	3.26E-03	6.45E-03	1.23E-02	2.27E-02	4.07E-02	7.09E-02	1.21E-01	2.01E-01	3.27E-01
<i>i17 – i22</i>	4.89E+03	8.36E+03	1.38E+04	2.22E+04	3.47E+04	5.30E+04	7.92E+04	1.16E+05	1.67E+05
<i>i23 – i17</i>	5.54E-02	8.29E-02	1.23E-01	1.79E-01	2.59E-01	3.70E-01	5.24E-01	7.35E-01	1.02E+00
<i>i17 – i23</i>	4.36E+07	5.34E+07	6.49E+07	7.82E+07	9.36E+07	1.11E+08	1.31E+08	1.54E+08	1.80E+08

<i>i19 – i16</i>	1.21E+08	1.36E+08	1.53E+08	1.71E+08	1.90E+08	2.11E+08	2.34E+08	2.59E+08	2.86E+08
<i>i16 – i19</i>	2.05E+09	2.27E+09	2.51E+09	2.76E+09	3.04E+09	3.33E+09	3.64E+09	3.98E+09	4.33E+09
<i>i22 – i23</i>	1.74E+09	1.91E+09	2.09E+09	2.29E+09	2.50E+09	2.72E+09	2.95E+09	3.21E+09	3.47E+09
<i>i23 – i22</i>	3.31E+06	3.85E+06	4.45E+06	5.13E+06	5.90E+06	6.77E+06	7.75E+06	8.84E+06	1.01E+07
<i>i3 – p21</i>	9.76E+03	1.60E+04	2.55E+04	3.98E+04	6.08E+04	9.12E+04	1.34E+05	1.95E+05	2.78E+05
<i>i77 – p24</i>	4.03E+06	4.94E+06	6.02E+06	7.30E+06	8.80E+06	1.06E+07	1.26E+07	1.50E+07	1.78E+07
<i>i74 – p25</i>	2.17E+04	2.91E+04	3.87E+04	5.11E+04	6.70E+04	8.70E+04	1.13E+05	1.45E+05	1.85E+05
<i>i11 – i16</i>	5.52E+07	6.20E+07	6.94E+07	7.74E+07	8.62E+07	9.56E+07	1.06E+08	1.17E+08	1.29E+08
<i>i16 – i11</i>	1.44E+08	1.67E+08	1.93E+08	2.22E+08	2.54E+08	2.90E+08	3.31E+08	3.75E+08	4.25E+08
<i>i16 – p20</i>	1.23E+09	1.38E+09	1.56E+09	1.75E+09	1.96E+09	2.18E+09	2.43E+09	2.70E+09	2.99E+09
<i>i70 – i74</i>	1.50E+11	1.59E+11	1.68E+11	1.77E+11	1.87E+11	1.97E+11	2.07E+11	2.17E+11	2.27E+11
<i>i74 – i70</i>	1.03E+06	1.24E+06	1.48E+06	1.77E+06	2.10E+06	2.49E+06	2.93E+06	3.44E+06	4.03E+06
<i>i20 – i13</i>	5.29E+05	6.89E+05	8.87E+05	1.13E+06	1.43E+06	1.78E+06	2.21E+06	2.72E+06	3.32E+06
<i>i13 – i20</i>	5.63E+04	7.80E+04	1.06E+05	1.44E+05	1.92E+05	2.53E+05	3.31E+05	4.29E+05	5.51E+05
<i>i18 – i14</i>	5.25E+00	1.04E+01	1.97E+01	3.55E+01	6.19E+01	1.04E+02	1.71E+02	2.72E+02	4.23E+02
<i>i14 – i18</i>	9.13E+02	1.72E+03	3.08E+03	5.29E+03	8.77E+03	1.41E+04	2.20E+04	3.36E+04	5.00E+04
<i>i10 – i14</i>	3.85E+02	6.03E+02	9.21E+02	1.38E+03	2.02E+03	2.91E+03	4.13E+03	5.76E+03	7.93E+03
<i>i14 – i10</i>	4.85E+05	7.08E+05	1.01E+06	1.42E+06	1.95E+06	2.65E+06	3.54E+06	4.66E+06	6.06E+06
<i>i7 – i4</i>	9.72E+10	1.07E+11	1.18E+11	1.29E+11	1.41E+11	1.54E+11	1.67E+11	1.81E+11	1.95E+11
<i>i4 – i7</i>	2.61E+08	3.06E+08	3.58E+08	4.16E+08	4.81E+08	5.54E+08	6.35E+08	7.24E+08	8.23E+08
<i>i7 – i20</i>	3.85E+10	4.31E+10	4.79E+10	5.31E+10	5.86E+10	6.45E+10	7.07E+10	7.72E+10	8.41E+10
<i>i20 – i7</i>	6.52E+08	7.64E+08	8.89E+08	1.03E+09	1.19E+09	1.36E+09	1.55E+09	1.76E+09	2.00E+09
<i>i18 – i12</i>	6.35E+03	9.66E+03	1.44E+04	2.09E+04	2.99E+04	4.21E+04	5.83E+04	7.97E+04	1.07E+05
<i>i12 – i18</i>	1.37E+03	2.16E+03	3.33E+03	5.04E+03	7.46E+03	1.09E+04	1.56E+04	2.20E+04	3.06E+04
<i>i13 – i14</i>	6.55E+04	8.40E+04	1.07E+05	1.35E+05	1.69E+05	2.09E+05	2.58E+05	3.17E+05	3.86E+05
<i>i14 – i13</i>	6.81E+08	7.77E+08	8.83E+08	9.98E+08	1.12E+09	1.26E+09	1.40E+09	1.56E+09	1.73E+09
<i>i3 – i8</i>	1.27E+02	2.11E+02	3.41E+02	5.41E+02	8.42E+02	1.29E+03	1.93E+03	2.86E+03	4.17E+03
<i>i8 – i3</i>	3.36E+01	5.69E+01	9.41E+01	1.53E+02	2.43E+02	3.79E+02	5.81E+02	8.77E+02	1.30E+03
<i>i1 – i107</i>	1.58E+06	2.11E+06	2.79E+06	3.64E+06	4.70E+06	6.02E+06	7.63E+06	9.60E+06	1.20E+07
<i>i107 – i1</i>	5.44E+03	7.81E+03	1.10E+04	1.54E+04	2.13E+04	2.91E+04	3.93E+04	5.26E+04	6.97E+04
<i>i107 – p2</i>	1.82E+04	2.66E+04	3.84E+04	5.47E+04	7.67E+04	1.06E+05	1.46E+05	1.98E+05	2.65E+05
<i>i1 – i25</i>	9.88E+03	1.41E+04	1.97E+04	2.71E+04	3.68E+04	4.94E+04	6.55E+04	8.57E+04	1.11E+05
<i>i25 – i1</i>	1.06E+07	1.48E+07	2.03E+07	2.74E+07	3.66E+07	4.82E+07	6.28E+07	8.09E+07	1.03E+08
<i>i25 – i26</i>	2.37E+06	3.24E+06	4.35E+06	5.77E+06	7.56E+06	9.79E+06	1.25E+07	1.59E+07	2.00E+07
<i>i26 – i25</i>	2.34E+02	3.43E+02	4.95E+02	7.02E+02	9.83E+02	1.36E+03	1.85E+03	2.49E+03	3.33E+03
<i>i26 – p16</i>	4.12E+04	6.21E+04	9.21E+04	1.34E+05	1.93E+05	2.73E+05	3.81E+05	5.25E+05	7.16E+05
<i>i26 – p18</i>	1.84E-01	4.72E-01	1.12E+00	2.50E+00	5.27E+00	1.06E+01	2.04E+01	3.79E+01	6.80E+01
<i>i26 – i27</i>	9.63E+06	1.16E+07	1.39E+07	1.65E+07	1.95E+07	2.30E+07	2.69E+07	3.14E+07	3.64E+07
<i>i27 – i26</i>	2.18E+09	2.48E+09	2.82E+09	3.19E+09	3.59E+09	4.03E+09	4.50E+09	5.02E+09	5.57E+09
<i>i27 – i28</i>	2.06E+12	2.09E+12	2.13E+12	2.17E+12	2.21E+12	2.25E+12	2.29E+12	2.32E+12	2.36E+12
<i>i28 – i27</i>	1.48E+12	1.52E+12	1.56E+12	1.60E+12	1.64E+12	1.68E+12	1.72E+12	1.76E+12	1.80E+12

<i>i28 – i29</i>	1.38E+10	1.48E+10	1.59E+10	1.70E+10	1.82E+10	1.94E+10	2.06E+10	2.19E+10	2.32E+10
<i>i29 – i28</i>	4.93E+04	6.19E+04	7.73E+04	9.60E+04	1.19E+05	1.46E+05	1.78E+05	2.17E+05	2.63E+05
<i>i29 – i91</i>	7.82E-02	1.22E-01	1.88E-01	2.86E-01	4.27E-01	6.30E-01	9.18E-01	1.32E+00	1.88E+00
<i>i91 – i29</i>	1.92E+02	2.82E+02	4.07E+02	5.80E+02	8.15E+02	1.13E+03	1.56E+03	2.11E+03	2.84E+03
<i>i91 – i23</i>	6.29E+05	7.84E+05	9.72E+05	1.20E+06	1.46E+06	1.78E+06	2.16E+06	2.60E+06	3.11E+06
<i>i23 – i91</i>	2.70E+01	3.65E+01	4.90E+01	6.53E+01	8.64E+01	1.13E+02	1.48E+02	1.92E+02	2.47E+02
<i>i29 – i94</i>	1.23E+05	1.48E+05	1.77E+05	2.12E+05	2.52E+05	2.98E+05	3.51E+05	4.13E+05	4.83E+05
<i>i94 – i29</i>	3.22E+10	3.52E+10	3.85E+10	4.19E+10	4.55E+10	4.94E+10	5.34E+10	5.77E+10	6.22E+10
<i>i94 – i95</i>	2.78E+03	4.14E+03	6.05E+03	8.72E+03	1.24E+04	1.74E+04	2.41E+04	3.30E+04	4.47E+04
<i>i95 – i94</i>	8.73E+02	1.30E+03	1.90E+03	2.74E+03	3.89E+03	5.47E+03	7.58E+03	1.04E+04	1.41E+04
<i>i95 – i23</i>	3.90E+10	4.21E+10	4.52E+10	4.86E+10	5.21E+10	5.57E+10	5.95E+10	6.35E+10	6.76E+10
<i>i23 – i95</i>	5.00E+04	6.02E+04	7.23E+04	8.65E+04	1.03E+05	1.22E+05	1.45E+05	1.70E+05	2.00E+05
<i>i29 – p20</i>	3.58E+07	4.21E+07	4.93E+07	5.74E+07	6.67E+07	7.73E+07	8.93E+07	1.03E+08	1.18E+08
<i>i26 – i89</i>	3.33E+01	5.87E+01	1.01E+02	1.70E+02	2.80E+02	4.52E+02	7.15E+02	1.11E+03	1.69E+03
<i>i89 – i26</i>	2.62E+03	4.37E+03	7.12E+03	1.14E+04	1.78E+04	2.72E+04	4.10E+04	6.07E+04	8.84E+04
<i>i89 – p16</i>	1.02E+05	1.55E+05	2.31E+05	3.37E+05	4.85E+05	6.87E+05	9.57E+05	1.32E+06	1.79E+06
<i>i89 – i90</i>	2.61E+12	2.64E+12	2.67E+12	2.70E+12	2.72E+12	2.75E+12	2.78E+12	2.80E+12	2.83E+12
<i>i90 – i89</i>	1.83E+12	1.88E+12	1.92E+12	1.97E+12	2.02E+12	2.07E+12	2.12E+12	2.17E+12	2.21E+12
<i>i90 – i93</i>	8.47E+09	9.10E+09	9.75E+09	1.04E+10	1.11E+10	1.19E+10	1.26E+10	1.34E+10	1.42E+10
<i>i93 – i90</i>	9.49E+07	1.11E+08	1.28E+08	1.48E+08	1.71E+08	1.96E+08	2.24E+08	2.55E+08	2.90E+08
<i>i93 – p20</i>	2.90E+09	3.25E+09	3.63E+09	4.05E+09	4.50E+09	4.99E+09	5.52E+09	6.09E+09	6.70E+09
<i>i25 – i80</i>	1.34E+03	2.17E+03	3.42E+03	5.29E+03	8.01E+03	1.19E+04	1.74E+04	2.50E+04	3.55E+04
<i>i80 – i25</i>	6.55E+02	1.05E+03	1.64E+03	2.51E+03	3.77E+03	5.55E+03	8.04E+03	1.15E+04	1.61E+04
<i>i80 – i82</i>	1.76E+02	3.04E+02	5.09E+02	8.23E+02	1.29E+03	1.98E+03	2.97E+03	4.36E+03	6.29E+03
<i>i82 – i80</i>	1.69E+04	2.86E+04	4.70E+04	7.47E+04	1.15E+05	1.74E+05	2.57E+05	3.71E+05	5.27E+05
<i>i82 – i84</i>	1.68E+05	2.61E+05	3.96E+05	5.86E+05	8.49E+05	1.21E+06	1.68E+06	2.31E+06	3.13E+06
<i>i84 – i82</i>	1.16E+03	1.91E+03	3.07E+03	4.79E+03	7.32E+03	1.09E+04	1.61E+04	2.32E+04	3.29E+04
<i>i84 – i24</i>	1.48E+08	1.81E+08	2.20E+08	2.66E+08	3.19E+08	3.79E+08	4.49E+08	5.29E+08	6.20E+08
<i>i24 – i84</i>	5.67E+00	8.14E+00	1.16E+01	1.62E+01	2.26E+01	3.11E+01	4.25E+01	5.76E+01	7.73E+01
<i>i84 – i87</i>	5.93E+08	7.08E+08	8.41E+08	9.93E+08	1.17E+09	1.36E+09	1.58E+09	1.82E+09	2.10E+09
<i>i87 – i84</i>	1.15E+05	1.42E+05	1.74E+05	2.11E+05	2.56E+05	3.07E+05	3.67E+05	4.37E+05	5.16E+05
<i>i87 – p17</i>	2.75E+04	4.22E+04	6.33E+04	9.34E+04	1.36E+05	1.94E+05	2.73E+05	3.80E+05	5.23E+05
<i>i29 – i30</i>	1.81E+08	2.02E+08	2.26E+08	2.52E+08	2.80E+08	3.10E+08	3.44E+08	3.80E+08	4.19E+08
<i>i30 – i29</i>	2.93E+08	3.25E+08	3.61E+08	4.00E+08	4.42E+08	4.87E+08	5.36E+08	5.89E+08	6.46E+08
<i>i30 – i19</i>	3.31E+07	3.77E+07	4.27E+07	4.82E+07	5.43E+07	6.11E+07	6.85E+07	7.67E+07	8.56E+07
<i>i19 – i30</i>	7.10E+08	7.80E+08	8.55E+08	9.35E+08	1.02E+09	1.11E+09	1.21E+09	1.31E+09	1.42E+09
<i>i1 – i79</i>	1.62E+09	1.79E+09	1.98E+09	2.18E+09	2.39E+09	2.62E+09	2.86E+09	3.11E+09	3.37E+09
<i>i79 – i1</i>	5.54E+11	5.94E+11	6.35E+11	6.77E+11	7.21E+11	7.66E+11	8.12E+11	8.59E+11	9.07E+11
<i>i79 – i83</i>	3.32E+01	8.35E+01	1.92E+02	4.15E+02	8.43E+02	1.63E+03	3.01E+03	5.35E+03	9.20E+03
<i>i83 – i79</i>	2.90E-01	7.74E-01	1.89E+00	4.31E+00	9.24E+00	1.88E+01	3.66E+01	6.85E+01	1.24E+02
<i>i83 – i26</i>	4.57E+09	5.25E+09	6.00E+09	6.83E+09	7.74E+09	8.74E+09	9.83E+09	1.10E+10	1.23E+10

<i>i26 – i83</i>	1.62E+08	1.91E+08	2.23E+08	2.61E+08	3.03E+08	3.50E+08	4.02E+08	4.61E+08	5.26E+08
<i>i79 – i25</i>	2.05E+01	4.15E+01	7.94E+01	1.45E+02	2.54E+02	4.30E+02	7.02E+02	1.12E+03	1.73E+03
<i>i25 – i79</i>	6.41E+01	1.32E+02	2.56E+02	4.73E+02	8.38E+02	1.43E+03	2.37E+03	3.81E+03	5.98E+03
<i>i83 – i25</i>	9.31E-02	2.10E-01	4.45E-01	8.94E-01	1.72E+00	3.17E+00	5.64E+00	9.72E+00	1.63E+01
<i>i25 – i83</i>	3.35E+01	7.20E+01	1.46E+02	2.80E+02	5.16E+02	9.14E+02	1.56E+03	2.59E+03	4.18E+03
<i>i27 – i80</i>	1.18E+03	1.82E+03	2.76E+03	4.08E+03	5.92E+03	8.44E+03	1.18E+04	1.64E+04	2.23E+04
<i>i80 – i27</i>	5.15E+04	7.75E+04	1.14E+05	1.64E+05	2.32E+05	3.23E+05	4.43E+05	5.98E+05	7.98E+05
<i>i83 – p19</i>	9.08E-03	3.15E-02	9.50E-02	2.58E-01	6.42E-01	1.49E+00	3.25E+00	6.72E+00	1.33E+01
<i>i30 – p20</i>	5.01E+07	5.85E+07	6.81E+07	7.89E+07	9.12E+07	1.05E+08	1.21E+08	1.38E+08	1.58E+08
<i>i29 – i93</i>	3.16E+06	3.69E+06	4.28E+06	4.96E+06	5.72E+06	6.59E+06	7.56E+06	8.65E+06	9.87E+06
<i>i93 – i29</i>	6.70E+09	7.29E+09	7.91E+09	8.57E+09	9.27E+09	1.00E+10	1.08E+10	1.16E+10	1.24E+10
<i>i16 – i93</i>	6.85E+07	7.91E+07	9.11E+07	1.05E+08	1.20E+08	1.36E+08	1.55E+08	1.75E+08	1.98E+08
<i>i93 – i16</i>	2.47E+08	2.82E+08	3.20E+08	3.62E+08	4.09E+08	4.60E+08	5.16E+08	5.78E+08	6.45E+08
<i>i26 – i81</i>	5.75E+05	7.38E+05	9.39E+05	1.18E+06	1.48E+06	1.84E+06	2.27E+06	2.78E+06	3.38E+06
<i>i81 – i26</i>	3.13E+12	3.24E+12	3.34E+12	3.44E+12	3.54E+12	3.64E+12	3.74E+12	3.84E+12	3.93E+12
<i>i92 – i26</i>	2.30E+03	3.53E+03	5.31E+03	7.85E+03	1.14E+04	1.64E+04	2.32E+04	3.24E+04	4.46E+04
<i>i26 – i92</i>	2.63E+01	4.21E+01	6.61E+01	1.02E+02	1.55E+02	2.31E+02	3.39E+02	4.90E+02	7.01E+02
<i>i92 – p21</i>	1.80E+04	3.13E+04	5.28E+04	8.64E+04	1.38E+05	2.15E+05	3.28E+05	4.90E+05	7.21E+05
<i>i81 – i85</i>	8.45E+12	8.53E+12	8.61E+12	8.68E+12	8.76E+12	8.82E+12	8.89E+12	8.95E+12	9.01E+12
<i>i85 – i81</i>	4.75E+05	5.91E+05	7.31E+05	8.98E+05	1.09E+06	1.32E+06	1.59E+06	1.90E+06	2.26E+06
<i>i85 – p14</i>	1.78E+02	3.00E+02	4.91E+02	7.85E+02	1.23E+03	1.88E+03	2.84E+03	4.20E+03	6.12E+03
<i>i85 – i11</i>	5.91E+02	8.95E+02	1.33E+03	1.95E+03	2.82E+03	4.01E+03	5.64E+03	7.82E+03	1.07E+04
<i>i11 – i85</i>	1.27E+02	1.97E+02	3.02E+02	4.55E+02	6.75E+02	9.87E+02	1.42E+03	2.02E+03	2.84E+03
<i>i85 – i86</i>	1.36E+04	1.80E+04	2.37E+04	3.09E+04	3.99E+04	5.10E+04	6.47E+04	8.15E+04	1.02E+05
<i>i86 – i85</i>	4.65E+08	5.38E+08	6.19E+08	7.08E+08	8.06E+08	9.12E+08	1.03E+09	1.15E+09	1.29E+09
<i>i86 – i88</i>	1.57E+12	1.59E+12	1.61E+12	1.63E+12	1.65E+12	1.67E+12	1.69E+12	1.71E+12	1.73E+12
<i>i88 – i86</i>	3.82E+12	3.88E+12	3.94E+12	4.01E+12	4.07E+12	4.12E+12	4.18E+12	4.24E+12	4.29E+12
<i>i88 – i91</i>	1.58E+10	1.70E+10	1.83E+10	1.96E+10	2.09E+10	2.23E+10	2.37E+10	2.51E+10	2.66E+10
<i>i91 – i88</i>	8.85E+05	1.15E+06	1.48E+06	1.89E+06	2.40E+06	3.02E+06	3.77E+06	4.68E+06	5.78E+06
<i>i85 – p18</i>	3.39E+00	6.80E+00	1.30E+01	2.40E+01	4.27E+01	7.36E+01	1.24E+02	2.02E+02	3.23E+02

Table S2 RRKM calculated rate constants ($k(E)$, s^{-1}) of the reaction of the phenylethynyl radical with propylene for unimolecular reaction steps at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$).

E_C	0	5	10	15	20	25	30	35	40
Reaction step	$k(E)$								
<i>i34 – i31</i>	1.19E+07	1.66E+07	2.28E+07	3.08E+07	4.10E+07	5.40E+07	7.03E+07	9.06E+07	1.16E+08
<i>i31 – i34</i>	2.51E+02	3.59E+02	5.05E+02	7.00E+02	9.57E+02	1.29E+03	1.72E+03	2.27E+03	2.96E+03
<i>i34 – i36</i>	3.51E+06	4.77E+06	6.39E+06	8.45E+06	1.10E+07	1.43E+07	1.83E+07	2.31E+07	2.91E+07
<i>i36 – i34</i>	4.94E+01	7.25E+01	1.04E+02	1.48E+02	2.08E+02	2.87E+02	3.92E+02	5.30E+02	7.08E+02
<i>i35 – i38</i>	9.52E+06	1.27E+07	1.67E+07	2.18E+07	2.80E+07	3.57E+07	4.50E+07	5.63E+07	6.98E+07
<i>i38 – i35</i>	3.27E+02	4.73E+02	6.73E+02	9.44E+02	1.31E+03	1.79E+03	2.42E+03	3.23E+03	4.28E+03
<i>i35 – i33</i>	1.48E+06	2.11E+06	2.94E+06	4.03E+06	5.46E+06	7.30E+06	9.63E+06	1.26E+07	1.62E+07
<i>i33 – i35</i>	1.44E+03	2.07E+03	2.93E+03	4.09E+03	5.62E+03	7.61E+03	1.02E+04	1.35E+04	1.76E+04
<i>i38 – i40</i>	1.31E+06	1.61E+06	1.96E+06	2.37E+06	2.86E+06	3.42E+06	4.07E+06	4.83E+06	5.70E+06
<i>i40 – i38</i>	3.61E+08	4.16E+08	4.77E+08	5.45E+08	6.20E+08	7.02E+08	7.92E+08	8.90E+08	9.97E+08
<i>i36 – i39</i>	1.36E+06	1.67E+06	2.04E+06	2.49E+06	3.01E+06	3.61E+06	4.32E+06	5.14E+06	6.08E+06
<i>i39 – i36</i>	1.05E+09	1.22E+09	1.40E+09	1.61E+09	1.83E+09	2.09E+09	2.36E+09	2.66E+09	2.99E+09
<i>i42 – i44</i>	8.21E+08	9.00E+08	9.82E+08	1.07E+09	1.16E+09	1.26E+09	1.36E+09	1.47E+09	1.58E+09
<i>i44 – i42</i>	3.08E+03	3.97E+03	5.09E+03	6.48E+03	8.21E+03	1.03E+04	1.29E+04	1.61E+04	1.99E+04
<i>i44 – i46</i>	3.21E+07	3.65E+07	4.15E+07	4.70E+07	5.30E+07	5.98E+07	6.72E+07	7.53E+07	8.43E+07
<i>i46 – i44</i>	2.06E+07	2.33E+07	2.62E+07	2.95E+07	3.31E+07	3.70E+07	4.13E+07	4.60E+07	5.12E+07
<i>i46 – i48</i>	1.46E+06	1.69E+06	1.95E+06	2.24E+06	2.57E+06	2.94E+06	3.35E+06	3.81E+06	4.32E+06
<i>i48 – i46</i>	4.58E+07	5.14E+07	5.76E+07	6.44E+07	7.18E+07	7.98E+07	8.86E+07	9.81E+07	1.08E+08
<i>i48 – i50</i>	4.61E+10	4.75E+10	4.89E+10	5.03E+10	5.17E+10	5.31E+10	5.45E+10	5.60E+10	5.74E+10
<i>i50 – i48</i>	3.70E+11	3.85E+11	4.00E+11	4.16E+11	4.31E+11	4.47E+11	4.63E+11	4.79E+11	4.96E+11
<i>i45 – i47</i>	5.38E+07	6.06E+07	6.81E+07	7.63E+07	8.53E+07	9.52E+07	1.06E+08	1.18E+08	1.31E+08
<i>i47 – i45</i>	1.67E+07	1.88E+07	2.11E+07	2.36E+07	2.64E+07	2.94E+07	3.27E+07	3.64E+07	4.03E+07
<i>i45 – i43</i>	1.51E+04	1.91E+04	2.40E+04	3.00E+04	3.73E+04	4.62E+04	5.68E+04	6.96E+04	8.49E+04
<i>i43 – i45</i>	9.19E+09	9.87E+09	1.06E+10	1.13E+10	1.21E+10	1.29E+10	1.37E+10	1.45E+10	1.54E+10
<i>i47 – i49</i>	3.80E+06	4.39E+06	5.05E+06	5.79E+06	6.62E+06	7.56E+06	8.60E+06	9.76E+06	1.10E+07
<i>i49 – i47</i>	2.65E+08	2.95E+08	3.28E+08	3.63E+08	4.01E+08	4.43E+08	4.88E+08	5.36E+08	5.88E+08
<i>i49 – i51</i>	6.92E+10	7.14E+10	7.36E+10	7.58E+10	7.80E+10	8.03E+10	8.26E+10	8.49E+10	8.72E+10
<i>i51 – i49</i>	1.93E+11	2.02E+11	2.11E+11	2.20E+11	2.30E+11	2.39E+11	2.49E+11	2.59E+11	2.70E+11
<i>i45 – i99</i>	6.82E+03	8.50E+03	1.05E+04	1.30E+04	1.60E+04	1.95E+04	2.37E+04	2.87E+04	3.46E+04
<i>i99 – i45</i>	1.97E+04	2.44E+04	3.00E+04	3.68E+04	4.49E+04	5.45E+04	6.58E+04	7.91E+04	9.48E+04
<i>i31 – p8</i>	3.46E+03	5.31E+03	7.98E+03	1.18E+04	1.71E+04	2.44E+04	3.43E+04	4.75E+04	6.50E+04
<i>i31 – p6</i>	1.69E+04	2.40E+04	3.37E+04	4.65E+04	6.35E+04	8.55E+04	1.14E+05	1.50E+05	1.95E+05
<i>i33 – i32</i>	1.35E+09	1.49E+09	1.63E+09	1.79E+09	1.96E+09	2.13E+09	2.32E+09	2.51E+09	2.72E+09
<i>i32 – i33</i>	1.65E+11	1.77E+11	1.90E+11	2.03E+11	2.16E+11	2.30E+11	2.44E+11	2.59E+11	2.74E+11
<i>i31 – i32</i>	6.55E+07	7.34E+07	8.19E+07	9.11E+07	1.01E+08	1.11E+08	1.23E+08	1.35E+08	1.47E+08
<i>i32 – i31</i>	2.13E+11	2.29E+11	2.46E+11	2.63E+11	2.81E+11	2.99E+11	3.18E+11	3.37E+11	3.57E+11
<i>i33 – p22</i>	4.30E+06	5.76E+06	7.63E+06	9.98E+06	1.29E+07	1.66E+07	2.10E+07	2.64E+07	3.30E+07

<i>i33 – p5</i>	2.39E+04	3.47E+04	4.94E+04	6.93E+04	9.57E+04	1.31E+05	1.76E+05	2.34E+05	3.08E+05
<i>i33 – i96</i>	1.08E+05	1.47E+05	1.96E+05	2.59E+05	3.38E+05	4.37E+05	5.60E+05	7.12E+05	8.97E+05
<i>i96 – i33</i>	6.32E+01	9.37E+01	1.37E+02	1.98E+02	2.81E+02	3.95E+02	5.50E+02	7.56E+02	1.03E+03
<i>i51 – i53</i>	1.35E+11	1.42E+11	1.49E+11	1.56E+11	1.64E+11	1.71E+11	1.79E+11	1.87E+11	1.95E+11
<i>i53 – i51</i>	1.52E+09	1.65E+09	1.79E+09	1.94E+09	2.09E+09	2.26E+09	2.44E+09	2.62E+09	2.82E+09
<i>i50 – i52</i>	8.81E+10	9.24E+10	9.68E+10	1.01E+11	1.06E+11	1.11E+11	1.16E+11	1.21E+11	1.26E+11
<i>i52 – i50</i>	4.57E+08	4.97E+08	5.40E+08	5.86E+08	6.35E+08	6.87E+08	7.42E+08	8.00E+08	8.61E+08
<i>i44 – p31</i>	8.01E+06	9.51E+06	1.13E+07	1.33E+07	1.56E+07	1.82E+07	2.13E+07	2.47E+07	2.87E+07
<i>i44 – p33</i>	8.29E+06	9.96E+06	1.19E+07	1.42E+07	1.69E+07	2.00E+07	2.35E+07	2.77E+07	3.24E+07
<i>i46 – p31</i>	7.56E+06	8.90E+06	1.04E+07	1.22E+07	1.42E+07	1.65E+07	1.92E+07	2.21E+07	2.55E+07
<i>i46 – p37</i>	8.49E+02	1.18E+03	1.64E+03	2.24E+03	3.03E+03	4.08E+03	5.44E+03	7.19E+03	9.45E+03
<i>i48 – p31</i>	1.96E+07	2.27E+07	2.62E+07	3.01E+07	3.45E+07	3.95E+07	4.50E+07	5.11E+07	5.79E+07
<i>i48 – p35</i>	1.02E+07	1.23E+07	1.46E+07	1.74E+07	2.06E+07	2.42E+07	2.84E+07	3.32E+07	3.87E+07
<i>i45 – p27</i>	1.97E+08	2.27E+08	2.61E+08	2.98E+08	3.41E+08	3.88E+08	4.40E+08	4.98E+08	5.62E+08
<i>i45 – p28</i>	5.26E+06	6.19E+06	7.26E+06	8.49E+06	9.88E+06	1.15E+07	1.33E+07	1.53E+07	1.76E+07
<i>i47 – p28</i>	1.78E+07	2.08E+07	2.42E+07	2.80E+07	3.24E+07	3.73E+07	4.29E+07	4.91E+07	5.61E+07
<i>i47 – p32</i>	1.67E+07	2.00E+07	2.38E+07	2.82E+07	3.33E+07	3.93E+07	4.61E+07	5.39E+07	6.29E+07
<i>i49 – p28</i>	7.04E+07	8.07E+07	9.22E+07	1.05E+08	1.19E+08	1.35E+08	1.53E+08	1.72E+08	1.93E+08
<i>i53 – p4</i>	3.51E+09	3.83E+09	4.18E+09	4.56E+09	4.96E+09	5.38E+09	5.84E+09	6.32E+09	6.84E+09
<i>i104 – i53</i>	8.18E+06	9.23E+06	1.04E+07	1.16E+07	1.30E+07	1.46E+07	1.62E+07	1.81E+07	2.01E+07
<i>i53 – i104</i>	3.16E+07	3.57E+07	4.01E+07	4.50E+07	5.04E+07	5.64E+07	6.29E+07	7.00E+07	7.77E+07
<i>i102 – p4</i>	6.06E+08	6.68E+08	7.34E+08	8.06E+08	8.84E+08	9.67E+08	1.06E+09	1.15E+09	1.26E+09
<i>i52 – p3</i>	3.39E+09	3.70E+09	4.04E+09	4.39E+09	4.77E+09	5.18E+09	5.61E+09	6.06E+09	6.55E+09
<i>i52 – p38</i>	2.94E+10	3.17E+10	3.40E+10	3.65E+10	3.91E+10	4.19E+10	4.48E+10	4.78E+10	5.10E+10
<i>i52 – i102</i>	3.93E+03	4.90E+03	6.08E+03	7.51E+03	9.23E+03	1.13E+04	1.37E+04	1.67E+04	2.01E+04
<i>i102 – i52</i>	1.04E+03	1.31E+03	1.65E+03	2.06E+03	2.55E+03	3.15E+03	3.88E+03	4.76E+03	5.81E+03
<i>i104 – p4</i>	1.38E+09	1.51E+09	1.64E+09	1.78E+09	1.94E+09	2.10E+09	2.27E+09	2.45E+09	2.65E+09
<i>i104 – i102</i>	3.91E+06	4.42E+06	4.99E+06	5.62E+06	6.31E+06	7.07E+06	7.91E+06	8.83E+06	9.84E+06
<i>i102 – i104</i>	6.96E+06	7.94E+06	9.04E+06	1.03E+07	1.16E+07	1.31E+07	1.48E+07	1.66E+07	1.87E+07
<i>i96 – p5</i>	3.79E+03	5.51E+03	7.91E+03	1.12E+04	1.57E+04	2.16E+04	2.96E+04	4.00E+04	5.37E+04
<i>i37 – i36</i>	3.28E+12	3.41E+12	3.55E+12	3.68E+12	3.82E+12	3.95E+12	4.08E+12	4.22E+12	4.35E+12
<i>i36 – i37</i>	7.37E+05	9.40E+05	1.19E+06	1.49E+06	1.86E+06	2.30E+06	2.82E+06	3.44E+06	4.17E+06
<i>i37 – i38</i>	2.00E+12	2.08E+12	2.17E+12	2.25E+12	2.34E+12	2.42E+12	2.50E+12	2.58E+12	2.66E+12
<i>i38 – i37</i>	6.32E+05	8.09E+05	1.03E+06	1.29E+06	1.61E+06	2.00E+06	2.46E+06	3.01E+06	3.65E+06
<i>i31 – p7</i>	1.34E+04	1.92E+04	2.70E+04	3.74E+04	5.12E+04	6.92E+04	9.24E+04	1.22E+05	1.60E+05
<i>i97 – i44</i>	9.52E+10	9.87E+10	1.02E+11	1.06E+11	1.10E+11	1.13E+11	1.17E+11	1.21E+11	1.25E+11
<i>i44 – i97</i>	1.08E+12	1.12E+12	1.15E+12	1.19E+12	1.22E+12	1.26E+12	1.30E+12	1.33E+12	1.37E+12
<i>i97 – p30</i>	1.74E+06	2.06E+06	2.43E+06	2.86E+06	3.35E+06	3.92E+06	4.56E+06	5.29E+06	6.13E+06
<i>i46 – i98</i>	5.05E+08	5.58E+08	6.15E+08	6.75E+08	7.41E+08	8.12E+08	8.89E+08	9.70E+08	1.06E+09
<i>i98 – i46</i>	3.93E+08	4.36E+08	4.83E+08	5.33E+08	5.88E+08	6.48E+08	7.11E+08	7.80E+08	8.54E+08
<i>i98 – p30</i>	1.17E+07	1.37E+07	1.61E+07	1.88E+07	2.18E+07	2.53E+07	2.93E+07	3.37E+07	3.88E+07

<i>i48 – p30</i>	4.25E+07	4.90E+07	5.63E+07	6.45E+07	7.36E+07	8.38E+07	9.51E+07	1.08E+08	1.22E+08
<i>i104 – p41</i>	2.18E+06	2.60E+06	3.09E+06	3.66E+06	4.31E+06	5.07E+06	5.94E+06	6.93E+06	8.07E+06
<i>i106 – i53</i>	2.95E+06	3.37E+06	3.84E+06	4.37E+06	4.95E+06	5.60E+06	6.33E+06	7.12E+06	8.00E+06
<i>i53 – i106</i>	2.98E+07	3.37E+07	3.80E+07	4.27E+07	4.79E+07	5.36E+07	5.99E+07	6.68E+07	7.44E+07
<i>i106 – p4</i>	7.32E+08	8.06E+08	8.86E+08	9.72E+08	1.06E+09	1.16E+09	1.27E+09	1.39E+09	1.51E+09
<i>i106 – p40</i>	7.86E+06	9.38E+06	1.12E+07	1.32E+07	1.56E+07	1.84E+07	2.16E+07	2.53E+07	2.96E+07
<i>i102 – p38</i>	1.74E+10	1.88E+10	2.04E+10	2.20E+10	2.37E+10	2.55E+10	2.74E+10	2.94E+10	3.15E+10
<i>i97 – p34</i>	7.87E+05	9.51E+05	1.14E+06	1.37E+06	1.64E+06	1.94E+06	2.30E+06	2.72E+06	3.20E+06
<i>i98 – p36</i>	5.42E+03	7.39E+03	1.00E+04	1.34E+04	1.79E+04	2.36E+04	3.09E+04	4.03E+04	5.20E+04
<i>i105 – p39</i>	6.80E+05	8.12E+05	9.66E+05	1.15E+06	1.35E+06	1.59E+06	1.87E+06	2.19E+06	2.55E+06
<i>i105 – p3</i>	3.68E+08	4.06E+08	4.46E+08	4.89E+08	5.36E+08	5.87E+08	6.41E+08	6.99E+08	7.62E+08
<i>i105 – i52</i>	2.76E+05	3.17E+05	3.62E+05	4.13E+05	4.69E+05	5.33E+05	6.03E+05	6.81E+05	7.67E+05
<i>i52 – i105</i>	3.13E+07	3.53E+07	3.96E+07	4.45E+07	4.97E+07	5.55E+07	6.19E+07	6.88E+07	7.64E+07
<i>i103 – p42</i>	2.87E+03	3.93E+03	5.34E+03	7.20E+03	9.63E+03	1.28E+04	1.68E+04	2.20E+04	2.87E+04
<i>i103 – p3</i>	4.42E+09	4.82E+09	5.26E+09	5.73E+09	6.22E+09	6.75E+09	7.32E+09	7.92E+09	8.56E+09
<i>i103 – i52</i>	7.90E+06	8.92E+06	1.00E+07	1.13E+07	1.26E+07	1.41E+07	1.57E+07	1.75E+07	1.95E+07
<i>i52 – i103</i>	4.12E+07	4.62E+07	5.17E+07	5.77E+07	6.43E+07	7.14E+07	7.92E+07	8.77E+07	9.70E+07
<i>i39 – i42</i>	2.35E+12	2.40E+12	2.45E+12	2.50E+12	2.55E+12	2.60E+12	2.65E+12	2.70E+12	2.75E+12
<i>i42 – i39</i>	2.53E+11	2.62E+11	2.72E+11	2.81E+11	2.91E+11	3.00E+11	3.10E+11	3.19E+11	3.29E+11
<i>i99 – p29</i>	1.17E+07	1.37E+07	1.59E+07	1.85E+07	2.14E+07	2.48E+07	2.85E+07	3.27E+07	3.75E+07
<i>i99 – p27</i>	3.19E+08	3.65E+08	4.17E+08	4.74E+08	5.39E+08	6.10E+08	6.89E+08	7.77E+08	8.73E+08
<i>i41 – i43</i>	1.88E+09	2.13E+09	2.40E+09	2.69E+09	3.00E+09	3.34E+09	3.71E+09	4.10E+09	4.53E+09
<i>i43 – i41</i>	1.60E+09	1.80E+09	2.02E+09	2.25E+09	2.51E+09	2.79E+09	3.08E+09	3.40E+09	3.74E+09
<i>i41 – i40</i>	1.25E+09	1.41E+09	1.59E+09	1.79E+09	2.00E+09	2.22E+09	2.47E+09	2.73E+09	3.01E+09
<i>i40 – i41</i>	3.03E+09	3.36E+09	3.72E+09	4.10E+09	4.50E+09	4.94E+09	5.39E+09	5.88E+09	6.39E+09
<i>i100 – i99</i>	1.01E+08	1.13E+08	1.25E+08	1.38E+08	1.52E+08	1.68E+08	1.85E+08	2.02E+08	2.22E+08
<i>i99 – i100</i>	1.85E+07	2.12E+07	2.42E+07	2.76E+07	3.13E+07	3.54E+07	4.00E+07	4.50E+07	5.06E+07
<i>i100 – i101</i>	3.71E+10	3.85E+10	3.98E+10	4.12E+10	4.26E+10	4.40E+10	4.54E+10	4.68E+10	4.83E+10
<i>i101 – i100</i>	2.57E+11	2.69E+11	2.82E+11	2.94E+11	3.07E+11	3.20E+11	3.33E+11	3.47E+11	3.61E+11
<i>i101 – i103</i>	7.50E+10	7.88E+10	8.27E+10	8.67E+10	9.08E+10	9.50E+10	9.94E+10	1.04E+11	1.08E+11
<i>i103 – i101</i>	1.55E+08	1.69E+08	1.85E+08	2.02E+08	2.19E+08	2.38E+08	2.59E+08	2.80E+08	3.03E+08
<i>i100 – p29</i>	3.15E+07	3.62E+07	4.14E+07	4.72E+07	5.37E+07	6.09E+07	6.88E+07	7.76E+07	8.73E+07

Table S3 Statistical branching ratios (%) for the reaction of the phenylethynyl radical with ethylene with *i1* as an initial intermediate at different collision energies (E_C , kJ·mol⁻¹).

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	0.0311	0.0318	0.0323	0.0328	0.0332	0.0335	0.0338	0.0339	0.0340
<i>p20</i>	0.1045	0.1084	0.1121	0.1154	0.1184	0.1212	0.1238	0.1260	0.1281
<i>p2</i>	99.8629	99.8579	99.8531	99.8486	99.8443	99.8403	99.8363	99.8326	99.8289
<i>p9-p19,</i> <i>p21,</i> <i>p23-p26</i>	<10 ⁻²	<10 ⁻²	<10 ⁻²	<10 ⁻²	<10 ⁻²	<10 ⁻²	<10 ⁻²	<10 ⁻²	<10 ⁻²

Table S4 Statistical branching ratios (%) for the reaction of the phenylethynyl radical with ethylene with *i25* as an initial intermediate at different collision energies (E_C , kJ·mol⁻¹).

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	3.7	3.6	3.4	3.3	3.1	3.0	2.9	2.8	2.7
<i>p20</i>	14.6	14.4	14.3	14.1	13.9	13.8	13.6	13.5	13.3
<i>p2</i>	81.6	81.9	82.2	82.5	82.7	83.0	83.2	83.4	83.6
<i>p9-p19,</i> <i>p21,</i> <i>p23-p26</i>	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹	<10 ⁻¹

Table S5 Statistical branching ratios (%) for the reaction of the phenylethynyl radical with ethylene with *i25* as an initial intermediate at different collision energies (E_C , kJ·mol⁻¹) having the values of *ts*[*i1-i25*], *ts*[*i29-p20*], and *ts*[*i30-p20*] increased by 4 kJ·mol⁻¹ and the values of *ts*[*i25-i26*], *ts*[*i29-i30*], and *ts*[*i30-i19*] decreased by 4 kJ·mol⁻¹.

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	17.8	16.8	15.8	14.9	14.1	13.3	12.6	11.9	11.3
<i>p20</i>	30.5	30.0	29.5	29.0	28.5	28.0	27.5	27.1	26.6
<i>p2</i>	51.5	53.0	54.4	55.7	57.0	58.1	59.2	60.2	61.2
<i>p9-p19,</i> <i>p21,</i> <i>p23-p26</i>	≤1.0	≤1.0	≤1.0	≤1.0	≤1.0	≤1.0	≤1.0	≤1.0	≤1.0

Table S6 Statistical branching ratios (%) at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$) for the reaction of the phenylethynyl radical with propylene with *i34* as an initial intermediate. Both atomic hydrogen and methyl loss channels are included.

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	0.3	0.3	0.3	0.2	0.2	0.2	0.2	0.2	0.2
<i>p2</i>	62.3	62.0	61.6	61.3	60.9	60.5	60.1	59.6	59.2
<i>p3</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p4</i>	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p5</i>	1.9	1.9	2.0	2.0	2.0	2.0	2.1	2.1	2.1
<i>p6</i>	6.5	6.8	7.1	7.4	7.6	7.9	8.1	8.4	8.6
<i>p7</i>	5.2	5.4	5.7	5.9	6.2	6.4	6.6	6.8	7.0
<i>p8</i>	1.3	1.5	1.7	1.9	2.1	2.2	2.5	2.7	2.9
<i>p20</i>	2.8	2.8	2.8	2.8	2.8	2.9	2.9	2.9	2.9
<i>p28</i>	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
<i>p29</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p30</i>	9.5	9.2	8.9	8.7	8.4	8.2	8.0	7.8	7.6
<i>p31</i>	4.2	4.1	4.0	3.9	3.8	3.8	3.7	3.6	3.5
<i>p32</i>	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.3
<i>p33</i>	2.6	2.6	2.6	2.6	2.5	2.5	2.5	2.5	2.5
<i>p34</i>	2.8	2.8	2.8	2.8	2.8	2.7	2.7	2.7	2.7
<i>p35</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p36</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p37</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p39</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p40</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p42</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S7 Statistical branching ratios (%) at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$) for the reaction of the phenylethynyl radical with propylene with *i35* as an initial intermediate. Both atomic hydrogen and methyl loss channels are included.

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
<i>p2</i>	10.9	11.4	11.8	12.2	12.7	13.0	13.4	13.8	14.1
<i>p3</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p4</i>	1.0	1.0	0.9	0.9	0.8	0.8	0.8	0.7	0.7
<i>p5</i>	0.3	0.4	0.4	0.4	0.4	0.4	0.5	0.5	0.5
<i>p6</i>	1.1	1.2	1.3	1.5	1.6	1.7	1.8	1.9	2.0
<i>p7</i>	0.9	1.0	1.1	1.2	1.3	1.4	1.4	1.5	1.6
<i>p8</i>	0.2	0.3	0.3	0.4	0.4	0.5	0.5	0.6	0.7
<i>p20</i>	55.0	54.0	53.1	52.3	51.4	50.6	49.8	49.1	48.4
<i>p28</i>	6.3	6.2	6.0	5.9	5.7	5.6	5.5	5.3	5.2
<i>p29</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p30</i>	9.6	9.7	9.9	10.0	10.1	10.2	10.2	10.3	10.4
<i>p31</i>	4.3	4.4	4.4	4.5	4.6	4.7	4.7	4.8	4.8
<i>p32</i>	4.6	4.5	4.5	4.4	4.4	4.3	4.3	4.2	4.2
<i>p33</i>	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4
<i>p34</i>	2.8	2.9	3.1	3.2	3.3	3.4	3.5	3.6	3.7
<i>p35</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p36</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p37</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p39</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p40</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p42</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S8 Statistical branching ratios (%) at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$) for the reaction of the phenylethynyl radical with propylene with *i3I* as an initial intermediate. Both atomic hydrogen and methyl loss channels are included.

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p2</i>	80.6	79.8	78.9	78.1	77.3	76.5	75.7	74.9	74.1
<i>p3</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p4</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p5</i>	8.5	8.8	9.1	9.4	9.7	10.0	10.3	10.5	10.8
<i>p6</i>	2.4	2.5	2.5	2.5	2.6	2.6	2.6	2.6	2.7
<i>p7</i>	6.7	7.0	7.3	7.6	7.8	8.1	8.3	8.6	8.8
<i>p8</i>	1.7	1.9	2.2	2.4	2.6	2.8	3.1	3.3	3.6
<i>p20</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p28</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p29</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p30</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p31</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p32</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p33</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p34</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p35</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p36</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p37</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p39</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p40</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p42</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S9 Statistical branching ratios (%) at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$) for the reaction of the phenylethynyl radical with propylene with *i33* as an initial intermediate. Both atomic hydrogen and methyl loss channels are included.

E_C	0	5	10	15	20	25	30	35	40
<i>p1</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p2</i>	80.7	79.9	79.1	78.3	77.5	76.8	76.0	75.3	74.6
<i>p3</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p4</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p5</i>	2.4	2.5	2.5	2.5	2.6	2.6	2.6	2.7	2.7
<i>p6</i>	8.4	8.7	9.0	9.3	9.6	9.8	10.1	10.3	10.6
<i>p7</i>	6.7	7.0	7.2	7.5	7.7	8.0	8.2	8.4	8.6
<i>p8</i>	1.7	1.9	2.1	2.4	2.6	2.8	3.0	3.3	3.5
<i>p20</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p28</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p29</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p30</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p31</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p32</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p33</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p34</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p35</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p36</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p37</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p39</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p40</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p42</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S10 Statistical branching ratios (%) at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$) for the reaction of the phenylethynyl radical with propylene with *i34* as an initial intermediate having the values of $ts[i34-i31]$, $ts[i44-p31]$, $ts[i44-p33]$, $ts[i97-p30]$, $ts[i97-p34]$, $ts[i46-p31]$, $ts[i48-p31]$, $ts[i48-p30]$, $ts[i98-p30]$, $ts[i36-i37]$, and $ts[i37-i38]$ increased by 5 kJ mol^{-1} and the values of $ts[i34-i36]$, $ts[i44-i46]$, $ts[i46-i48]$, and $ts[i36-i39]$ decreased by 5 kJ mol^{-1} . Only H loss channels are included.

E_C	0	5	10	15	20	25	30	35	40
<i>p3</i>	4.5	4.2	4.0	3.7	3.5	3.3	3.1	2.9	2.7
<i>p4</i>	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
<i>p5</i>	4.1	4.2	4.2	4.3	4.4	4.4	4.5	4.5	4.6
<i>p6</i>	14.0	14.6	15.2	15.8	16.3	16.8	17.2	17.7	18.1
<i>p7</i>	11.1	11.7	12.2	12.7	13.2	13.6	14.0	14.4	14.8
<i>p8</i>	2.9	3.2	3.6	4.0	4.4	4.8	5.2	5.6	6.0
<i>p28</i>	1.6	1.7	1.8	1.8	1.9	1.9	2.0	2.0	2.1
<i>p29</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p30</i>	31.4	30.4	29.5	28.5	27.6	26.8	25.9	25.2	24.4
<i>p31</i>	14.2	13.8	13.4	13.1	12.8	12.4	12.1	11.8	11.5
<i>p32</i>	1.2	1.2	1.3	1.4	1.4	1.5	1.5	1.6	1.6
<i>p33</i>	7.1	7.0	7.0	6.9	6.9	6.8	6.8	6.7	6.7
<i>p34</i>	7.6	7.6	7.5	7.5	7.4	7.4	7.3	7.3	7.2
<i>p35</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p36</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p37</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p39</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p40</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p42</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Table S11 Statistical branching ratios (%) at different collision energies (E_C , $\text{kJ}\cdot\text{mol}^{-1}$) for the reaction of the phenylethynyl radical with propylene with *i35* as an initial intermediate having the values of *ts*[*i35-i33*], *ts*[*i36-i37*], *ts*[*i37-i38*], *ts*[*i45-p28*], *ts*[*i47-p28*], *ts*[*i47-p32*], and *ts*[*i49-p28*] increased by 5 kJ mol^{-1} and the values of *ts*[*i35-i38*], *ts*[*i38-i40*], and *ts*[*i47-i49*] decreased by 5 kJ mol^{-1} . Only H loss channels are included.

E_C	0	5	10	15	20	25	30	35	40
<i>p3</i>	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.2
<i>p4</i>	21.4	20.6	19.8	19.1	18.3	17.6	16.9	16.3	15.7
<i>p5</i>	0.3	0.3	0.3	0.3	0.4	0.4	0.4	0.4	0.5
<i>p6</i>	0.9	1.0	1.1	1.2	1.3	1.5	1.6	1.7	1.8
<i>p7</i>	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
<i>p8</i>	0.2	0.2	0.3	0.3	0.4	0.4	0.5	0.5	0.6
<i>p28</i>	39.7	39.4	39.1	38.9	38.6	38.3	38.0	37.6	37.3
<i>p29</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p30</i>	3.6	3.8	4.0	4.2	4.4	4.6	4.8	5.0	5.2
<i>p31</i>	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4
<i>p32</i>	29.4	29.8	30.1	30.4	30.6	30.8	31.0	31.2	31.4
<i>p33</i>	1.0	1.1	1.2	1.2	1.3	1.4	1.5	1.6	1.7
<i>p34</i>	1.1	1.1	1.2	1.3	1.4	1.5	1.6	1.8	1.9
<i>p35</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p36</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p37</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p39</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p40</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p42</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) for all intermediates, transition states, reactants, and products involved in the C₈H₅ + C₂H₄ reaction at the ωB97X-D/6-311G(d,p) level.

Reactants

C₈H₅

C	0.045775	1.219540	0.013382
C	1.426126	1.212650	-0.006714
C	2.115813	-0.000010	-0.017253
C	1.426105	-1.212662	-0.006715
C	0.045755	-1.219531	0.013384
C	-0.671544	0.000009	0.023596
C	-2.068345	0.000016	0.040729
C	-3.340546	-0.000008	-0.055969
H	-0.510694	2.148691	0.019942
H	1.973361	2.147570	-0.015716
H	3.199878	-0.000024	-0.035097
H	1.973339	-2.147581	-0.015717
H	-0.510719	-2.148680	0.019947

Frequencies

109.1212	143.9347	246.8164
390.7115	476.4153	484.9854
507.4479	629.6306	687.8436
783.4529	788.1472	862.7349
967.3232	1013.8868	1014.0002
1029.0644	1049.7885	1112.7315
1182.8967	1188.0328	1227.9584
1322.9787	1353.0819	1478.2436
1508.7173	1612.2257	1638.8824
1988.9682	3202.8066	3213.5662
3220.9948	3230.0795	3233.7590

C₂H₄

C	0.000000	0.662198	0.000000
C	0.000000	-0.662198	0.000000
H	0.923912	1.231530	0.000000
H	-0.923912	1.231530	0.000000
H	-0.923912	-1.231530	0.000000
H	0.923912	-1.231530	0.000000

Frequencies

840.2909	984.0439	992.4718
1073.0004	1241.7128	1388.2692
1471.4635	1715.7398	3140.3746
3160.4646	3221.8080	3248.2257

Intermediates

il

C	-1.345863	-1.218640	-0.097181
C	-2.724791	-1.085054	-0.165984
C	-3.311753	0.172143	-0.080525
C	-2.512000	1.298743	0.074572
C	-1.132521	1.172022	0.145076
C	-0.534148	-0.089709	0.058832
C	0.889930	-0.223165	0.129383
C	2.085702	-0.334561	0.190216
C	3.541162	-0.453452	0.251222
C	4.264130	0.664349	-0.425751
H	-0.883731	-2.196293	-0.164903
H	-3.343690	-1.966869	-0.286827
H	-4.389445	0.274657	-0.136511
H	-2.965358	2.281081	0.142622
H	-0.505287	2.047181	0.266567
H	3.832079	-1.418979	-0.193219
H	3.852809	-0.522485	1.302344
H	5.332438	0.772288	-0.286977
H	3.751089	1.313369	-1.122262

Frequencies

40.6883	71.4505	89.9451
157.4300	180.5943	254.7042
366.0796	396.2745	413.9126
442.6408	506.7196	552.1792
580.1497	643.2804	712.5823
713.0481	782.3346	862.7401
867.3673	922.0025	946.0055
1000.5798	1018.7924	1023.2238
1048.8582	1066.4048	1096.7857
1111.9453	1188.7094	1196.9174
1207.8522	1285.7189	1316.7141
1355.2746	1360.4162	1451.7355
1458.0067	1488.6045	1542.5515
1647.6796	1680.4070	2383.2052
2979.4729	3028.0559	3169.7797
3192.4475	3202.8730	3211.3198
3221.1806	3225.9686	3288.3395

i25

C	0.845540	1.163339	0.000041
C	2.232917	1.233897	0.000030
C	2.989693	0.069617	-0.000012

C	2.352111	-1.168258	-0.000041
C	0.968885	-1.240938	-0.000019
C	0.197681	-0.073315	0.000021
C	-1.254981	-0.141701	0.000034
C	-2.203901	-1.078044	0.000109
C	-3.414840	-0.181048	-0.000003
C	-2.329091	0.947826	-0.000094
H	0.257044	2.074869	0.000065
H	2.723265	2.200828	0.000052
H	4.072334	0.123800	-0.000021
H	2.939041	-2.079873	-0.000091
H	0.469511	-2.203698	-0.000036
H	-4.039576	-0.221847	0.893831
H	-4.039532	-0.222023	-0.893860
H	-2.343063	1.569754	-0.899335
H	-2.343106	1.569948	0.899010

Frequencies

61.4799	106.5777	135.7041
237.4640	360.2704	403.9223
416.1258	461.3321	555.3573
636.8058	697.9122	716.2066
778.5753	826.9229	867.6962
868.9957	901.3179	945.9109
1000.9335	1005.7244	1022.0071
1023.8635	1029.6241	1055.9982
1072.0197	1072.1416	1115.5638
1160.7746	1164.8641	1187.7593
1209.0196	1234.3647	1298.6691
1333.9115	1359.3664	1465.6853
1489.4077	1493.6298	1538.6702
1652.0319	1678.0117	1713.2018
3048.5303	3081.6494	3114.7638
3139.0344	3183.0009	3188.3038
3197.3611	3205.2920	3215.5185

i107

C	1.394049	-1.226542	-0.000633
C	2.769357	-1.066350	0.003575
C	3.329645	0.207793	0.004346
C	2.502134	1.327130	0.000617
C	1.125453	1.179273	-0.003747
C	0.547890	-0.103044	-0.004131
C	-0.855427	-0.260348	-0.006595
C	-2.075478	-0.402616	-0.004363
C	-3.427807	-0.545679	-0.001504

C	-4.380939	0.607183	0.005118
H	0.953486	-2.216336	-0.000981
H	3.410869	-1.940336	0.006405
H	4.406778	0.328611	0.008044
H	2.935382	2.320867	0.001289
H	0.477566	2.047786	-0.006347
H	-4.980678	0.611654	0.923006
H	-3.838057	-1.551102	0.007958
H	-5.084513	0.538473	-0.831835
H	-3.854088	1.559585	-0.063640

Frequencies

51.3850	65.9619	71.4690
100.6108	187.7647	254.9682
383.6860	411.8541	419.4212
505.6448	525.9694	585.4743
618.2989	640.6454	703.3719
726.6233	772.4583	859.3004
920.6969	933.7061	997.9663
1013.6249	1015.5695	1017.1927
1055.5888	1096.0126	1111.9968
1131.8366	1186.7226	1204.3442
1303.3904	1313.3084	1353.8609
1411.2604	1444.2912	1480.3958
1484.7517	1503.4050	1547.6931
1631.6075	1656.0961	2081.7768
3027.1737	3081.1471	3143.2596
3182.2358	3190.8136	3200.0693
3210.2550	3220.8978	3225.6844

i26

C	1.022098	1.140637	0.386313
C	2.371329	0.819758	0.456881
C	2.810669	-0.442202	0.076792
C	1.890817	-1.382619	-0.371333
C	0.542439	-1.061703	-0.442482
C	0.092796	0.204854	-0.068659
C	-1.359040	0.557086	-0.151650
C	-2.268644	-0.389437	0.178019
C	-1.758347	1.829631	-0.564457
C	-3.142351	-1.291494	0.502632
H	0.683211	2.120146	0.705238
H	3.080599	1.556355	0.817232
H	3.863993	-0.692103	0.133426
H	2.224766	-2.369893	-0.670351
H	-0.172836	-1.796221	-0.796075

H	-1.028311	2.559864	-0.888467
H	-2.807257	2.092287	-0.603261
H	-3.517993	-1.383970	1.520490
H	-3.536764	-1.993534	-0.230562

Frequencies

49.4040	107.4429	143.3186
200.5035	246.6933	362.8649
417.3543	423.9670	487.3812
500.6977	534.0033	596.8835
634.6479	641.0395	719.4051
736.0245	747.0760	793.8667
870.1824	903.5490	936.3020
949.3271	982.9754	1002.1661
1020.9001	1024.7231	1060.6319
1113.9945	1125.1130	1188.6310
1215.0439	1230.3733	1331.2101
1345.5440	1360.3434	1450.2173
1485.6840	1500.3791	1545.4484
1656.4615	1682.0600	1926.1143
3096.7613	3168.6334	3173.4616
3187.5649	3193.4443	3203.4932
3210.3435	3219.8090	3280.3077

i27

C	1.119620	1.180928	-0.202449
C	2.472023	0.869944	-0.153955
C	2.897263	-0.437844	0.061573
C	1.954383	-1.454540	0.226620
C	0.636206	-1.085543	0.168879
C	0.142550	0.188642	-0.022653
C	-1.315672	0.462781	-0.041118
C	-2.180192	-0.662413	-0.458989
C	-1.823166	1.649734	0.304102
C	-3.347727	-0.964954	0.100170
H	0.808029	2.201063	-0.401518
H	3.205048	1.655450	-0.297110
H	3.956064	-0.670337	0.095668
H	2.258112	-2.482063	0.392370
H	-1.796820	-1.282540	-1.266125
H	-1.196512	2.454721	0.670535
H	-2.886912	1.841616	0.228461
H	-3.733350	-0.404338	0.945724
H	-3.945390	-1.793972	-0.261094

Frequencies

50.3484	93.0086	127.7086
204.7911	305.4297	348.9540
392.3076	426.7500	463.6820
526.4050	629.6392	633.1027
679.0168	736.2501	762.4126
775.4407	783.6141	878.4800
916.3161	945.8850	968.5859
968.8605	994.2404	1006.0303
1031.1424	1053.2405	1094.0572
1129.7017	1139.0224	1186.6351
1241.6793	1313.3773	1326.0023
1342.9640	1438.8850	1451.3478
1464.8520	1495.9702	1605.7998
1666.6482	1706.2406	1723.1431
3157.4022	3167.7379	3173.0977
3187.5248	3197.0994	3206.6375
3215.9283	3250.5561	3258.4217

i28

C	0.891041	1.112767	0.539892
C	2.251748	0.831784	0.583456
C	2.757770	-0.326398	0.004199
C	1.890392	-1.222383	-0.626317
C	0.560971	-0.891713	-0.637189
C	-0.007394	0.241265	-0.093819
C	-1.459399	0.549331	-0.186163
C	-2.448646	-0.492844	0.132152
C	-1.866687	1.768901	-0.554324
C	-2.195134	-1.700837	0.629705
H	0.504175	2.009638	1.012684
H	2.922598	1.521611	1.082268
H	3.820436	-0.539705	0.043159
H	2.260359	-2.132479	-1.085122
H	-3.481634	-0.208136	-0.054359
H	-2.922353	2.010782	-0.614290
H	-1.161583	2.548727	-0.817402
H	-3.002712	-2.393459	0.836396
H	-1.187261	-2.036221	0.847117

Frequencies

50.5681	117.7444	134.0627
189.2279	270.8664	359.4772
427.0605	440.9197	498.0399
525.8111	599.7893	633.6418
689.0911	736.5130	740.3001
776.0642	792.9438	875.6975

921.5071	945.9407	964.9528
967.2489	995.9386	1008.6619
1035.1721	1052.9426	1065.6636
1134.3131	1161.4412	1185.1189
1254.0032	1324.2900	1338.0211
1362.2374	1433.5838	1450.7516
1468.7992	1495.1580	1605.9664
1665.5470	1682.6322	1734.8643
3153.5494	3156.5864	3167.2718
3183.2484	3190.1032	3200.5367
3213.2486	3247.4491	3250.2095

i29

C	-0.739393	-1.477716	-0.000058
C	-2.103047	-1.206715	-0.000044
C	-2.565463	0.107330	0.000026
C	-1.669531	1.172724	0.000052
C	-0.310713	0.903583	0.000024
C	0.154305	-0.414625	-0.000001
C	1.637075	-0.406426	-0.000015
C	2.036583	0.929595	-0.000072
C	2.454711	-1.518029	0.000060
C	0.858585	1.856008	-0.000005
H	-0.385229	-2.503039	-0.000149
H	-2.814859	-2.024543	-0.000074
H	-3.632392	0.300358	0.000046
H	-2.033761	2.194906	0.000091
H	3.066068	1.263622	-0.000136
H	3.532717	-1.412094	-0.000030
H	2.046210	-2.521041	0.000415
H	0.851262	2.513748	-0.878720
H	0.851317	2.513700	0.878755

Frequencies

136.3047	189.4945	239.5075
263.2066	410.7532	458.7483
466.4354	508.7321	541.4524
566.0077	611.0631	669.7883
706.3354	732.0947	754.9153
763.1824	790.8442	849.1698
879.4536	927.2943	952.6808
967.7389	1006.7270	1018.2367
1058.2681	1108.3191	1154.3506
1163.1007	1187.1174	1223.5284
1241.3556	1256.5336	1330.3493
1353.3452	1404.2330	1414.6188

1446.8792	1503.6229	1516.2330
1534.3172	1660.0262	1688.5872
3027.7871	3055.9345	3167.7455
3187.4879	3194.2203	3205.2099
3219.2169	3225.9019	3265.7747

i30

C	0.767364	-1.466595	0.000003
C	2.128143	-1.179499	0.000016
C	2.579526	0.150730	0.000004
C	1.690662	1.205127	-0.000015
C	0.304082	0.931331	-0.000017
C	-0.144881	-0.421864	-0.000019
C	-1.611099	-0.440100	-0.000009
C	-2.070467	1.012541	0.000020
C	-2.407867	-1.509841	-0.000009
C	-0.794749	1.799484	-0.000001
H	0.427712	-2.496923	0.000016
H	2.850464	-1.987497	0.000048
H	3.646136	0.346897	0.000004
H	2.045292	2.229858	-0.000019
H	-2.689055	1.232674	-0.878746
H	-3.487484	-1.408779	0.000030
H	-2.005135	-2.516679	-0.000042
H	-2.688994	1.232655	0.878831
H	-0.743222	2.879898	0.000034

Frequencies

87.9455	174.1895	243.9669
271.5666	397.0393	464.6546
464.7829	537.8253	548.9594
555.5000	593.4712	674.1077
688.7714	752.2330	760.9315
786.5686	868.2032	879.2624
888.4220	909.1195	931.6947
956.3228	991.8804	1008.1789
1043.7491	1105.7666	1141.0326
1157.0716	1164.5601	1205.9258
1251.0689	1287.6237	1322.1123
1338.2531	1390.7768	1445.8481
1451.3538	1464.5590	1520.1417
1610.5238	1632.6880	1713.4951
3030.3993	3059.6714	3159.4709
3189.5223	3194.6314	3207.7982
3221.0112	3235.5874	3246.7456

i19

C	-2.545399	0.206100	0.152356
C	-2.154539	-1.113188	-0.062239
C	-0.810414	-1.434044	-0.245323
C	0.125979	-0.416959	-0.212027
C	-0.264737	0.909907	0.010850
C	-1.603996	1.230404	0.192296
C	1.629485	-0.481656	-0.373088
C	2.016640	0.982674	-0.207298
C	0.939940	1.746129	0.010245
H	-3.595712	0.435452	0.293689
H	-2.903284	-1.896856	-0.085735
H	-0.505961	-2.462832	-0.407000
H	-1.911772	2.256263	0.363645
H	1.884022	-0.802178	-1.392117
H	3.043951	1.318788	-0.257455
H	0.940135	2.818335	0.161759
C	2.307166	-1.368767	0.617488
H	3.243941	-1.856811	0.378315
H	1.963928	-1.373765	1.645339

Frequencies

108.5501	137.3659	167.5256
265.7176	288.4505	408.6356
433.4271	510.6967	549.6100
560.3516	588.3160	621.8364
734.3390	753.4957	769.1912
790.7654	816.1190	876.1648
907.3521	964.8548	976.5198
987.5906	1010.4964	1018.7193
1051.7045	1086.7011	1117.0660
1143.4320	1181.0462	1192.0933
1215.2460	1233.4065	1297.5186
1315.2803	1349.5289	1388.4510
1453.2231	1507.5479	1509.6695
1634.8496	1670.9122	1688.8449
3041.5305	3157.1850	3190.3078
3197.0856	3207.6934	3216.8968
3220.2904	3242.4242	3271.4330

i21

C	-1.422576	1.347642	0.117323
C	1.468354	-0.921612	-0.340991
C	-1.069897	-1.441512	-0.143444
C	-2.342805	-0.890312	0.030419
C	-2.509545	0.490769	0.164329

C	-0.137538	0.809388	-0.079142
C	1.118848	1.442070	-0.197529
C	2.177661	0.422669	-0.339127
C	2.347768	-0.541824	0.827807
C	0.023114	-0.601682	-0.193530
H	-1.558684	2.418979	0.215972
H	3.044749	0.611043	-0.960637
H	1.785936	-1.732545	-0.984867
H	-0.946577	-2.515150	-0.237645
H	-3.209417	-1.540656	0.065184
H	-3.505721	0.896240	0.302736
H	1.295596	2.508378	-0.155454
H	3.303616	-1.046072	0.909199
H	1.870200	-0.293788	1.768824

Frequencies

157.0211	179.5436	346.0895
379.4315	405.7589	454.0335
532.8004	574.0139	596.6209
629.8181	707.6991	766.5738
768.0599	781.2244	806.0281
848.7460	881.9285	888.7611
914.1291	960.6685	991.1848
1005.0679	1011.1676	1045.8661
1054.3991	1067.1397	1093.0902
1134.4117	1171.8963	1183.0258
1201.0450	1224.0659	1273.1698
1320.3356	1352.3511	1365.3637
1400.7079	1473.2181	1490.6056
1516.3411	1621.1964	1642.0189
3144.1423	3184.5249	3190.7351
3192.7689	3199.4789	3203.5240
3213.7273	3235.7252	3240.9670

i24

C	1.283668	1.388010	0.000017
C	2.486486	0.693123	-0.000001
C	2.480440	-0.708192	-0.000019
C	1.290284	-1.399184	-0.000013
C	0.045050	-0.714290	0.000011
C	0.064979	0.717528	0.000019
C	-1.203319	1.430367	0.000008
C	-2.379604	0.796678	-0.000026
C	-2.492414	-0.697565	-0.000008
C	-1.174336	-1.394912	0.000032
H	1.286492	2.473756	0.000010

H	3.426463	1.232327	-0.000008
H	3.419623	-1.250181	-0.000044
H	1.287257	-2.484439	-0.000016
H	-3.304303	1.364890	-0.000062
H	-3.090725	-1.020660	-0.867772
H	-3.090787	-1.020648	0.867718
H	-1.169448	2.515879	-0.000008
H	-1.171968	-2.480305	0.000060

Frequencies

112.4482	170.7736	250.1623
360.4332	392.8512	455.8980
500.3201	507.5132	543.8828
616.9063	672.3312	698.2719
759.4651	762.2901	789.9630
790.5593	867.7925	912.2476
926.6007	932.5825	953.5834
990.2184	1005.8169	1047.3480
1064.1666	1148.6144	1165.0778
1183.5253	1197.2030	1209.2784
1250.6573	1298.9099	1342.1915
1375.6978	1418.8875	1442.7992
1451.9968	1468.6649	1518.7430
1592.3826	1632.6732	1717.1351
2969.8156	2975.2340	3176.5657
3185.9324	3189.4531	3191.5868
3199.2068	3205.3327	3220.3949

i2

C	1.205900	-1.222666	0.085440
C	2.568669	-1.207152	-0.120481
C	3.262539	0.000866	-0.225839
C	2.567433	1.208142	-0.120081
C	1.204651	1.222190	0.085834
C	0.476828	-0.000631	0.194537
C	-0.877389	-0.001200	0.394665
C	-2.167958	-0.000560	0.585076
C	-3.168754	-0.000219	-0.490314
C	-4.481336	0.000707	-0.270737
H	0.669139	-2.160187	0.167153
H	3.104901	-2.146072	-0.202142
H	4.333694	0.001448	-0.388634
H	3.102705	2.147635	-0.201423
H	0.666920	2.159127	0.167860
H	-2.559200	-0.000348	1.606347
H	-2.783164	-0.000734	-1.505988

H	-5.191912	0.001013	-1.088564
H	-4.886587	0.001263	0.736779

Frequencies

26.2751	57.1538	120.4206
182.5064	191.7777	333.3949
357.7504	410.6631	477.5464
537.0903	580.2279	629.1343
639.1082	688.6138	760.4569
784.1091	832.7685	862.2372
906.8512	938.1098	949.5170
989.6479	990.2006	1005.4543
1031.9117	1044.7452	1110.1958
1129.6896	1176.4739	1178.1850
1216.9525	1301.4324	1301.5799
1330.8752	1349.7460	1455.2580
1468.5828	1498.6797	1587.5195
1614.7875	1712.1421	1895.1082
3085.0672	3157.8262	3184.6623
3193.3015	3199.4244	3213.9800
3218.9233	3225.5610	3252.0521

i3

C	0.945984	1.150939	-0.457453
C	2.246888	1.230984	-0.003168
C	2.921916	0.087450	0.426520
C	2.275524	-1.149134	0.397473
C	0.974932	-1.253472	-0.052632
C	0.269443	-0.098854	-0.488134
H	0.421144	2.037865	-0.792048
H	2.746296	2.193091	0.019851
H	3.943306	0.159786	0.781095
H	2.797062	-2.038834	0.732310
C	-1.025987	-0.193158	-0.963093
C	-2.333119	-0.205435	-0.967474
C	-3.192005	-0.001363	0.220929
C	-2.765814	0.336487	1.435416
H	0.472029	-2.212825	-0.075710
H	-2.854402	-0.380481	-1.908879
H	-4.256061	-0.144998	0.052250
H	-1.712835	0.497016	1.645837
H	-3.463121	0.462715	2.254993

Frequencies

26.5450	47.7828	90.5056
174.7614	213.6633	329.0934

407.1881	438.4007	482.8425
548.9882	620.4186	633.8160
641.1552	686.6213	756.8650
771.0031	835.4876	857.9095
905.4988	941.3853	967.5081
987.7781	995.8302	1000.8934
1045.7898	1048.5013	1081.8888
1112.0672	1165.3529	1181.2644
1215.5626	1304.4424	1345.0736
1352.2721	1353.1136	1449.5153
1473.7070	1501.5911	1599.1272
1622.7720	1709.6856	1855.0554
3121.0956	3155.4358	3175.5537
3194.2392	3201.5954	3213.5307
3220.4465	3226.1428	3251.1220

i8

C	0.462095	-0.471135	-0.055394
C	0.599177	0.916097	-0.159035
C	1.850785	1.506494	-0.092245
C	2.989366	0.723964	0.079308
C	2.864002	-0.654677	0.183826
C	1.609120	-1.246876	0.116184
C	-0.859147	-1.132439	-0.122169
C	-2.006927	-0.532064	-0.272299
C	-3.182854	0.107716	-0.424182
C	-3.977817	0.572771	0.617828
H	-0.286790	1.528533	-0.290815
H	1.942381	2.583686	-0.175553
H	3.967025	1.189056	0.132352
H	3.744817	-1.272475	0.317993
H	1.515022	-2.324997	0.199497
H	-0.849936	-2.220203	-0.032514
H	-3.526658	0.263627	-1.445806
H	-3.678756	0.437811	1.649793
H	-4.913906	1.075860	0.414118

Frequencies

32.4631	61.6545	147.5847
176.4166	274.7095	307.9799
401.0141	415.6961	505.0897
537.6101	570.4492	623.6466
639.3448	713.8345	756.0617
763.8331	817.3230	840.3392
867.2973	942.0097	944.4236
951.9174	998.6180	1018.5770

1024.3115	1061.6573	1085.9198
1118.8319	1188.8488	1193.2817
1210.1997	1223.3138	1295.1701
1344.9341	1363.8044	1411.2279
1494.8386	1501.9738	1542.3393
1657.9584	1680.0209	1921.1893
3109.5471	3146.7650	3172.7249
3184.1392	3190.4168	3202.3288
3210.1763	3221.6753	3278.2823

i4

C	0.382724	0.148582	-0.018059
C	1.207730	1.273479	0.081585
C	2.590309	1.150787	0.088741
C	3.177822	-0.103419	-0.011831
C	2.370815	-1.231327	-0.124545
C	0.990407	-1.107362	-0.132604
C	-1.073873	0.332230	-0.005129
C	-1.993490	-0.614929	0.212233
C	-3.443514	-0.385608	0.194738
C	-4.070924	0.636142	-0.343196
H	0.753549	2.255911	0.161561
H	3.209200	2.037238	0.170391
H	4.257172	-0.203845	-0.010215
H	2.822497	-2.212578	-0.218094
H	0.379323	-1.995559	-0.247309
H	-1.421170	1.350988	-0.166366
H	-1.682070	-1.630321	0.440481
H	-5.093384	0.965297	-0.456300
H	-4.053145	-1.158578	0.674250

Frequencies

28.8474	70.9172	128.6632
170.5186	224.2665	294.1014
409.0222	415.8253	485.5045
523.9300	631.0975	637.1571
652.0164	712.0540	771.0241
824.2021	834.9319	865.9053
901.2962	908.7470	946.5309
999.9543	1009.8462	1018.8719
1023.2167	1031.8952	1066.7062
1118.3429	1188.6417	1216.5660
1239.3576	1266.7407	1313.6448
1343.3359	1353.2694	1369.8514
1494.1325	1545.6855	1651.7033
1657.5186	1681.7848	1722.2159

3068.8190	3163.0345	3181.5161
3184.3183	3190.1753	3202.3798
3211.6823	3219.8842	3266.8551

i5

C	0.000000	0.689333	0.000000
C	0.608118	1.957926	0.000000
C	1.989429	2.100733	0.000000
C	2.818868	0.984798	0.000000
C	2.254830	-0.294529	0.000000
C	0.888828	-0.369647	0.000000
C	-1.463377	0.586132	0.000000
C	-2.228254	-0.516084	0.000000
C	-1.782729	-1.901104	0.000000
C	-2.622467	-2.936757	0.000000
H	-0.025418	2.840081	0.000000
H	2.422982	3.094027	0.000000
H	3.897008	1.101182	0.000000
H	2.878756	-1.181358	0.000000
H	-1.974786	1.544923	0.000000
H	-3.306350	-0.371700	0.000000
H	-0.710076	-2.081540	0.000000
H	-2.262530	-3.958775	0.000000
H	-3.699055	-2.791639	0.000000

Frequencies

35.3229	104.4357	116.3847
169.4628	271.7674	355.3286
374.1476	419.7996	521.7080
523.4814	630.2303	659.6829
717.9908	725.2800	763.9428
812.0068	830.1886	875.6822
947.6340	957.4937	961.7484
994.5459	1004.0824	1011.1910
1047.5367	1057.6847	1130.1382
1156.0217	1183.3768	1227.6541
1256.0118	1303.3240	1324.6528
1333.6981	1411.8105	1457.3053
1482.8200	1498.7396	1602.5449
1664.6804	1682.4864	1738.2879
3143.2537	3149.8784	3156.1019
3174.8013	3178.1852	3186.8778
3199.5856	3213.3491	3241.8447

i6

C	0.902564	1.227958	0.000185
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C	2.284529	1.190352	0.000125
C	2.958288	-0.030386	-0.000067
C	2.230134	-1.217577	-0.000179
C	0.846387	-1.189778	-0.000091
C	0.148776	0.035070	0.000067
C	-1.272449	0.055200	0.000079
C	-2.328586	-1.052034	0.000313
C	-3.304452	0.120167	-0.000128
C	-2.291723	1.044966	-0.000293
H	0.386700	2.182069	0.000342
H	2.846464	2.117861	0.000235
H	4.041858	-0.055093	-0.000137
H	2.748411	-2.170072	-0.000336
H	0.285090	-2.118178	-0.000186
H	-2.345251	-1.683844	0.893897
H	-2.345099	-1.684403	-0.892880
H	-4.383878	0.179928	-0.000311
H	-2.275106	2.128100	-0.000691

Frequencies

86.4943	96.7103	142.3937
244.3479	366.0382	412.0038
414.0259	452.5271	512.9851
631.7243	636.1646	698.3619
699.2137	769.4771	846.8540
890.8721	904.9600	916.7590
945.1194	989.6268	994.0189
999.2643	1006.3345	1006.3913
1054.7994	1073.2961	1097.6711
1125.9830	1161.7065	1182.6265
1205.4541	1216.0935	1306.3115
1327.9772	1361.1692	1395.6659
1458.2785	1486.4858	1509.8134
1557.3234	1624.9573	1646.0903
3050.4568	3099.8938	3188.3880
3192.3007	3204.1201	3210.2988
3217.1048	3222.1028	3250.8602

i7

C	-0.313957	-0.239850	-0.000017
C	-1.266995	-1.291429	0.000010
C	-2.623137	-1.035552	0.000027
C	-3.093941	0.277969	0.000017
C	-2.179413	1.330056	-0.000012
C	-0.819039	1.085621	-0.000030
C	1.066626	-0.552080	-0.000023

C	2.183069	0.396704	-0.000070
C	3.507473	0.008062	0.642460
C	3.507540	0.007915	-0.642367
H	-0.910032	-2.316509	0.000014
H	-3.326193	-1.861344	0.000052
H	-4.159065	0.477848	0.000036
H	-2.537397	2.353980	-0.000016
H	-0.133514	1.924220	-0.000051
H	1.339255	-1.605077	0.000011
H	1.920218	1.452880	-0.000202
H	3.998606	-0.175064	1.582564
H	3.998770	-0.175432	-1.582377

Frequencies

50.4357	79.3454	143.6653
206.6274	317.0834	399.0618
413.0953	427.4205	488.8250
599.3566	630.7811	649.5604
685.8274	697.0331	760.9824
788.2431	839.1783	861.3000
883.1767	902.5290	934.3951
986.1062	999.9611	1002.0238
1017.8256	1048.1381	1049.0326
1080.7971	1121.6576	1166.3501
1180.6806	1190.6876	1244.4432
1322.6124	1346.5614	1351.9588
1456.1750	1499.3831	1515.2501
1611.3296	1630.8673	1748.7298
3118.8343	3158.8548	3184.1980
3190.9933	3203.2154	3215.7567
3222.6975	3268.8885	3319.3717

i9

C	0.442822	-0.211589	0.000052
C	1.352222	-1.290669	0.000009
C	2.719061	-1.079843	-0.000044
C	3.229556	0.215618	-0.000048
C	2.350552	1.296466	0.000017
C	0.982464	1.092306	0.000073
C	-0.963101	-0.489104	0.000083
C	-2.002575	0.470371	-0.000105
C	-3.298434	0.162594	-0.000035
C	-4.560297	-0.142123	0.000009
H	0.962016	-2.303361	0.000006
H	3.394369	-1.928206	-0.000084
H	4.300408	0.382332	-0.000094

H	2.740298	2.308437	0.000032
H	0.323405	1.952675	0.000153
H	-1.257999	-1.533920	0.000227
H	-1.755096	1.529173	-0.000363
H	-5.110521	-0.275471	0.928557
H	-5.110496	-0.275813	-0.928505

Frequencies

63.6880	76.5767	104.4415
220.6014	232.6290	296.8828
381.1474	411.6689	496.9029
514.0467	555.7547	631.9250
638.4404	695.4492	745.4074
794.7323	847.4470	867.8900
901.4852	902.5112	917.4003
989.6346	995.7368	1007.5194
1008.0685	1052.6178	1069.6124
1110.3708	1178.7058	1186.8145
1197.0254	1243.2703	1303.2360
1338.7819	1358.7992	1433.4922
1474.3476	1506.2199	1524.0517
1628.2554	1645.5642	1973.8314
3120.6042	3159.6378	3181.1488
3188.0489	3194.6844	3197.1348
3204.3885	3212.1761	3222.5905

il0

C	-0.424628	0.150415	-0.064722
C	-1.054132	-1.074515	0.068496
C	-2.400083	-1.295720	0.149385
C	-3.231207	-0.170388	0.092586
C	-2.669970	1.093468	-0.041190
C	-1.291329	1.253701	-0.119096
C	1.027767	0.327699	-0.143297
C	1.923710	-0.665218	-0.146389
C	3.375668	-0.478926	-0.195314
C	4.040461	0.533132	0.360106
H	1.562522	-1.691854	-0.133854
H	-2.815583	-2.291734	0.255325
H	-4.307118	-0.290718	0.154760
H	-3.312074	1.965601	-0.084419
H	-0.865885	2.247544	-0.223295
H	1.375940	1.355228	-0.221074
H	3.936866	-1.252601	-0.714718
H	3.531294	1.297103	0.939279
H	5.116497	0.619529	0.264608

Frequencies

43.3363	81.1987	113.3613
197.7469	224.7111	280.8740
404.2174	420.5542	490.2042
535.7623	620.9613	637.1575
673.9305	714.7180	758.4958
863.5839	872.6218	903.6178
955.7507	962.2586	985.7798
996.0580	1003.8358	1009.9002
1035.9906	1055.3793	1088.6874
1134.4609	1179.7270	1230.2876
1260.3928	1313.8746	1329.2904
1341.5294	1357.1665	1454.0643
1466.1829	1490.9181	1605.8418
1666.4059	1709.7108	1729.3166
3150.9678	3156.3590	3168.3885
3170.6198	3176.5428	3188.6038
3200.5657	3214.9457	3247.0116

iii

C	0.360092	-0.597858	0.000039
C	1.631783	-1.209834	-0.000057
C	2.793003	-0.459277	-0.000093
C	2.726317	0.931924	-0.000027
C	1.482884	1.556589	0.000076
C	0.315703	0.810983	0.000107
C	-0.800406	-1.443644	0.000062
C	-2.174234	-1.103271	0.000056
C	-2.764662	0.093011	-0.000024
C	-3.409912	1.220381	-0.000116
H	1.692887	-2.293597	-0.000112
H	3.756090	-0.957281	-0.000172
H	3.635438	1.522248	-0.000054
H	1.422288	2.639380	0.000137
H	-0.638714	1.319074	0.000190
H	-0.596769	-2.509828	0.000075
H	-2.863681	-1.945996	0.000116
H	-3.685464	1.716077	0.928084
H	-3.685485	1.715911	-0.928399

Frequencies

26.2195	125.5060	139.5444
231.2039	256.8305	306.1755
384.3649	411.9245	496.0026
529.4436	543.6408	634.2261

697.4401	718.6136	746.4164
790.8709	811.5543	843.8222
893.1841	926.4016	928.9139
986.4287	993.2077	996.7728
1009.1790	1015.7569	1061.7574
1123.9095	1158.9480	1185.7975
1208.2649	1255.3332	1330.0372
1360.6684	1389.3913	1442.9066
1472.2683	1507.8381	1532.8153
1632.3293	1651.7460	1959.2058
3117.6673	3147.8617	3184.6019
3188.8969	3192.4306	3193.7385
3205.5601	3218.0991	3250.4664

il2

C	-1.841285	1.104149	-0.478759
C	2.578745	-1.096625	-0.870066
C	-0.710963	-1.338784	0.564183
C	-2.046087	-1.256803	0.128582
C	-2.586053	-0.067079	-0.375564
C	-0.511054	1.020085	-0.049229
C	0.710136	1.715035	0.130027
C	1.390363	0.456341	0.709356
C	2.581039	-0.058623	-0.044495
C	0.022557	-0.185664	0.461392
H	-2.277274	2.014772	-0.871899
H	1.676771	-1.670929	-1.056296
H	3.479101	-1.400374	-1.392128
H	-0.306400	-2.265296	0.955616
H	-2.678647	-2.135690	0.183286
H	-3.622666	-0.064471	-0.695125
H	1.066005	2.717464	-0.063389
H	3.504054	0.496407	0.113232
H	1.634671	0.555929	1.774133

Frequencies

80.1150	116.4987	161.2558
259.9420	318.2344	398.1823
425.7971	492.9199	530.6705
550.1909	617.1772	626.8870
706.4850	740.1631	765.2426
840.9555	877.5188	889.6353
937.0113	958.3317	969.8034
995.8599	996.8710	1022.3337
1045.5291	1075.3332	1114.2453
1144.1719	1167.6256	1183.2627

1199.3482	1238.5587	1307.9580
1329.4279	1348.4142	1395.6689
1449.8893	1461.9203	1505.5315
1611.2048	1665.8602	1732.5477
3046.5458	3150.9940	3165.6700
3184.5577	3195.3022	3208.0131
3215.5994	3244.3190	3246.3159

il3

C	1.138243	-1.284812	0.000184
C	2.477670	-0.909497	-0.000004
C	2.822290	0.434952	-0.000168
C	1.820656	1.400967	-0.000148
C	0.486128	1.023047	0.000031
C	0.127867	-0.326766	0.000201
C	-1.323254	-0.735619	0.000338
C	-2.252351	-0.059559	-1.015110
C	-3.033790	0.486142	-0.000334
C	-2.252484	-0.058647	1.015042
H	0.874760	-2.338068	0.000322
H	3.250743	-1.669771	-0.000018
H	3.865350	0.730715	-0.000314
H	2.082099	2.453455	-0.000277
H	-0.292449	1.779055	0.000039
H	-1.407401	-1.827473	0.000821
H	-2.255991	-0.025310	-2.095644
H	-3.926672	1.099557	-0.000670
H	-2.256277	-0.023417	2.095544

Frequencies

37.6455	128.7244	136.1109
314.3176	319.8304	392.9103
418.0645	526.0567	529.1744
578.5066	638.8641	670.5239
718.3859	779.5277	841.3909
865.8048	918.1259	920.5966
928.7789	951.9252	963.6418
964.1454	997.9345	1015.1622
1023.6952	1064.4333	1115.7811
1150.0778	1180.9582	1187.3025
1202.3371	1216.6974	1232.5232
1305.0288	1333.4647	1356.9143
1382.8992	1462.6178	1499.5859
1546.8647	1659.7899	1683.6624
3069.2660	3177.8176	3184.6840
3197.0372	3206.4435	3207.2459

3217.2399	3242.3910	3255.9247
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il4

C	1.136119	-1.251276	-0.187730
C	2.475623	-0.913429	-0.023262
C	2.857062	0.412083	0.150372
C	1.885587	1.417230	0.159451
C	0.584802	1.019704	-0.003116
C	0.135426	-0.271728	-0.178877
C	-1.320821	-0.614633	-0.320534
C	-2.241106	0.435195	-0.916674
C	-3.002781	0.541565	0.171607
C	-2.208323	-0.465685	0.973436
H	0.854370	-2.290880	-0.329755
H	3.228969	-1.692700	-0.035160
H	3.903240	0.668855	0.276612
H	2.157431	2.458952	0.289599
H	-1.424143	-1.603214	-0.778951
H	-2.246539	0.911371	-1.890018
H	-3.881202	1.128771	0.411901
H	-2.736862	-1.374127	1.276929
H	-1.664788	-0.061181	1.830809

Frequencies

27.0534	111.2126	123.4362
283.6198	320.6557	378.5029
423.8505	544.9055	570.8475
633.9321	705.6523	720.5897
765.4421	819.1594	870.9910
876.8651	929.1236	939.3918
963.9803	969.7858	994.9181
1010.5376	1018.0233	1023.2990
1056.6853	1110.8196	1133.5709
1151.0404	1184.4556	1206.7692
1231.4824	1238.7000	1252.3695
1320.5819	1327.9887	1374.0523
1465.7818	1481.9401	1494.7701
1608.4892	1669.2578	1671.3789
3062.7958	3068.4273	3121.0336
3181.1845	3193.7845	3197.5543
3207.1175	3220.8504	3232.7068

il5

C	0.334211	0.531482	0.254460
C	1.418591	1.238375	-0.275213
C	2.632495	0.609727	-0.509781

C	2.791433	-0.737253	-0.203391
C	1.730569	-1.445612	0.346628
C	0.513770	-0.817169	0.577037
C	-0.941996	1.231665	0.492146
C	-2.177160	0.780108	0.237062
C	-2.518148	-0.487689	-0.420398
C	-3.741946	-0.955914	-0.522806
H	1.299149	2.290408	-0.513351
H	3.458577	1.171796	-0.930664
H	3.741225	-1.228392	-0.381403
H	1.852771	-2.491217	0.606106
H	-0.299406	-1.367312	1.036594
H	-0.852091	2.233028	0.906374
H	-3.016586	1.417217	0.500876
H	-1.698312	-1.051419	-0.864296
H	-4.736245	-0.660432	-0.214697

Frequencies

47.9510	88.4467	147.5377
199.7705	264.4742	323.0657
419.1024	430.8138	503.4107
523.6111	638.9048	677.0685
709.3839	725.7139	767.8013
799.8843	834.1181	856.6072
875.1425	913.1554	958.9807
1006.8441	1017.7751	1024.8453
1027.1958	1061.7422	1076.0098
1117.3217	1191.2845	1212.3181
1220.0577	1249.0262	1276.4527
1336.7776	1361.2192	1428.2134
1492.9340	1542.0917	1645.3634
1654.5143	1681.1985	1712.3006
3144.1085	3157.9035	3182.6763
3189.0013	3195.0954	3203.3793
3213.0094	3221.9710	3244.1206

il6

C	2.540011	0.106375	-0.081495
C	2.020634	-1.230632	-0.190271
C	0.708907	-1.501395	-0.018875
C	-0.204083	-0.415266	0.450451
C	0.319093	0.967132	0.158366
C	1.686879	1.190961	0.032831
C	-1.663878	-0.339244	0.030680
C	-1.943546	1.073094	-0.155722
C	-0.793064	1.813138	-0.075198

C	-2.514038	-1.363308	-0.110125
H	3.604663	0.266915	-0.203640
H	2.707099	-2.028811	-0.451833
H	0.321548	-2.508069	-0.132046
H	2.069818	2.201311	-0.069664
H	-0.240519	-0.497122	1.555799
H	-2.929360	1.464034	-0.372954
H	-0.726495	2.883515	-0.226053
H	-3.548990	-1.197564	-0.387124
H	-2.199251	-2.389347	0.043663

Frequencies

104.1669	173.9830	232.1649
308.6354	389.2392	443.5118
514.8261	516.9495	535.4041
607.0438	656.0039	693.2932
708.0058	727.7785	792.5515
826.0434	845.7819	858.0284
894.6507	935.8789	948.5363
968.0872	990.0227	995.9246
1020.7526	1049.5765	1076.9946
1132.2869	1166.7202	1215.3886
1234.4908	1242.5224	1298.6053
1333.6995	1366.8163	1400.7613
1431.3813	1451.3671	1517.4489
1536.0982	1640.2059	1684.4325
2905.7696	3162.3559	3185.6059
3189.8002	3205.9082	3217.5162
3218.0334	3237.7981	3250.9751

il7

C	0.069099	0.767410	0.086512
C	-1.195664	1.463949	-0.029349
C	-2.361220	0.796939	-0.100708
C	-2.392358	-0.660305	-0.085896
C	-1.280521	-1.373372	0.114854
C	0.042822	-0.722533	0.399610
C	1.258807	1.396908	-0.009880
C	2.514526	0.641522	0.028889
C	2.438937	-0.674904	-0.086739
C	1.209778	-1.474117	-0.281132
H	-1.173407	2.546703	-0.105019
H	-3.294593	1.336308	-0.214780
H	-3.339992	-1.160479	-0.253699
H	-1.311849	-2.459005	0.120255
H	0.226320	-0.803857	1.486995

H	1.301055	2.474063	-0.139941
H	3.459850	1.169878	0.097045
H	1.289727	-2.475586	0.149968
H	1.017646	-1.597010	-1.357786

Frequencies

116.5076	152.3444	279.6072
337.8675	408.5177	415.5212
466.9683	483.1596	515.8128
594.3302	652.9472	717.8878
746.4606	764.5010	803.3397
827.0005	908.4914	919.4710
954.4965	981.7565	991.4943
1001.4147	1011.4272	1049.0665
1070.3750	1088.7872	1170.8731
1185.1462	1211.3551	1227.6481
1267.2286	1292.9262	1323.8561
1341.4373	1387.2511	1413.5307
1463.1027	1476.6231	1599.5174
1644.3806	1702.7105	1733.6802
2940.4083	3010.1973	3093.9306
3178.0949	3180.3466	3184.8267
3194.2407	3200.9727	3216.3711

il8

C	1.483576	-1.272660	0.083749
C	2.679879	-0.570018	0.023899
C	2.682651	0.816801	-0.080701
C	1.468815	1.508245	-0.121904
C	0.321334	0.763298	-0.063956
C	0.242188	-0.612717	0.041391
C	-0.992684	-1.405782	0.083417
C	-2.265505	-1.022973	-0.091727
C	-2.807447	0.321491	-0.305582
C	-2.487326	1.416214	0.382722
H	1.499130	-2.355540	0.168412
H	3.619249	-1.109466	0.060767
H	3.619783	1.360779	-0.128055
H	1.443912	2.589720	-0.200720
H	-0.822331	-2.470709	0.221065
H	-3.006681	-1.818965	-0.120793
H	-3.576439	0.393937	-1.072616
H	-1.780212	1.387353	1.203899
H	-2.949290	2.371510	0.160188

Frequencies

41.3420	113.8391	128.9593
194.0852	224.3086	366.2973
412.9427	423.5210	495.1273
556.0444	625.9662	630.8651
716.1721	745.6631	772.6082
817.3519	823.7959	874.2508
955.8257	960.1797	973.6825
992.6864	1002.3096	1025.7488
1046.1198	1054.9574	1099.3602
1138.7913	1182.3156	1216.5733
1241.9260	1302.2247	1333.4056
1337.7612	1442.4051	1459.5567
1481.0722	1496.9824	1602.2052
1665.1896	1712.6376	1721.2438
3145.5019	3155.1401	3166.6379
3176.8713	3179.7610	3189.2187
3202.5860	3217.8578	3254.5851

i20

C	1.220391	-1.284859	-0.358653
C	2.445673	-0.671384	-0.571310
C	2.653094	0.637197	-0.146983
C	1.629960	1.320994	0.495558
C	0.398687	0.709221	0.698855
C	0.171242	-0.597084	0.260057
C	-1.115746	-1.283599	0.467814
C	-2.353933	-0.835463	0.217086
C	-2.783438	0.427323	-0.397936
C	-2.100579	1.536033	-0.579175
H	1.063457	-2.307712	-0.685992
H	3.243158	-1.215157	-1.065205
H	3.612391	1.115999	-0.307592
H	1.790094	2.333865	0.847681
H	-0.384717	1.236271	1.230001
H	-1.034825	-2.304442	0.835002
H	-3.167172	-1.524502	0.426639
H	-3.815205	0.415816	-0.766203
H	-2.299290	2.499589	-1.026214

Frequencies

34.8457	67.2445	116.2335
211.2960	231.0083	365.0804
419.6812	437.5942	498.8994
538.1895	637.1105	660.8501
706.1641	725.8571	755.1996
783.3422	812.5295	867.2899

878.0943	904.2960	961.5382
986.0905	1000.3544	1011.0681
1022.5138	1026.5113	1063.3440
1116.3799	1190.4810	1212.2558
1221.2246	1269.6671	1288.7234
1342.3600	1360.5867	1448.6583
1491.6389	1543.6152	1650.8178
1663.9887	1679.3778	1716.0340
3059.8229	3156.1054	3183.7002
3185.1463	3193.3797	3201.3521
3208.6819	3218.5979	3255.3108

i22

C	1.235713	-1.424222	0.029278
C	2.412346	-0.727389	-0.099857
C	2.400008	0.707884	-0.199584
C	1.266485	1.406196	-0.008342
C	0.000009	0.723011	0.425237
C	-0.000005	-0.762265	0.142668
C	-1.235733	-1.424211	0.029320
C	-2.412357	-0.727371	-0.099818
C	-2.400003	0.707898	-0.199598
C	-1.266454	1.406192	-0.008427
H	1.240105	-2.509006	-0.024128
H	3.349614	-1.258230	-0.217320
H	3.318563	1.222093	-0.460944
H	1.251388	2.487536	-0.100642
H	-0.000076	0.800823	1.540923
H	-1.240126	-2.508996	-0.024099
H	-3.349633	-1.258200	-0.217280
H	-3.318546	1.222120	-0.460977
H	-1.251340	2.487525	-0.100798

Frequencies

107.7030	151.9538	328.4130
347.2162	440.7623	467.9232
471.6819	518.5103	564.6763
610.0774	673.7756	687.9006
719.0919	775.5777	787.9625
803.0329	879.4914	923.2253
941.3933	967.3315	986.4372
990.0127	1002.9479	1005.3458
1081.8460	1083.7036	1084.8521
1171.0281	1182.7969	1188.3995
1215.4518	1259.5554	1273.6275
1330.1603	1361.4293	1406.9266

1428.2042	1477.0608	1519.9583
1536.9164	1666.8010	1667.2222
2766.1408	3179.6907	3181.6467
3182.7435	3184.8433	3202.6157
3203.4706	3218.2359	3219.1718

i23

C	1.292522	-1.389226	0.000074
C	2.479851	-0.683504	-0.000067
C	2.457667	0.710537	-0.000163
C	1.241494	1.379517	-0.000077
C	0.036030	0.686295	0.000090
C	0.052236	-0.725243	0.000133
C	-1.183414	-1.455506	0.000135
C	-2.414534	-0.785472	-0.000195
C	-2.490717	0.578043	-0.000247
C	-1.271875	1.443386	0.000308
H	1.304210	-2.474603	0.000143
H	3.426196	-1.212434	-0.000120
H	3.385782	1.270575	-0.000301
H	1.225716	2.465699	-0.000159
H	-1.149720	-2.538986	0.000281
H	-3.330070	-1.368021	-0.000493
H	-3.456429	1.071403	-0.000630
H	-1.300724	2.116242	0.870423
H	-1.300521	2.117163	-0.869087

Frequencies

85.7484	170.4013	249.4885
360.5168	428.0984	473.0299
489.5576	508.7781	541.1099
615.8392	652.9615	713.1920
753.4373	757.8847	792.2572
799.3637	875.2184	927.2674
939.0256	965.5215	970.5635
979.1856	1001.8662	1068.2459
1098.4388	1148.9622	1182.1522
1187.3789	1216.0358	1219.7733
1236.9906	1283.9622	1317.7709
1364.5099	1398.1524	1443.7483
1449.6148	1487.1125	1530.4176
1578.1875	1634.0190	1664.3835
2993.6372	3008.8562	3180.0262
3181.7029	3189.3254	3203.0534
3203.7867	3213.1571	3218.8766

i64

C	-0.913795	-1.275494	0.000022
C	-0.371785	1.138932	0.000036
C	-1.708071	1.411438	0.000004
C	-2.670597	0.380352	-0.000024
C	-2.241950	-0.960991	-0.000010
C	0.125824	-0.239263	0.000033
C	1.437866	-0.661326	-0.750644
C	2.480449	0.429180	-0.670026
C	2.480469	0.429161	0.670004
C	1.437884	-0.661346	0.750619
H	-0.594690	-2.313526	0.000027
H	0.353506	1.943065	0.000053
H	-2.038217	2.444959	0.000007
H	-3.727391	0.616709	-0.000043
H	-2.978880	-1.756967	-0.000019
H	1.415993	-1.520209	-1.408735
H	2.907934	1.081206	-1.421505
H	2.907964	1.081182	1.421481
H	1.416016	-1.520278	1.408646

Frequencies

82.8197	182.0521	217.3687
338.7573	377.5692	417.2518
440.3508	494.8455	608.7609
631.4815	690.7256	700.8810
739.4720	763.0611	784.9233
837.0874	841.0355	868.1242
901.0808	918.1094	953.9185
985.7856	988.5268	1000.4101
1014.3402	1019.3826	1031.4545
1084.6246	1112.8503	1154.4162
1188.6415	1204.9733	1207.4906
1272.7984	1316.0534	1330.5000
1341.0559	1438.2573	1473.2903
1565.2203	1613.6046	1621.8532
3175.4254	3186.5316	3200.3501
3201.5408	3211.7438	3216.4500
3219.3490	3227.5050	3239.2965

i65

C	1.235707	1.438843	-0.061045
C	2.461377	0.728255	-0.106231
C	2.461540	-0.688786	0.012238
C	1.313173	-1.422905	0.004483
C	0.020294	-0.753816	-0.318087

C	0.078299	0.737772	-0.160386
C	-1.278509	0.860765	0.489405
C	-1.264775	-0.719337	0.611224
C	-2.542972	-0.683522	-0.191278
C	-2.524192	0.642285	-0.353365
H	1.230292	2.500479	0.167985
H	3.402798	1.263913	-0.084008
H	3.413918	-1.192376	0.144133
H	1.341772	-2.501206	0.123897
H	-0.297649	-1.074040	-1.322975
H	-1.356208	1.521817	1.353556
H	-3.166910	-1.472668	-0.596131
H	-3.132956	1.332001	-0.926331
H	-1.194702	-1.215246	1.578131

Frequencies

116.1955	174.6834	287.2334
338.6518	372.6430	396.9051
511.9635	553.5489	610.9857
678.3610	708.8334	762.4595
780.2604	811.7758	854.1196
869.0308	895.5909	928.4683
941.0885	977.8517	984.2984
987.5336	995.5434	1012.6887
1062.0732	1070.9902	1109.5455
1132.7178	1160.1079	1166.1147
1179.8182	1206.7181	1223.9754
1242.4281	1289.7826	1326.9273
1341.4720	1389.4728	1433.0623
1553.4284	1626.4564	1652.8112
2971.3954	3116.9829	3143.6723
3175.8630	3178.4395	3195.9468
3196.6993	3217.2574	3228.6237

i66

C	0.000160	-0.576391	-1.253042
C	0.000160	-0.576391	1.253042
C	0.000160	-1.934294	1.222774
C	0.000136	-2.646467	0.000000
C	0.000160	-1.934294	-1.222774
C	0.000065	0.263728	0.000000
C	-1.176157	1.228743	0.000000
C	-0.734518	2.492557	0.000000
C	0.733898	2.492802	0.000000
C	1.175962	1.229135	0.000000
H	0.000178	-0.036247	-2.193822

H	0.000178	-0.036247	2.193822
H	0.000185	-2.485681	2.157270
H	0.000116	-3.729361	0.000000
H	0.000185	-2.485681	-2.157270
H	-2.201450	0.884834	0.000000
H	-1.349171	3.383795	0.000000
H	1.348254	3.384246	0.000000
H	2.201374	0.885580	0.000000

Frequencies

58.4033	116.2008	206.7306
362.2169	372.1922	423.9053
513.1293	593.3098	598.5247
598.6245	665.8072	668.5733
742.9352	766.2853	789.6496
807.4471	811.9956	850.5723
955.9485	976.1018	979.6249
979.9028	981.8012	995.7566
999.3409	1059.5552	1080.6733
1082.8147	1131.0066	1141.3374
1152.4003	1211.9488	1257.0422
1295.5746	1325.5966	1391.7009
1395.6308	1454.2887	1555.0850
1588.2505	1621.0137	1668.6670
3184.8470	3186.7625	3205.4680
3206.6081	3207.6871	3219.3823
3225.1641	3244.6874	3249.6641

i67

C	-0.851540	1.414007	0.214161
C	-0.125367	-0.949467	-0.540185
C	-1.548034	-1.257892	-0.502699
C	-2.458229	-0.407010	0.010979
C	-2.107003	0.954917	0.357507
C	0.271450	0.528453	-0.103014
C	0.632805	-0.663727	0.755978
C	2.100351	-0.768086	0.673950
C	2.592292	0.209300	-0.180857
C	1.557644	1.008936	-0.648794
H	-0.634321	2.471152	0.325183
H	0.468011	-1.399313	-1.329913
H	-1.869020	-2.194967	-0.946131
H	-3.503496	-0.693808	0.045287
H	-2.901795	1.639126	0.632687
H	0.094704	-0.864499	1.675052
H	2.682278	-1.525703	1.180886

H	3.631841	0.316803	-0.462936
H	1.645587	1.834620	-1.342263

Frequencies

173.5193	213.2582	245.1610
343.2876	399.2940	447.7006
526.6847	553.1888	599.3802
631.1116	658.6932	686.7694
707.1532	771.6756	788.3702
819.2964	837.8794	906.8047
938.8059	948.5574	979.5723
988.7443	995.6384	1004.2105
1034.9000	1047.9460	1090.0483
1095.3318	1099.0443	1188.4459
1206.5733	1212.6834	1255.4012
1298.8976	1346.3110	1365.7388
1403.9542	1431.5546	1473.8847
1493.0074	1617.2181	1709.0886
3170.0821	3182.5672	3190.2447
3190.4168	3202.2400	3215.9088
3221.6726	3234.2100	3248.3629

i68

C	-1.338913	1.351848	0.003612
C	1.365667	-1.294822	-0.305513
C	-1.148284	-1.412398	-0.005600
C	-2.395517	-0.804230	0.100375
C	-2.490565	0.580363	0.100654
C	-0.087912	0.748511	-0.096535
C	1.157507	1.548282	-0.156882
C	2.300094	0.933242	0.069714
C	2.504325	-0.502610	0.368867
C	0.010064	-0.653772	-0.106646
H	-1.408209	2.434942	0.012393
H	1.567375	-1.335927	-1.383289
H	-1.075972	-2.495741	-0.012971
H	-3.289307	-1.412385	0.180606
H	-3.458704	1.061308	0.181843
H	1.084783	2.616952	-0.336533
H	3.471524	-0.863355	0.009310
H	2.490102	-0.647177	1.456679
H	1.359607	-2.325096	0.059680

Frequencies

131.0203	163.4462	272.0853
361.9905	379.9651	422.2461

482.7219	509.5685	541.0971
597.1255	696.4982	752.7792
757.7374	764.7157	814.3051
847.9683	896.5092	913.3988
947.6894	962.9599	1002.3716
1008.2003	1029.4373	1074.0635
1141.0778	1185.0268	1188.7578
1206.3063	1211.1932	1235.1768
1261.9098	1322.8074	1337.3999
1343.7810	1377.1397	1465.4690
1475.7725	1499.4586	1531.9909
1647.0924	1679.8851	1720.2106
3036.3522	3041.0303	3096.1932
3105.4502	3179.2639	3181.9277
3187.8610	3201.5853	3216.7498

i69

C	0.821399	-0.861796	-0.746875
C	0.821400	-0.861788	0.746884
C	1.854256	0.111108	1.139977
C	2.422300	0.665445	-0.000005
C	1.854256	0.111093	-1.139981
C	-0.423200	-0.286972	0.000007
C	-1.680070	-1.049368	0.000004
C	-2.706671	-0.175327	-0.000004
C	-2.170240	1.184734	-0.000005
C	-0.824550	1.131401	-0.000001
H	0.625200	-1.747561	-1.337094
H	0.625211	-1.747554	1.337107
H	2.083264	0.373117	2.163328
H	3.171154	1.447043	-0.000009
H	2.083278	0.373079	-2.163335
H	-1.737562	-2.129820	0.000003
H	-3.759163	-0.426250	-0.000001
H	-2.770256	2.085126	-0.000015
H	-0.134410	1.961645	-0.000002

Frequencies

126.6773	159.0578	178.6932
346.6259	362.6424	468.8989
577.7114	578.3127	609.4928
708.5248	723.9011	727.2688
748.0564	793.6502	804.8630
822.3165	830.8525	870.3497
912.5759	937.9159	947.8282
960.6316	960.8891	966.9309

1015.3578	1047.2566	1053.7339
1086.6948	1091.9909	1108.4423
1118.4925	1200.0681	1266.5969
1288.5588	1338.1637	1341.0075
1361.5459	1413.2229	1425.5602
1486.0801	1554.1253	1646.0529
3201.8361	3209.9155	3215.1111
3225.3221	3225.5471	3238.3498
3243.8289	3251.8437	3263.7354

i70

C	1.385522	-1.430256	0.022207
C	-1.164952	1.159930	-0.285227
C	1.351953	1.447434	0.022002
C	2.497775	0.748803	0.157692
C	2.514435	-0.704793	0.157838
C	0.123640	-0.743421	-0.125794
C	-1.139432	-1.201700	-0.271780
C	-2.083313	-0.036298	-0.379958
C	-3.126732	-0.007107	0.692143
C	0.107293	0.730980	-0.127307
H	1.411049	-2.514375	0.024446
H	-1.513964	2.183004	-0.318088
H	1.351518	2.531858	0.023837
H	3.441957	1.269789	0.272014
H	3.470249	-1.204090	0.272492
H	-1.461301	-2.233938	-0.298238
H	-2.565676	-0.044040	-1.368327
H	-4.101661	0.425340	0.504116
H	-2.829302	-0.194985	1.716861

Frequencies

84.6215	163.0496	203.9181
219.1886	305.6464	413.3058
449.8900	503.6882	523.1516
551.2633	574.4424	589.9567
705.2676	707.3911	744.2807
782.4806	812.9648	855.3557
859.4572	901.8056	909.2477
980.7986	991.5818	1000.2865
1018.1447	1047.2918	1105.5441
1142.1001	1186.4575	1190.7595
1204.4561	1218.9293	1259.8549
1305.0116	1405.5922	1410.0756
1451.3530	1463.4645	1582.3217
1617.0107	1651.3785	1735.3825

3031.5820	3156.4241	3187.6712
3197.0995	3210.7264	3218.1505
3235.9122	3240.2820	3270.7393

i71

C	0.725981	-0.826826	-0.000606
C	1.512389	-0.300232	1.175765
C	2.561321	0.407991	0.733896
C	2.561416	0.408998	-0.733154
C	1.512536	-0.298605	-1.176131
C	-0.688904	-0.339992	-0.000298
C	-1.856464	-1.101904	-0.000479
C	-2.932028	-0.213884	0.000038
C	-2.417364	1.149924	0.000559
C	-1.065465	1.080017	0.000365
H	0.733139	-1.924402	-0.001366
H	1.227674	-0.478363	2.203386
H	3.301102	0.903403	1.349539
H	3.301283	0.905248	-1.348019
H	1.227980	-0.475360	-2.204035
H	-1.910927	-2.180921	-0.000936
H	-3.980498	-0.482941	0.000062
H	-3.023680	2.044289	0.001010
H	-0.356582	1.896129	0.000628

Frequencies

50.1010	89.6927	118.6551
295.3928	315.4648	400.7846
521.6835	529.1808	551.3963
661.2776	696.7370	728.5520
741.9217	757.7991	818.9734
821.2239	839.2478	865.8560
904.4746	926.6882	943.2957
964.8373	970.4376	977.5441
1017.8860	1031.6084	1032.3392
1098.7911	1114.3054	1121.8730
1148.3778	1219.3991	1231.8935
1284.3266	1312.5106	1331.0798
1406.4135	1436.1417	1472.8065
1585.4956	1598.2426	1669.8610
3059.5573	3220.3805	3221.3715
3231.6482	3235.5936	3250.4825
3251.4501	3257.6637	3259.4276

i72

C	-0.694754	0.966098	0.430397
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C	-0.577036	-0.568877	0.729607
C	-1.892936	-1.137893	0.321210
C	-2.622650	-0.166489	-0.354169
C	-1.963216	1.050999	-0.368576
C	0.644184	0.785360	-0.251248
C	1.906256	1.141068	0.058654
C	2.741869	-0.057170	-0.029510
C	1.972023	-1.150179	-0.229586
C	0.565577	-0.703875	-0.407558
H	-0.682935	1.654534	1.279549
H	-0.196362	-0.833472	1.714719
H	-2.177950	-2.173244	0.453131
H	-3.584261	-0.341937	-0.821567
H	-2.320247	1.957069	-0.839489
H	2.229991	2.090389	0.466324
H	3.820495	-0.059551	0.074816
H	2.333131	-2.155143	-0.406026
H	0.102247	-1.092883	-1.316785

Frequencies

135.4081	164.6495	266.6090
318.5973	366.3500	506.1003
554.3413	636.4487	663.7517
682.5749	735.7432	762.8986
784.6116	810.9692	845.7030
858.9307	871.4058	889.6056
917.8812	968.1063	975.3328
980.6088	1015.7682	1027.6847
1036.2471	1066.1858	1094.4123
1110.9395	1129.4582	1166.0851
1182.7585	1189.8339	1245.3522
1269.2976	1290.5149	1321.7521
1333.1601	1385.7633	1401.6988
1476.6933	1567.6483	1663.8808
3085.5561	3113.3154	3147.4726
3207.4240	3207.9509	3223.3870
3233.5779	3237.4237	3244.0224

i73

C	-0.659491	0.050345	0.000015
C	-1.487452	1.165502	-0.000016
C	-2.860657	0.750992	-0.000026
C	-2.929755	-0.601775	-0.000005
C	-1.546362	-1.174131	0.000029
C	0.736772	0.025663	0.000014
C	1.571917	-1.155565	-0.000020

C	2.868718	-0.749214	-0.000026
C	2.901806	0.714747	0.000006
C	1.628176	1.176763	0.000029
H	-1.362322	-1.801751	-0.879366
H	-1.149549	2.193103	-0.000049
H	-3.705360	1.427483	-0.000041
H	-3.831926	-1.198073	0.000001
H	-1.362359	-1.801667	0.879494
H	1.211228	-2.174436	-0.000030
H	3.741557	-1.388245	-0.000057
H	3.802771	1.313135	0.000008
H	1.313933	2.210488	0.000043

Frequencies

99.7107	106.9230	156.0852
235.5678	386.7345	387.6362
444.8116	529.9976	561.8906
641.7537	703.2228	714.6615
767.0780	782.4091	817.7912
832.8873	845.2506	897.4196
911.0727	925.0061	933.4309
972.7773	977.7185	978.5324
1030.4096	1050.0864	1096.1032
1114.8471	1122.5350	1147.1448
1168.2644	1261.4076	1297.9642
1309.4906	1351.1942	1393.6105
1411.7255	1424.7150	1499.2359
1532.9620	1582.6382	1589.2545
3057.5138	3094.9504	3218.7028
3221.3470	3229.3609	3235.7425
3247.1151	3248.6122	3254.2812

i74

C	1.381531	1.424415	-0.000002
C	-1.223967	-1.213360	0.000047
C	1.387744	-1.393774	-0.000029
C	2.584598	-0.674990	-0.000006
C	2.576562	0.720584	0.000012
C	0.178002	0.709352	-0.000013
C	-1.178953	1.162325	0.000005
C	-2.059621	0.059020	-0.000004
C	-3.421646	0.098612	-0.000028
C	0.192362	-0.703056	-0.000029
H	1.377950	2.508916	0.000006
H	-1.436225	-1.826335	-0.881534
H	1.402610	-2.478807	-0.000041

H	3.530373	-1.204784	0.000003
H	3.517819	1.258897	0.000045
H	-1.491510	2.198866	-0.000001
H	-1.436109	-1.826017	0.881855
H	-4.013105	-0.809591	-0.000076
H	-3.951473	1.044090	0.000024

Frequencies

105.7625	194.3209	269.3983
274.4518	420.8864	448.6927
461.2861	492.0710	546.1825
600.5918	603.9570	670.9433
725.6218	747.4218	792.3266
816.2108	818.9222	872.4211
883.3225	894.8919	938.8130
970.9154	982.7901	999.5543
1047.4485	1127.3023	1170.8285
1176.4076	1191.5035	1208.0673
1230.5654	1286.1323	1333.8479
1352.5450	1384.6522	1410.0015
1447.9413	1490.0347	1517.6665
1551.7292	1639.3929	1658.7209
3060.6174	3100.7042	3157.8567
3189.8567	3196.5265	3208.3125
3220.0850	3221.4949	3253.8503

i75

C	-0.656493	-0.018787	0.000124
C	-1.528454	1.171480	-0.000117
C	-2.811113	0.793491	-0.000206
C	-2.901958	-0.705505	0.000008
C	-1.467796	-1.125922	0.000262
C	0.761713	-0.003815	0.000113
C	1.633460	-1.169177	-0.000127
C	2.914280	-0.728321	-0.000211
C	2.900658	0.737716	0.000023
C	1.605829	1.161789	0.000223
H	-1.164340	2.190081	-0.000305
H	-3.672444	1.447728	-0.000446
H	-3.439301	-1.087473	-0.877832
H	-1.138063	-2.155582	0.000483
H	-3.439620	-1.087223	0.877755
H	1.301995	-2.197299	-0.000277
H	3.806504	-1.339359	-0.000422
H	3.781607	1.365503	0.000065
H	1.262906	2.185923	0.000429

Frequencies

73.9798	109.8469	166.2102
261.3120	365.2336	389.7165
439.9013	551.0520	581.7665
642.6677	707.7028	714.1671
738.5017	741.1574	788.3954
811.8248	835.6513	906.6764
917.5854	924.6569	929.2483
948.7326	971.8532	987.9399
1003.0524	1051.7144	1082.5086
1105.6855	1129.5832	1132.4907
1152.9360	1254.6718	1298.1038
1306.3888	1353.5054	1386.9255
1425.8624	1454.4488	1495.4100
1526.7298	1583.5712	1653.4367
3040.2326	3070.4122	3219.9660
3224.4440	3231.3497	3241.2802
3248.3387	3253.0456	3258.2585

i76

C	0.645052	1.592793	-0.012076
C	0.447415	-1.536298	-0.260762
C	1.766851	-1.296688	-0.353075
C	2.471163	-0.117080	0.081281
C	1.971277	1.155996	0.204054
C	-0.490749	0.789338	-0.007332
C	-1.792096	1.150461	-0.338322
C	-2.667749	0.035205	-0.128448
C	-1.962291	-1.023115	0.336719
C	-0.514439	-0.647968	0.482666
H	0.497853	2.654315	-0.190987
H	0.044598	-2.439172	-0.709204
H	2.381445	-2.062474	-0.819591
H	3.545560	-0.227092	0.196044
H	2.702076	1.938382	0.390779
H	-2.093216	2.123485	-0.705023
H	-3.732972	0.046540	-0.320839
H	-2.353959	-2.001837	0.580782
H	-0.237996	-0.648014	1.549812

Frequencies

112.3959	151.5214	294.8917
313.2322	373.8157	382.4380
501.3214	551.7831	577.2442
608.9480	701.8556	712.3818

721.4221	787.5078	803.1380
821.7471	860.1615	880.4012
911.8927	950.7442	972.7443
977.5167	997.4721	1007.3411
1038.6111	1058.9549	1109.4493
1135.4370	1213.3372	1219.5572
1242.4859	1257.6557	1268.8939
1341.7288	1360.8297	1403.4071
1425.9102	1440.2796	1500.8758
1567.2747	1596.4376	1678.0177
2982.0364	3157.1775	3164.3711
3176.4024	3186.0947	3194.0718
3218.0536	3230.3119	3246.4671

i77

C	0.641705	1.593032	0.000035
C	0.541438	-1.579464	0.000026
C	1.948149	-1.263596	-0.000047
C	2.556947	-0.056117	-0.000033
C	1.959167	1.265879	0.000058
C	-0.493720	0.731057	-0.000048
C	-1.861583	1.188153	-0.000060
C	-2.722823	0.149844	-0.000014
C	-1.954231	-1.139991	0.000045
C	-0.503681	-0.697010	0.000007
H	0.410616	2.656238	0.000094
H	0.294320	-2.637039	0.000098
H	2.607482	-2.127628	-0.000125
H	3.642950	-0.065312	-0.000123
H	2.664994	2.090361	0.000163
H	-2.137801	2.236144	-0.000118
H	-3.802130	0.210437	-0.000037
H	-2.174339	-1.757052	-0.879197
H	-2.174295	-1.756873	0.879427

Frequencies

105.6216	161.3101	229.0701
331.6396	361.4844	402.7205
420.3815	495.8657	574.9246
589.3018	630.0285	674.0528
675.0119	744.8472	770.8520
799.5772	852.9713	901.8360
931.1395	935.3984	946.4879
948.7525	983.1018	999.2529
1016.1769	1066.9883	1091.1712
1138.2408	1161.5988	1215.0336

1255.6247	1269.4396	1303.7352
1351.4309	1391.6771	1433.1604
1449.7022	1473.5873	1540.6773
1572.1910	1646.7152	1681.3688
3041.3449	3075.0918	3155.2560
3158.7427	3174.9226	3185.6416
3200.6584	3205.9520	3245.8949

i78

C	0.616650	-1.613198	0.000007
C	0.616649	1.613197	0.000016
C	1.945374	1.273858	0.000009
C	2.546354	0.000000	-0.000013
C	1.945375	-1.273857	-0.000015
C	-0.528663	-0.744102	0.000011
C	-1.814888	-1.167244	0.000023
C	-2.748587	0.000001	-0.000007
C	-1.814885	1.167246	-0.000030
C	-0.528664	0.744097	-0.000002
H	0.383102	-2.674402	-0.000003
H	0.383099	2.674400	0.000053
H	2.642258	2.107495	0.000017
H	3.632087	0.000001	-0.000019
H	2.642260	-2.107494	-0.000017
H	-2.134464	-2.201339	0.000021
H	-3.411090	0.000030	0.876947
H	-2.134447	2.201342	-0.000026
H	-3.411109	-0.000024	-0.876960

Frequencies

123.1288	170.3438	277.4431
338.5070	395.8204	398.4562
401.1630	493.1176	573.9882
662.1471	688.7264	699.3609
726.2314	769.9050	774.3729
822.1327	831.3687	865.4913
912.7235	928.8842	940.4824
977.0651	990.0580	993.5680
1007.0609	1088.7267	1132.2554
1135.9069	1205.3320	1233.6071
1250.9788	1261.1314	1316.9342
1356.2664	1418.4480	1430.1081
1441.4279	1479.7030	1553.5743
1592.9912	1598.7355	1633.7375
3020.3790	3045.5204	3161.6454
3164.3733	3176.9245	3184.7229

3198.6385	3224.1850	3226.6597
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i79

C	-1.132520	1.219402	0.000001
C	-2.511877	1.206529	-0.000005
C	-3.214890	0.000002	-0.000006
C	-2.511879	-1.206528	0.000000
C	-1.132522	-1.219402	0.000007
C	-0.398274	-0.000001	0.000008
C	0.978283	-0.000003	0.000013
C	2.253316	-0.000001	0.000007
C	3.530359	0.000009	0.759805
C	3.530343	-0.000008	-0.759821
H	-0.588798	2.156600	0.000002
H	-3.053579	2.145979	-0.000009
H	-4.298369	0.000003	-0.000011
H	-3.053584	-2.145976	-0.000002
H	-0.588802	-2.156602	0.000011
H	3.810288	0.915633	1.269756
H	3.810292	-0.915601	1.269779
H	3.810263	-0.915631	-1.269777
H	3.810262	0.915603	-1.269800

Frequencies

43.5937	83.8231	117.6491
197.0845	264.3301	358.8670
404.1580	412.7218	486.9767
542.1157	635.0881	675.5699
690.6635	758.2471	779.7460
832.5957	846.9953	864.6780
871.3994	903.0011	989.5768
994.5436	1002.8886	1045.2277
1048.2323	1068.6126	1074.7031
1076.3828	1110.8220	1178.1379
1179.0490	1197.0975	1305.6499
1331.1189	1349.6598	1450.8509
1471.9583	1481.6945	1508.7490
1595.7123	1620.2494	1993.8064
3127.7387	3130.0765	3185.7026
3191.9853	3206.4576	3211.5302
3212.9194	3218.3870	3226.7638

i80

C	0.902295	1.148714	0.000002
C	2.292363	1.178351	0.000009
C	3.027532	-0.001201	0.000017

C	2.365568	-1.234551	0.000017
C	0.998684	-1.200933	0.000010
C	0.205250	-0.068964	0.000002
C	-1.252740	-0.106878	-0.000006
C	-2.173011	-1.080422	-0.000013
C	-2.276334	1.012231	-0.000012
C	-3.346655	-0.127934	-0.000020
H	0.338368	2.076587	-0.000004
H	2.806408	2.132530	0.000009
H	4.111705	0.029122	0.000023
H	2.919022	-2.167049	0.000024
H	-2.104656	-2.161890	-0.000014
H	-2.281354	1.646677	-0.890937
H	-2.281365	1.646675	0.890914
H	-3.982928	-0.156569	0.889204
H	-3.982915	-0.156568	-0.889252

Frequencies

43.6459	97.9037	137.2763
229.5706	358.7522	388.2744
421.6417	450.0461	540.9143
629.6990	689.8963	702.5814
742.6103	788.6605	869.2840
881.6676	897.9326	929.8361
953.7337	956.0865	997.7936
999.0441	1042.4416	1052.8386
1083.3086	1104.5968	1134.6717
1179.1629	1184.4707	1211.5004
1232.2297	1255.6118	1293.3394
1324.3338	1337.1333	1460.9271
1462.2705	1487.2493	1495.7493
1602.0581	1668.3846	1720.8066
3052.2557	3058.3204	3097.4308
3112.3107	3184.9530	3192.9262
3206.0092	3216.8514	3220.8429

i81

C	-0.773758	1.247100	0.205635
C	-1.986285	1.214960	-0.416499
C	-2.616967	-0.007547	-0.730646
C	-1.985947	-1.223333	-0.392013
C	-0.773408	-1.242694	0.230608
C	-0.071433	0.005705	0.557968
H	-0.288653	2.188918	0.438389
H	-2.476878	2.148004	-0.672203
H	-3.579655	-0.012690	-1.226023

H	-2.476289	-2.161462	-0.628882
H	-0.288036	-2.179507	0.482234
C	1.449964	0.004719	0.444158
C	2.423117	-0.003867	-0.389021
C	0.884414	0.018179	1.783009
C	3.390636	-0.012886	-1.265692
H	0.927518	0.941726	2.352318
H	0.927815	-0.893535	2.371074
H	3.806131	0.912294	-1.650443
H	3.806044	-0.945760	-1.631497

Frequencies

59.7056	84.2604	163.8638
287.2360	294.8972	358.0100
396.3506	428.9466	469.4150
529.7449	593.3978	595.0324
608.4902	657.5047	730.2382
755.4778	772.6113	831.7702
868.3064	871.5195	910.1973
976.8592	979.6538	984.9960
1008.1506	1012.4611	1027.2285
1053.1247	1094.1820	1109.1761
1156.5256	1212.4691	1326.8004
1335.6044	1372.5955	1430.5263
1451.4838	1472.6772	1541.2430
1561.8705	1615.2228	2126.4371
3119.1840	3146.6288	3190.1184
3191.7918	3208.2362	3209.8312
3212.8197	3229.0612	3230.1616

i82

C	1.268636	1.448340	-0.081375
C	2.426594	0.732425	0.227399
C	2.441159	-0.663900	0.274211
C	1.294174	-1.423794	0.015421
C	0.161323	-0.714526	-0.326240
C	0.146464	0.688060	-0.372265
C	-1.298452	0.718100	-0.656996
C	-1.328733	-0.830796	-0.608694
C	-2.368844	0.865509	0.412427
C	-2.267108	-0.680851	0.634044
H	1.267756	2.532078	-0.103930
H	3.344032	1.270203	0.440626
H	3.368949	-1.168543	0.520671
H	1.315333	-2.506002	0.080738
H	-1.674219	-1.458495	-1.428304

H	-3.342774	1.149797	0.005964
H	-2.131063	1.515056	1.256789
H	-1.782399	-0.955488	1.571979
H	-3.216889	-1.210007	0.547880

Frequencies

119.0562	132.0242	229.7199
349.9163	410.6652	442.4085
544.7293	552.6801	613.6499
720.3007	746.2479	758.2223
764.5758	798.2447	846.7782
884.4721	893.1725	945.6262
959.6875	971.5173	1007.3580
1026.7434	1040.5443	1063.5690
1111.6308	1124.7616	1128.1678
1167.7196	1188.6687	1204.7424
1222.0234	1230.9949	1264.7762
1270.8285	1306.5029	1389.4185
1468.3660	1470.5900	1489.9206
1504.8959	1646.6164	1663.6344
3071.2932	3088.4561	3125.8107
3140.1303	3156.3086	3188.4181
3198.9692	3210.2305	3218.0198

i83

C	-1.098652	-1.223051	0.000023
C	-2.466833	-1.016045	0.000027
C	-2.980732	0.278724	0.000004
C	-2.113599	1.370385	-0.000019
C	-0.744729	1.174030	-0.000021
C	-0.211249	-0.130312	-0.000003
C	1.187760	-0.343743	-0.000015
C	2.469938	0.126542	-0.000004
C	3.363359	1.131496	0.000040
C	2.269987	-1.366814	-0.000038
H	-0.690610	-2.227661	0.000043
H	-3.141271	-1.864941	0.000045
H	-4.052938	0.437675	0.000002
H	-2.514136	2.377901	-0.000039
H	-0.065970	2.019429	-0.000038
H	4.427941	0.931992	0.000054
H	3.038041	2.165534	0.000069
H	2.473731	-1.923615	0.915520
H	2.473716	-1.923590	-0.915616

Frequencies

70.0947	95.3855	102.1134
246.4786	285.6410	391.8982
398.6291	418.5321	497.2426
502.9477	593.5912	631.9832
699.3227	714.7850	772.5126
806.8962	821.3485	855.9041
927.9428	995.7886	996.8473
1006.7892	1011.6093	1012.9768
1021.0040	1046.5628	1051.9942
1090.3066	1114.6083	1167.1642
1184.8647	1198.8542	1321.7843
1352.9850	1406.4636	1462.0513
1486.1920	1500.8499	1544.0703
1619.2350	1627.7025	1682.3046
3065.3258	3138.2976	3158.1171
3192.3662	3199.0892	3208.9439
3215.3584	3223.5626	3254.8573

i84

C	1.356518	-1.429357	0.149025
C	2.494730	-0.712793	0.082171
C	2.463143	0.726874	-0.088083
C	1.297021	1.397148	-0.148273
C	0.023369	0.709284	-0.031703
C	0.062479	-0.778982	0.043242
C	-1.109911	-1.412117	-0.058711
C	-2.427358	-0.796339	-0.322252
C	-2.439495	0.607429	0.316005
C	-1.160852	1.353548	0.052808
H	1.376962	-2.507388	0.258161
H	3.455852	-1.209883	0.146703
H	3.403000	1.262930	-0.157567
H	1.281950	2.476983	-0.256933
H	-3.254117	-1.394324	0.068754
H	-2.561519	0.500183	1.404860
H	-3.306704	1.167083	-0.043108
H	-2.566943	-0.722089	-1.411103
H	-1.186351	2.438349	0.024867

Frequencies

129.0229	158.0376	267.2777
305.0506	357.6472	438.2961
461.8810	503.4325	507.0345
609.0603	635.2162	716.6861
722.1963	746.0888	810.4929
833.6113	854.2355	903.5994

918.1352	992.2084	996.4973
1008.5059	1021.3025	1040.1570
1081.9370	1166.1154	1175.3326
1184.4093	1201.9193	1228.6786
1254.1621	1334.5769	1357.2125
1378.4833	1409.2010	1468.6282
1469.1528	1476.8064	1488.2437
1619.3677	1670.3831	1718.3778
2992.1989	3006.6735	3099.8591
3102.9986	3184.5317	3190.6651
3196.5354	3209.5972	3220.7985

i85

C	1.696720	-1.200912	0.109507
C	2.894438	-0.504094	0.178550
C	2.900937	0.882078	0.066974
C	1.702863	1.559230	-0.112930
C	0.503439	0.858887	-0.182570
C	0.489551	-0.527154	-0.072988
H	1.697716	-2.283145	0.201448
H	3.824556	-1.042158	0.323339
H	3.835403	1.428573	0.123461
H	1.697627	2.640087	-0.199365
H	-0.431034	1.392094	-0.317319
C	-2.028215	-0.577904	-0.049636
C	-3.068224	0.052869	0.056771
C	-0.792683	-1.338242	-0.175096
C	-4.236318	0.756903	0.175417
H	-0.802190	-1.867241	-1.136195
H	-0.780679	-2.119730	0.594358
H	-5.161189	0.363647	-0.227950
H	-4.255272	1.717908	0.674228

Frequencies

22.0985	71.9552	154.3356
177.8052	198.6269	252.3268
332.8031	410.7030	418.5708
437.1457	475.8514	608.4524
637.9696	682.6134	720.9232
749.1605	803.2554	848.5987
875.3059	906.1560	971.0456
1005.4496	1024.8320	1025.5099
1033.0886	1062.9126	1116.4061
1186.4826	1210.5644	1216.0387
1234.6509	1245.0452	1315.6356
1355.1450	1373.5861	1464.8780

1468.9444	1498.7820	1543.3767
1662.3337	1684.1367	2165.8697
3033.8507	3064.4962	3161.8446
3179.2251	3192.4419	3203.6117
3212.7884	3221.1926	3260.4997

i86

C	-1.520376	-1.213676	0.014328
C	-2.773289	-0.670124	0.284699
C	-2.977372	0.702761	0.227231
C	-1.914366	1.548960	-0.105027
C	-0.708062	0.952805	-0.357807
C	-0.435062	-0.397297	-0.321805
C	1.929908	-0.604053	0.484847
C	3.017675	0.083043	0.285112
C	0.941335	-0.958974	-0.602325
C	4.101340	0.772790	0.073940
H	-1.376370	-2.289508	0.060805
H	-3.596443	-1.326884	0.541503
H	-3.955547	1.121226	0.437719
H	-2.049166	2.623598	-0.157687
H	1.694408	-0.934475	1.494038
H	0.869013	-2.048432	-0.684397
H	1.307866	-0.583815	-1.560349
H	5.038590	0.285073	-0.173869
H	4.097261	1.855797	0.143081

Frequencies

12.7407	40.7570	126.1621
183.9745	282.6392	321.5937
351.1946	422.0059	477.5560
520.2613	582.0343	627.1596
635.8748	718.4345	756.2352
833.0042	871.3220	886.1603
891.3421	925.0178	958.1910
996.8607	1005.7444	1023.5996
1032.9630	1056.5562	1132.8835
1152.5931	1180.9185	1198.4091
1229.3877	1279.6942	1322.0670
1338.2273	1382.6434	1464.3376
1484.6016	1487.9801	1493.6005
1611.4134	1670.1586	2091.1646
3055.6047	3112.6094	3141.1926
3156.9793	3171.7051	3185.6955
3198.6325	3211.9028	3223.6524

i87

C	1.046114	-1.474763	0.042713
C	2.323017	-0.976537	0.038530
C	2.534033	0.407801	-0.006182
C	1.444185	1.264782	-0.038376
C	0.121939	0.816497	-0.025204
C	-0.099140	-0.609609	0.004285
C	-1.319914	-1.214757	-0.016736
C	-2.419765	-1.900370	-0.057654
C	-2.245590	1.717520	0.094687
C	-0.923023	1.840197	-0.042065
H	0.870082	-2.543460	0.071078
H	3.165872	-1.657640	0.065902
H	3.539920	0.810030	-0.014230
H	1.617735	2.335704	-0.070259
H	-2.952196	-2.183897	0.849953
H	-2.870522	-2.202642	-1.002606
H	-2.741120	0.768465	0.240276
H	-2.871538	2.602223	0.066645
H	-0.529380	2.846647	-0.170745

Frequencies

41.4456	107.1086	159.8404
177.7442	250.0090	258.5911
392.0891	400.5588	474.3641
502.9175	515.4879	542.5939
622.5700	646.1522	706.1558
748.6357	770.4331	841.3672
860.7477	901.4806	954.3230
955.7506	976.2375	994.2498
1041.7709	1044.3352	1060.3098
1140.2587	1156.6484	1187.9248
1226.8273	1280.2404	1322.5115
1374.6336	1429.0894	1446.3534
1472.9246	1481.5790	1562.0585
1625.2437	1697.2931	1913.2816
3090.7777	3149.3089	3160.1601
3174.7757	3189.8062	3199.6866
3216.4403	3225.6901	3275.9943

i88

C	-0.736835	-0.330254	1.184883
C	-1.930330	0.381458	1.157780
C	-2.586814	0.619545	-0.045166
C	-2.043370	0.140591	-1.239241
C	-0.863758	-0.552062	-1.144678

C	-0.164927	-0.826477	0.007001
C	1.148579	-1.564658	0.015060
C	2.358641	-0.653801	-0.023285
C	2.312041	0.646735	-0.073835
C	2.250723	1.945188	-0.126270
H	-0.230664	-0.506278	2.129821
H	-2.353566	0.752915	2.083956
H	-3.519764	1.172621	-0.059998
H	-2.537328	0.311823	-2.189125
H	1.211077	-2.191438	0.911725
H	1.194075	-2.245253	-0.840558
H	3.331629	-1.139848	-0.011214
H	2.213834	2.465586	-1.077650
H	2.227006	2.542292	0.779549

Frequencies

33.8048	66.8137	84.1596
176.5503	309.5495	319.4256
332.3675	424.4311	502.6715
521.0596	524.4821	635.6800
668.7851	735.1604	765.4245
812.9760	880.4520	882.6082
887.8820	941.7819	949.3002
970.1707	999.2178	1009.4811
1024.0884	1059.4136	1132.9531
1146.4275	1183.3257	1202.1407
1236.1053	1301.1361	1328.2751
1333.6674	1383.5257	1467.5001
1479.6800	1491.5699	1502.0297
1612.8535	1675.0757	2092.1076
3049.0624	3092.3651	3144.7856
3164.5718	3177.7369	3189.7187
3201.6864	3214.2420	3228.3184

i89

C	0.860231	1.149155	0.371344
C	2.236514	1.028662	0.511594
C	2.872252	-0.158650	0.171873
C	2.121757	-1.224947	-0.308969
C	0.745771	-1.105086	-0.446565
C	0.096489	0.086196	-0.114637
C	-1.375471	0.234033	-0.283411
C	-2.227848	-0.855806	0.269609
C	-1.899827	1.296646	-0.898290
C	-3.398608	-0.675032	0.829203
H	0.363924	2.070256	0.656065

H	2.812133	1.863202	0.895971
H	3.945797	-0.255731	0.285785
H	2.609798	-2.154123	-0.580773
H	0.176490	-1.940791	-0.839143
H	-1.266255	2.081064	-1.296326
H	-2.969589	1.393162	-1.043444
H	-4.048720	0.154315	1.072081
H	-1.811146	-1.862377	0.239278

Frequencies

57.3303	64.7865	131.6024
205.0827	286.9922	327.3899
376.7653	418.6706	520.2192
544.5045	612.1642	638.7599
711.3700	724.4887	746.0631
762.0078	805.8302	868.0762
878.7175	889.0476	948.0172
955.9647	965.3948	999.8474
1022.8476	1024.1144	1061.9429
1110.8691	1132.6580	1189.1365
1216.3470	1260.9413	1306.6920
1334.5761	1363.2479	1442.4575
1490.2334	1543.2298	1650.6207
1662.2861	1680.6723	1711.3079
3136.7251	3164.8248	3191.4906
3198.1731	3205.8140	3214.9502
3223.1661	3250.5336	3256.0773

i90

C	0.843745	1.139922	0.516572
C	2.208530	0.891346	0.583995
C	2.731972	-0.276546	0.044301
C	1.881684	-1.194349	-0.561071
C	0.517136	-0.948100	-0.624470
C	-0.018675	0.226129	-0.090451
C	-1.475681	0.515705	-0.180380
C	-2.435676	-0.526765	0.227154
C	-1.920346	1.701965	-0.608371
C	-2.140692	-1.692303	0.754001
H	0.433773	2.043011	0.955343
H	2.863026	1.608634	1.066447
H	3.796838	-0.472573	0.098867
H	2.283243	-2.106022	-0.989056
H	-0.139002	-1.664070	-1.105792
H	-3.491023	-0.274030	0.080944
H	-1.234852	2.477301	-0.929811

H	-2.981656	1.920737	-0.657569
H	-2.682335	-2.555019	1.112947

Frequencies

60.4393	116.4147	159.8182
203.1593	256.3097	359.8085
421.2931	438.3888	517.8687
540.2668	599.9071	639.1041
695.0226	723.9449	741.3743
760.1403	796.9025	823.2248
873.6904	883.6726	943.1665
955.4354	983.2051	1003.9036
1022.2708	1025.4276	1063.5197
1119.0131	1151.1541	1192.0658
1219.8266	1262.0360	1320.3719
1357.8534	1366.9437	1449.2724
1491.5794	1546.3113	1651.9250
1662.2849	1682.1220	1710.4268
3071.5660	3161.0455	3189.5686
3196.2254	3206.5046	3214.7225
3221.9028	3253.4598	3267.3895

i91

C	1.297754	1.347431	0.000008
C	2.471900	0.613479	0.000015
C	2.409761	-0.776235	0.000011
C	1.176283	-1.404577	0.000000
C	-0.015644	-0.675453	-0.000011
C	0.051320	0.719339	-0.000008
C	-2.415005	0.750594	0.000035
C	-2.549078	-0.550538	0.000045
C	-1.202851	1.588625	-0.000034
C	-1.324198	-1.438839	-0.000036
H	1.340455	2.432670	0.000012
H	3.430322	1.120011	0.000025
H	3.320212	-1.364764	0.000017
H	1.125837	-2.489560	-0.000002
H	-3.522813	-1.033212	0.000113
H	-1.191788	2.245824	-0.877303
H	-1.191754	2.245934	0.877154
H	-1.355977	-2.099860	-0.874901
H	-1.355942	-2.099992	0.874729

Frequencies

53.6497	148.2388	242.6365
352.9849	360.2140	441.9099

462.7558	504.6180	508.3531
607.5882	706.3194	731.4195
741.9039	769.8123	770.7281
879.1747	893.3233	939.9716
943.8682	982.3492	985.4828
1009.3275	1019.5725	1077.0148
1137.3719	1188.3923	1201.7848
1214.7622	1226.1082	1230.9601
1260.5496	1276.4479	1333.2948
1357.4981	1373.6780	1468.6248
1469.1462	1497.5533	1541.3922
1656.2894	1682.8256	1776.3181
3029.5147	3037.1808	3058.4973
3068.1174	3171.9706	3178.4639
3183.0307	3199.6849	3217.9004

i92

C	-0.798945	1.043117	0.683877
C	-2.154285	0.753720	0.791444
C	-2.698299	-0.309361	0.082774
C	-1.881561	-1.084220	-0.734036
C	-0.527910	-0.797574	-0.840813
C	0.025211	0.271461	-0.133104
C	1.482658	0.595565	-0.267583
C	2.493265	-0.373665	0.191829
C	1.831263	1.751996	-0.798829
C	2.230836	-1.504499	0.843602
H	-0.369058	1.867709	1.241542
H	-2.784698	1.359769	1.432299
H	-3.755277	-0.535279	0.166051
H	-2.301555	-1.913379	-1.292278
H	0.109503	-1.400546	-1.478027
H	1.314258	2.610056	-1.206170
H	3.522661	-0.101277	-0.022356
H	1.217262	-1.805733	1.084950
H	3.033501	-2.160569	1.159029

Frequencies

41.4587	110.4863	145.7980
197.1705	255.5610	324.9820
417.5138	450.6151	496.3891
524.4835	603.6216	637.3896
711.5025	723.8836	740.9519
761.8640	792.6995	840.4363
874.5340	949.9511	966.2834
1003.9643	1013.5755	1023.5559

1025.6286	1040.4615	1062.1789
1111.7229	1142.0383	1188.3061
1211.0256	1301.4935	1323.3424
1331.8589	1356.0158	1450.1997
1486.7843	1538.1912	1644.8829
1657.4094	1677.4957	1714.0677
3157.7893	3179.1411	3184.6450
3191.6532	3200.3296	3207.2637
3215.8174	3247.7226	3250.7238

i93

C	0.675711	-1.500685	0.093575
C	2.039728	-1.251381	-0.045597
C	2.518834	0.087682	-0.222199
C	1.700897	1.157498	-0.096060
C	0.308567	0.956478	0.416062
C	-0.204728	-0.444290	0.210286
C	-1.636330	-0.383559	-0.020015
C	-1.943797	1.046754	-0.214365
C	-2.517910	-1.400965	-0.070923
C	-0.859273	1.804228	-0.029892
H	0.302013	-2.516144	0.004952
H	2.733728	-2.077321	-0.145558
H	3.557316	0.233329	-0.500111
H	2.065685	2.166413	-0.257110
H	0.380728	1.120160	1.513667
H	-2.933691	1.407971	-0.464452
H	-2.210001	-2.426827	0.095256
H	-3.566960	-1.222473	-0.275331
H	-0.819017	2.884328	-0.096547

Frequencies

102.9418	173.0972	239.5328
290.5783	381.3900	426.8736
503.2079	519.1758	544.1551
632.6735	638.0662	700.3801
707.2993	718.7570	767.1201
784.7501	823.8392	875.7821
884.6929	930.5845	938.8590
978.4770	982.2413	999.2325
1040.3567	1084.8226	1089.2715
1123.5136	1147.5024	1173.7859
1241.6906	1244.9354	1285.7270
1329.5754	1353.1185	1396.3782
1434.1948	1445.1276	1532.1493
1617.1121	1643.8472	1673.4510

2865.3180	3163.9864	3184.6891
3188.2816	3205.3776	3213.3554
3219.6459	3237.4244	3255.1076

i94

C	-1.121197	-1.444043	-0.191839
C	-2.372004	-0.869551	0.006451
C	-2.499770	0.505691	0.181515
C	-1.377708	1.330985	0.159247
C	-0.131275	0.768788	-0.063238
C	-0.003480	-0.619190	-0.233711
C	1.413316	-0.954636	-0.392605
C	2.200230	0.300535	-0.340292
C	2.368281	-0.799320	0.724111
C	1.220605	1.450393	-0.121998
H	-1.015884	-2.515196	-0.319725
H	-3.255383	-1.497805	0.030299
H	-3.481519	0.938822	0.336879
H	-1.484117	2.400973	0.305770
H	3.064367	0.460193	-0.975094
H	3.320560	-1.318328	0.680797
H	1.970053	-0.658922	1.726430
H	1.268707	2.165273	-0.949044
H	1.431226	2.007076	0.797838

Frequencies

132.6156	178.4098	304.7651
358.3621	384.0130	444.7072
519.5530	566.7726	589.0195
679.1991	733.9954	755.7903
787.2988	808.6711	837.1753
851.9180	905.6975	921.0438
971.3557	997.7867	1016.9857
1021.4697	1050.9742	1056.8356
1065.7627	1084.2146	1130.2655
1170.9435	1183.7716	1198.9431
1223.4377	1264.3322	1302.0892
1332.1684	1349.3159	1389.1541
1471.5544	1480.1585	1506.7271
1511.8022	1647.2262	1678.1205
3053.1296	3094.8734	3113.3790
3182.2019	3184.9654	3192.1242
3204.7124	3206.4110	3214.4924

i95

C	-1.126767	-1.422869	-0.139040
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C	-2.367218	-0.810684	0.015223
C	-2.460188	0.571251	0.142447
C	-1.313673	1.361640	0.106371
C	-0.077647	0.757193	-0.060395
C	0.014195	-0.634261	-0.173899
C	1.439481	-1.057267	-0.300690
C	2.254563	0.248478	-0.255620
C	2.270946	-0.695572	0.863915
C	1.277084	1.423478	-0.184704
H	-1.052372	-2.501217	-0.229040
H	-3.267087	-1.415117	0.040671
H	-3.431411	1.037039	0.265694
H	-1.392146	2.440165	0.197336
H	3.139793	0.343028	-0.876828
H	1.712873	-1.881644	-0.951915
H	2.008929	-0.584851	1.908895
H	1.326103	2.028356	-1.096104
H	1.490662	2.085907	0.659643

Frequencies

133.8011	177.8451	308.4953
359.4677	375.9834	446.7621
522.5459	560.4032	597.0814
671.8794	704.6276	747.0604
786.7536	804.1116	837.9148
841.2493	882.5180	900.2979
954.3369	967.2443	988.2697
998.0379	1016.4698	1057.6891
1060.3614	1077.2014	1128.2546
1176.8934	1182.9689	1187.2891
1201.2056	1232.9487	1261.5574
1280.2077	1334.9628	1349.1579
1395.1268	1479.9746	1506.2017
1524.7701	1657.2328	1682.7255
3052.8843	3094.6085	3162.8015
3170.2889	3180.8730	3189.0768
3199.6323	3210.8034	3214.8969

Transition states

i20 – i22

C	1.109908	-1.375792	-0.293887
C	2.313667	-0.728059	-0.533780
C	2.482886	0.603317	-0.140858
C	1.463186	1.270637	0.507263
C	0.220954	0.638133	0.721081

C	0.048817	-0.709013	0.317028
C	-1.271791	-1.324319	0.432766
C	-2.398923	-0.672162	0.097070
C	-2.429787	0.662851	-0.508968
C	-1.434740	1.532119	-0.478183
H	0.976748	-2.407241	-0.604512
H	3.124243	-1.255291	-1.023490
H	3.429968	1.100911	-0.317537
H	1.611667	2.284042	0.862912
H	-0.448391	1.039840	1.473582
H	-1.329390	-2.371453	0.717001
H	-3.345854	-1.198348	0.161757
H	-3.334304	0.908271	-1.069676
H	-1.309748	2.512988	-0.917225

Frequencies

-444.9725	101.8462	155.7967
231.7625	297.3937	396.3532
411.3717	441.4406	518.2777
543.3788	622.4175	660.9115
705.7507	738.9610	763.8462
776.4932	832.2012	853.4286
871.6885	917.8960	950.0033
967.0368	990.0439	1007.4677
1013.4835	1034.5771	1053.7720
1102.6711	1184.8614	1200.2018
1207.3928	1232.2837	1271.8662
1332.1854	1343.2516	1435.7078
1470.8645	1532.0080	1600.4266
1630.1174	1646.1778	1685.5667
3097.8404	3169.7560	3180.5349
3186.0038	3195.6726	3198.0156
3206.0502	3216.3276	3230.9503

i22 - p1

C	-1.240572	1.411320	0.003150
C	-2.420540	0.719185	-0.041992
C	-2.421237	-0.698621	-0.097320
C	-1.252160	-1.392050	-0.037542
C	0.000000	-0.703529	0.131841
C	0.000000	0.733701	0.028530
C	1.240572	1.411320	0.003149
C	2.420540	0.719185	-0.041992
C	2.421237	-0.698621	-0.097319
C	1.252161	-1.392050	-0.037542
H	-1.241326	2.496583	-0.002224

H	-3.363025	1.253585	-0.072774
H	-3.362502	-1.226725	-0.198294
H	-1.243232	-2.475943	-0.076200
H	-0.000001	-0.754044	1.821219
H	1.241326	2.496583	-0.002225
H	3.363026	1.253585	-0.072775
H	3.362502	-1.226725	-0.198294
H	1.243232	-2.475943	-0.076200

Frequencies

-1178.7575	165.5330	171.6795
352.8371	375.9986	456.0747
478.0229	492.4845	523.7307
555.6797	568.3950	626.9919
641.3127	726.4476	756.2495
791.2739	808.1668	815.2411
841.3392	910.0251	947.7777
970.9400	987.5068	1006.6625
1011.1319	1034.0554	1046.9308
1151.9215	1160.9327	1184.7228
1194.4033	1230.1927	1266.8267
1283.7672	1390.9755	1407.5570
1421.4051	1494.1275	1494.2343
1552.3903	1623.6621	1670.7887
1695.3509	3189.7365	3190.6159
3195.0983	3196.6980	3208.9450
3209.7493	3220.9558	3221.8408

i23 – p1

C	1.285219	-1.398704	0.042261
C	2.455722	-0.689561	0.010789
C	2.431194	0.720507	-0.045820
C	1.236307	1.389870	-0.065235
C	0.013056	0.683152	-0.034617
C	0.034662	-0.733524	0.017091
C	-1.195726	-1.442626	0.024769
C	-2.392570	-0.777736	-0.046722
C	-2.424477	0.626910	-0.103537
C	-1.249865	1.354960	-0.035352
H	1.300142	-2.482931	0.085635
H	3.407225	-1.208597	0.029521
H	3.364316	1.271653	-0.070878
H	1.213886	2.474258	-0.098995
H	-1.172179	-2.526563	0.068788
H	-3.322717	-1.334066	-0.066233
H	-3.374857	1.143435	-0.167598

H	-1.310983	1.835202	1.830076
H	-1.265958	2.428118	-0.192078

Frequencies

-844.9443	167.6721	177.1165
278.2910	359.5746	386.7427
418.1505	486.7427	515.3666
520.9670	525.5281	632.3793
643.5900	738.5966	783.4572
794.2095	807.6307	810.7940
870.3548	909.8999	952.6827
977.9710	997.9352	1012.3514
1024.2558	1044.5009	1058.5118
1155.9300	1162.3479	1177.0145
1195.8927	1234.9225	1266.4836
1290.2090	1389.2281	1416.9479
1421.9948	1495.8032	1499.4083
1562.0041	1634.8520	1654.0788
1701.5603	3188.6663	3190.0207
3193.1773	3195.7998	3207.3878
3207.9687	3220.7080	3221.5093

i18 – i23

C	-1.392880	-1.320220	-0.038593
C	-2.586562	-0.620282	0.070516
C	-2.589448	0.770686	0.116154
C	-1.381970	1.468545	0.044739
C	-0.226209	0.735598	-0.059118
C	-0.160594	-0.648416	-0.106885
C	1.087812	-1.417941	-0.162623
C	2.325561	-0.955373	0.094019
C	2.625038	0.440230	0.363427
C	2.066961	1.453111	-0.331885
H	-1.405229	-2.405994	-0.072100
H	-3.523673	-1.162823	0.120183
H	-3.525804	1.311750	0.200991
H	-1.365767	2.552962	0.071244
H	0.963628	-2.486572	-0.315519
H	3.131852	-1.677874	0.190957
H	3.263520	0.659718	1.215939
H	1.632984	1.287234	-1.310139
H	2.222229	2.485976	-0.040063

Frequencies

-294.7325	85.9890	140.7037
228.8112	265.6429	381.4682

407.4920	428.4119	506.8727
557.4679	597.9694	644.0023
718.7891	742.6863	777.9500
805.1164	837.1448	870.0525
897.2217	956.4281	967.4970
984.0153	1002.0528	1006.4019
1012.4168	1055.2881	1091.1952
1140.0362	1181.4448	1203.8076
1239.2501	1280.5603	1298.9866
1333.7191	1423.3587	1459.1220
1471.9420	1494.8553	1602.8168
1623.0715	1652.6320	1682.6661
3155.0025	3160.5254	3168.0774
3179.1674	3184.6933	3188.0744
3201.1933	3216.2149	3250.9100

il - p2

C	-1.347245	-1.219396	-0.045216
C	-2.728705	-1.100381	-0.033528
C	-3.323382	0.155540	0.009994
C	-2.529467	1.296599	0.040884
C	-1.147254	1.185717	0.029110
C	-0.541539	-0.075214	-0.013902
C	0.882322	-0.194026	-0.023776
C	2.083104	-0.290949	-0.026521
C	3.505613	-0.420802	-0.054994
C	4.342523	0.641249	-0.101240
H	-0.878572	-2.195606	-0.078286
H	-3.344132	-1.992452	-0.057315
H	-4.403570	0.245727	0.019911
H	-2.989569	2.277412	0.075463
H	-0.523828	2.071588	0.053234
H	3.890504	-1.413269	-0.270772
H	3.691315	-1.012694	1.769408
H	5.409872	0.496868	-0.211640
H	3.972152	1.652406	0.015128

Frequencies

-913.6455	40.2692	68.3787
84.9998	197.0871	222.1081
358.3425	379.5748	413.2929
426.5611	443.8544	513.2457
552.8849	591.4563	642.1677
679.7883	710.6046	721.5035
780.9139	867.5223	923.6632
945.9066	951.7891	1002.0565

1019.0596	1023.2164	1030.8664
1060.5381	1102.3846	1112.7911
1189.2764	1209.2300	1292.5734
1299.2056	1318.2783	1356.6258
1443.1103	1488.9018	1541.9748
1606.5160	1646.5650	1680.6165
2358.5339	3169.5314	3180.0291
3191.0952	3200.2140	3209.6428
3220.5553	3225.2510	3272.4032

i20 – i66

C	0.519439	-0.483781	1.215607
C	0.519439	-0.483781	-1.215607
C	0.519439	-1.864261	-1.206736
C	0.497899	-2.565205	0.000000
C	0.519439	-1.864261	1.206736
C	0.422459	0.249933	0.000000
C	0.725854	1.712356	0.000000
C	-0.279574	2.588398	0.000000
C	-1.634240	2.016155	0.000000
C	-1.704302	0.700127	0.000000
H	0.548981	0.063114	2.151482
H	0.548981	0.063114	-2.151482
H	0.555853	-2.405939	-2.145593
H	0.504231	-3.649050	0.000000
H	0.555853	-2.405939	2.145593
H	1.766735	2.016875	0.000000
H	-0.121692	3.660888	0.000000
H	-2.507767	2.667282	0.000000
H	-2.486296	-0.044437	0.000000

Frequencies

-557.9147	95.5853	110.6635
174.0287	319.2024	339.1191
417.3841	432.1211	514.7898
599.2463	626.7259	676.5833
681.2312	709.6783	744.6211
745.4296	824.2694	838.7889
879.7555	899.7347	914.7615
982.8343	986.8317	999.1000
1002.9816	1007.0695	1047.1663
1108.2457	1158.5865	1176.5702
1195.6386	1211.0096	1241.7461
1294.5900	1346.3998	1402.6492
1470.9780	1506.5537	1596.7680
1625.2298	1632.4975	1706.4313

3125.8062	3188.4690	3191.3489
3193.5777	3205.8537	3210.6202
3218.9925	3221.4517	3273.5911

i1 – i2

C	-1.354683	-1.222046	0.064280
C	-2.732329	-1.088851	0.027235
C	-3.319862	0.171647	-0.025722
C	-2.512919	1.305547	-0.040707
C	-1.133668	1.187372	-0.006871
C	-0.530182	-0.082249	0.043917
C	0.874276	-0.210018	0.077394
C	2.093180	-0.330761	-0.047093
C	3.526458	-0.441206	-0.046546
C	4.411796	0.606728	0.121879
H	-0.898006	-2.203558	0.109592
H	-3.354634	-1.976685	0.040629
H	-4.398686	0.270379	-0.054265
H	-2.963922	2.290622	-0.081443
H	-0.506096	2.070664	-0.019125
H	2.750765	-0.416389	-1.223616
H	3.900325	-1.460701	-0.084611
H	5.475722	0.426273	0.054275
H	4.062129	1.622418	0.251971

Frequencies

-1863.6187	57.6394	65.3941
91.6418	182.7984	242.9618
361.6748	412.1253	416.4078
509.5103	512.8793	576.1121
605.8833	638.0511	687.1751
705.6649	714.6866	747.8430
768.4446	857.5646	925.3854
940.4645	995.5467	1011.2763
1013.9683	1039.8134	1057.6714
1101.6747	1113.1028	1186.2008
1205.1581	1237.6634	1309.8638
1313.3354	1356.3027	1424.9992
1484.6290	1511.4598	1539.5851
1629.7004	1639.2515	1671.3223
2177.1222	3174.8963	3180.6822
3188.1312	3196.2052	3207.8452
3216.5726	3222.4610	3284.4453

i23 – i68

C	1.304997	1.374204	-0.000229
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C	-1.330461	-1.356235	0.310087
C	1.185601	-1.397673	-0.007759
C	2.414763	-0.754956	-0.115626
C	2.472852	0.634265	-0.104779
C	0.062294	0.740920	0.104321
C	-1.195555	1.474487	0.218071
C	-2.306999	0.871972	-0.307667
C	-2.419315	-0.531011	-0.338881
C	0.010063	-0.669575	0.108873
H	1.344362	2.458652	-0.005259
H	-1.520907	-1.455868	1.387044
H	1.143642	-2.482681	-0.005071
H	3.324554	-1.337612	-0.204088
H	3.428917	1.139148	-0.184504
H	-1.202563	2.482996	0.616397
H	-3.271506	0.240565	0.325066
H	-3.120352	-0.994237	-1.029108
H	-1.315575	-2.369348	-0.098946

Frequencies

-1684.7854	120.0513	175.0777
271.1037	357.6857	420.1910
442.5069	500.1654	501.9590
549.0287	612.7534	694.8418
721.5393	737.5920	766.4152
775.4706	798.8742	873.9396
906.9443	927.2071	963.4906
997.8292	1006.6763	1069.9126
1090.2868	1135.2944	1185.6546
1196.7852	1203.6151	1224.9854
1236.7921	1273.0944	1299.4427
1329.8396	1355.2202	1392.4850
1454.2336	1465.9210	1500.2251
1529.3013	1639.2229	1667.2121
2159.8568	3026.1230	3105.7609
3160.1538	3183.1776	3190.4749
3198.1325	3203.9244	3218.4093

$i2 - p2$

C	1.231234	-1.204206	-0.068158
C	2.615319	-1.215591	0.010313
C	3.322610	-0.020417	0.081234
C	2.640012	1.191134	0.074175
C	1.256058	1.212181	-0.003944
C	0.537034	0.012336	-0.076264
C	-0.885371	0.028754	-0.154106

C	-2.099662	0.029004	-0.105057
C	-3.487218	0.071254	-0.460950
C	-4.517640	-0.065614	0.369452
H	0.673968	-2.131662	-0.121914
H	3.144726	-2.161365	0.017340
H	4.404715	-0.033171	0.142736
H	3.188681	2.124149	0.131057
H	0.718079	2.152512	-0.007838
H	-2.229223	-0.168699	1.931217
H	-3.669741	0.229669	-1.521056
H	-5.533708	-0.021105	-0.003730
H	-4.371754	-0.223329	1.432024

Frequencies

-636.7895	13.2741	66.4523
73.9293	97.0732	224.7714
299.2881	344.8392	398.5241
413.5289	498.9233	540.4674
544.9908	594.0462	641.7914
712.8825	719.0209	729.7844
785.8582	869.5145	950.2449
952.5576	978.8605	1004.5025
1017.2227	1023.7866	1025.1118
1061.4384	1105.3965	1112.9565
1189.3250	1209.3217	1290.6251
1319.3452	1326.8356	1356.5011
1445.3938	1487.8022	1539.7059
1645.7146	1675.2976	1714.1008
2272.0586	3156.2058	3167.2978
3189.9135	3199.1601	3208.8220
3216.5872	3221.6290	3257.3816

i3 – i4

C	-1.035809	-1.163428	0.202687
C	-2.422200	-1.141282	0.212546
C	-3.105337	0.056425	0.030181
C	-2.393070	1.234985	-0.160959
C	-1.006339	1.216955	-0.175679
C	-0.306725	0.016094	-0.006475
C	1.138473	0.002255	-0.039036
C	2.090739	-0.848660	-0.409084
C	3.442480	-0.302350	-0.114386
C	3.376407	0.900954	0.432465
H	-0.504061	-2.094183	0.365738
H	-2.972256	-2.061882	0.372378
H	-4.189182	0.072053	0.045413

H	-2.919907	2.172575	-0.297536
H	-0.450137	2.136012	-0.323647
H	1.922506	-1.811092	-0.881672
H	4.358244	-0.843747	-0.329730
H	1.976489	0.995814	0.406259
H	4.106585	1.602766	0.809226

Frequencies

-2066.8907	42.0738	95.1082
111.8294	280.4478	341.8632
389.9956	413.9517	442.4895
519.1505	630.2312	633.1289
656.3225	713.2804	729.9336
778.2113	865.5981	871.7047
906.0403	935.0797	940.4949
949.0227	1004.5458	1006.2797
1020.4920	1021.6354	1061.6366
1066.2118	1111.4075	1185.9096
1193.4710	1213.4681	1264.9235
1301.5263	1323.8719	1356.5985
1484.9507	1532.8008	1631.0589
1641.5846	1670.7849	1715.2742
1754.1899	3182.0959	3192.5264
3195.5301	3199.1234	3208.1320
3215.1230	3223.8666	3251.9610

i3 – i18

C	-0.624020	-1.125042	-0.138873
C	-1.990257	-1.395356	-0.140121
C	-2.942653	-0.380105	-0.013970
C	-2.575018	0.963073	0.114016
C	-1.216417	1.204606	0.110612
C	-0.257919	0.210879	-0.010894
H	0.104487	-1.919934	-0.240698
H	-2.329848	-2.420224	-0.240342
H	-3.995440	-0.642480	-0.015849
H	-3.318797	1.744564	0.206440
C	0.906676	1.080888	0.011679
C	2.229164	1.125550	-0.093498
C	3.107554	-0.046475	-0.216271
C	2.905723	-1.232938	0.354229
H	-0.093320	2.065353	0.142074
H	2.709077	2.100054	-0.116515
H	4.005989	0.104821	-0.811010
H	2.057365	-1.413408	1.006120
H	3.603493	-2.049239	0.208321

Frequencies

-2320.8839	58.7260	79.9731
127.3532	174.1297	252.6368
371.6017	413.0203	441.0814
494.8990	529.3484	616.4809
634.8796	717.3256	761.6882
769.0643	780.5208	851.4665
893.1802	954.2474	967.6625
968.5873	1004.7809	1014.3522
1030.9713	1038.9771	1043.6927
1086.1172	1131.8909	1171.7377
1190.9633	1279.3569	1320.8348
1332.9425	1376.4261	1448.4976
1475.9945	1491.6375	1627.4339
1661.3940	1700.8166	1747.0711
1908.5694	3156.6162	3166.9320
3180.3552	3185.1697	3205.3456
3217.6377	3223.2827	3253.9683

i69 – i71

C	0.842441	-0.854938	-0.700256
C	0.952142	-0.899838	0.780287
C	1.882982	0.074285	1.172383
C	2.416313	0.695279	0.007691
C	1.843486	0.159463	-1.108696
C	-0.483450	-0.276683	-0.237709
C	-1.692824	-1.054423	-0.094411
C	-2.722536	-0.186211	0.103636
C	-2.196674	1.171616	0.105694
C	-0.857408	1.124606	-0.094490
H	0.743170	-1.769917	-1.276705
H	0.533922	-1.673098	1.404591
H	2.129105	0.324770	2.194407
H	3.139499	1.500470	0.015635
H	2.014077	0.460456	-2.132489
H	-1.747633	-2.132416	-0.160466
H	-3.763002	-0.450022	0.238340
H	-2.787094	2.066218	0.249208
H	-0.168868	1.954603	-0.137295

Frequencies

-498.4762	122.5160	143.3869
180.8741	347.6216	413.0468
520.0297	574.8330	589.1963
653.3751	723.5040	741.6692

765.1263	771.3308	810.5893
817.6907	837.3106	866.9914
911.8662	917.7972	935.4848
966.4135	975.0220	997.8517
1023.8629	1056.2275	1081.7642
1091.3321	1100.0003	1110.8896
1130.6214	1217.7507	1261.9401
1290.3975	1328.6339	1337.3209
1369.7067	1429.8454	1431.6240
1512.1264	1542.8111	1597.7155
3170.5614	3224.4432	3227.6786
3237.4878	3242.4689	3249.8122
3257.1869	3268.6794	3276.4687

i66 – i69

C	0.673624	-0.911970	-0.830443
C	0.705009	-0.493185	1.107988
C	1.865188	0.395475	1.093177
C	2.427848	0.579871	-0.123764
C	1.870440	-0.293323	-1.127989
C	-0.357653	-0.259564	0.107899
C	-1.629929	-1.030010	0.254352
C	-2.666540	-0.211699	0.033147
C	-2.161328	1.135952	-0.269702
C	-0.823227	1.128196	-0.224960
H	0.359043	-1.818053	-1.334400
H	0.589862	-1.282050	1.843198
H	2.227566	0.850921	2.007426
H	3.271194	1.231921	-0.309858
H	2.446841	-0.597459	-1.994472
H	-1.664103	-2.083512	0.499584
H	-3.713565	-0.482974	0.070740
H	-2.787424	1.989109	-0.497165
H	-0.150004	1.953630	-0.403291

Frequencies

-736.1675	126.2210	171.9409
186.7303	390.0887	405.6721
475.7980	547.7713	568.6210
609.7764	648.2138	676.3624
719.0479	744.2341	750.5206
782.5540	816.8239	859.0505
871.8571	886.6889	924.9041
965.1749	969.7385	981.6161
1004.0078	1032.9508	1050.5916
1097.6109	1109.2502	1129.8874

1150.3029	1194.5396	1262.8768
1305.7571	1329.3635	1387.4973
1410.1785	1425.5558	1461.2343
1600.1490	1603.3350	1676.6697
3190.1533	3192.2616	3206.3262
3211.3120	3213.7025	3223.4683
3234.6831	3241.8084	3264.4887

i71 – i73

C	0.689237	0.019814	0.127391
C	1.552864	1.160297	0.099705
C	2.852190	0.731884	-0.065941
C	2.886256	-0.675766	-0.150284
C	1.588567	-1.160375	-0.048702
C	-0.752696	0.004899	0.041346
C	-1.599675	-1.159226	0.054340
C	-2.889758	-0.728861	-0.026482
C	-2.887739	0.735508	-0.095734
C	-1.597089	1.167187	-0.050737
H	1.056202	-0.671866	1.121139
H	1.220644	2.179446	0.230904
H	3.723854	1.372435	-0.072316
H	3.771601	-1.287151	-0.246519
H	1.234017	-2.174550	-0.157075
H	-1.262305	-2.183662	0.119457
H	-3.775078	-1.349704	-0.040933
H	-3.771383	1.353813	-0.173180
H	-1.250490	2.189074	-0.090883

Frequencies

-1205.0527	50.8839	116.0776
147.9583	302.5007	393.2855
423.3850	542.5139	597.7430
620.9836	671.0919	684.0299
711.4806	749.2254	788.0760
793.8201	847.7356	852.3680
895.4775	911.4107	917.9691
921.4533	966.1831	978.1552
1036.1779	1044.0938	1086.8384
1088.1061	1096.7797	1124.5348
1146.3809	1198.1866	1245.4730
1286.7752	1324.3835	1370.6725
1437.7882	1466.8939	1509.5131
1542.6909	1552.4446	1559.9770
2115.7830	3225.1266	3225.9055
3238.4966	3250.5535	3252.2781

3260.6717	3263.4700	3270.4996
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i71 – i72

C	-0.729892	1.000005	0.335815
C	-0.691365	-0.402714	0.921201
C	-1.880322	-1.071087	0.525864
C	-2.589226	-0.239677	-0.381036
C	-1.944895	0.953407	-0.545012
C	0.614336	0.710535	-0.266650
C	1.852182	1.106482	0.153486
C	2.735716	-0.020768	0.044444
C	2.028223	-1.136211	-0.344650
C	0.670033	-0.743954	-0.543909
H	-0.729196	1.826258	1.048811
H	-0.112753	-0.626577	1.807567
H	-2.144504	-2.084359	0.795502
H	-3.504349	-0.525236	-0.884605
H	-2.247565	1.761409	-1.196653
H	2.093614	2.056192	0.611467
H	3.801053	0.009381	0.238822
H	2.443970	-2.106047	-0.579213
H	0.010994	-1.247126	-1.239016

Frequencies

-593.9724	139.3965	175.9926
231.3886	330.1877	368.9442
522.0801	590.3307	659.4477
679.9230	745.4822	762.6325
780.2133	801.7311	817.8064
833.1545	855.8227	872.2945
895.3876	931.6728	946.1503
955.3943	972.2095	1004.4861
1039.8110	1056.6281	1061.1473
1077.2950	1103.2417	1116.0496
1157.0739	1201.7914	1251.4082
1286.0682	1308.0919	1325.7916
1351.8303	1413.6569	1427.5362
1467.3494	1520.5981	1595.6728
3116.6629	3214.2189	3219.6320
3227.5114	3230.3698	3238.4210
3240.0804	3250.8154	3251.6005

i72 – i76

C	-0.673252	1.183588	0.409012
C	-0.536413	-0.866192	0.688269
C	-1.894034	-1.125502	0.434002

C	-2.525968	-0.160255	-0.415222
C	-1.891573	1.035797	-0.431421
C	0.631799	0.816067	-0.105085
C	1.918929	1.102865	0.198179
C	2.703682	-0.106939	-0.045827
C	1.895519	-1.137981	-0.370441
C	0.490558	-0.630905	-0.457510
H	-0.730164	1.943132	1.191296
H	-0.088582	-1.230936	1.609321
H	-2.474485	-1.803028	1.052211
H	-3.469005	-0.333738	-0.920957
H	-2.262654	1.891494	-0.988283
H	2.292082	2.002991	0.668353
H	3.782208	-0.161592	0.043503
H	2.211875	-2.132871	-0.654855
H	0.023243	-0.838714	-1.424322

Frequencies

-850.2329	147.6494	192.0030
295.8588	337.3646	373.7527
472.7124	552.8985	581.7871
651.6224	671.9502	714.2497
734.4340	775.7268	803.6036
842.7492	851.4538	888.0993
921.8695	940.8859	959.4296
972.9699	979.9393	1012.0323
1019.2896	1039.7733	1062.4003
1116.0368	1143.0568	1154.9999
1192.3334	1228.8669	1245.6452
1314.0848	1328.5013	1358.3576
1388.8042	1413.7186	1438.0131
1553.6900	1580.3627	1647.1056
3092.2169	3112.8202	3167.2718
3180.1334	3187.5140	3208.5070
3213.4671	3232.3775	3240.6255

i76 – p24

C	0.569366	1.601224	-0.000267
C	0.554090	-1.587664	-0.071003
C	1.900248	-1.263173	-0.099135
C	2.496247	-0.004468	-0.015416
C	1.916077	1.260285	0.033142
C	-0.539051	0.763070	-0.004494
C	-1.873911	1.159889	-0.084196
C	-2.685837	0.016212	-0.083320
C	-1.899955	-1.126313	0.004751

C	-0.543247	-0.733078	0.077422
H	0.346974	2.665421	-0.029729
H	0.312643	-2.645684	-0.136802
H	2.586324	-2.099939	-0.186573
H	3.582949	-0.011057	-0.015670
H	2.612433	2.092537	0.063762
H	-2.214831	2.184673	-0.134999
H	-3.766293	0.023414	-0.146004
H	-2.247024	-2.149823	0.015294
H	-0.577340	-0.575452	2.025813

Frequencies

-886.1413	153.9646	170.2020
278.2728	329.3451	346.4733
400.9659	415.4359	432.3417
500.4191	580.3158	611.9027
674.2275	709.5390	723.8094
741.4480	782.0392	805.2436
836.5064	879.9498	917.3258
955.8506	959.8293	971.3322
991.9793	1003.9044	1021.4364
1069.4336	1086.2153	1178.8583
1224.2209	1255.1576	1304.6146
1316.6542	1330.6766	1415.2727
1439.9880	1490.6694	1505.4533
1533.3503	1592.9567	1650.1354
1656.3892	3163.3673	3167.1258
3174.8259	3191.2998	3200.6908
3224.2973	3241.0304	3251.4292

i73 – p26

C	0.652816	0.030721	-0.007510
C	1.525950	1.207962	0.039247
C	2.803956	0.782387	-0.029636
C	2.821806	-0.678726	-0.123184
C	1.548182	-1.140578	-0.076624
C	-0.697142	0.017976	-0.013491
C	-1.567281	-1.166273	-0.053392
C	-2.842531	-0.739464	-0.041293
C	-2.856955	0.734648	0.004936
C	-1.590290	1.186039	0.022442
H	1.365582	-1.606027	2.042829
H	1.182781	2.228184	0.123248
H	3.687044	1.406816	-0.017821
H	3.716227	-1.280404	-0.207490
H	1.221886	-2.160664	-0.210559

H	-1.219610	-2.188103	-0.078220
H	-3.727516	-1.361139	-0.058748
H	-3.754064	1.338710	0.022268
H	-1.263395	2.214481	0.055520

Frequencies

-589.4789	96.8045	124.6102
172.1905	212.8904	239.6587
274.1345	409.2190	447.6773
529.1947	581.2304	613.4465
667.3945	730.1618	764.4376
787.0948	801.5701	814.7296
820.2448	840.3770	909.0629
945.8019	953.9241	958.4222
965.5439	966.8632	1014.8704
1032.4651	1097.5750	1115.4219
1120.4831	1142.8916	1163.1711
1246.3268	1331.1102	1341.6432
1389.8897	1400.0224	1510.1472
1571.7282	1619.6347	1650.1153
1751.0426	3222.7314	3226.5722
3234.1208	3242.9732	3259.7063
3263.6434	3267.0427	3272.4489

i22 – i67

C	-0.843574	1.409888	0.291217
C	-0.104974	-0.824280	-0.626174
C	-1.533610	-1.207835	-0.535329
C	-2.452044	-0.389095	0.006579
C	-2.110381	0.945565	0.444171
C	0.194968	0.579976	-0.234644
C	0.706338	-1.010810	0.657358
C	2.083779	-0.787605	0.677557
C	2.553173	0.265203	-0.169396
C	1.541939	1.069440	-0.588194
H	-0.591125	2.429850	0.562230
H	0.414407	-1.192765	-1.513414
H	-1.824447	-2.174893	-0.931828
H	-3.486514	-0.708709	0.073719
H	-2.883719	1.584813	0.852624
H	0.176304	-1.431915	1.503944
H	2.711205	-1.247527	1.432049
H	3.600689	0.451948	-0.367215
H	1.669515	1.986514	-1.150976

Frequencies

-772.7594	156.1263	199.4278
265.0405	385.8483	432.3233
446.6680	514.5415	582.9772
607.5256	656.5414	691.1822
708.7235	724.6228	748.9094
810.4695	839.9488	866.3264
932.9560	952.2371	967.7660
987.9153	1005.5242	1013.1241
1038.9539	1047.3638	1118.0963
1138.4517	1160.6838	1180.3234
1202.1605	1238.0641	1289.9430
1313.7516	1365.8455	1403.2939
1415.4870	1433.7949	1481.5847
1553.3187	1573.4901	1693.0010
3085.0258	3184.8771	3189.0391
3196.6219	3206.7947	3208.5317
3214.3894	3221.5760	3233.1741

i67 – i76

C	-0.318668	0.615726	-0.068484
C	-0.586317	-0.619477	0.726596
C	-2.056517	-0.801795	0.659483
C	-2.598145	0.164924	-0.161140
C	-1.597592	1.031962	-0.616922
C	0.830869	1.447185	0.139568
C	2.080678	0.955411	0.364628
C	2.442358	-0.388864	0.059960
C	1.560240	-1.262361	-0.515902
C	0.155282	-1.077000	-0.502702
H	0.676973	2.519967	0.084221
H	-0.057291	-0.766259	1.664352
H	-2.587872	-1.613000	1.137529
H	-3.643290	0.232135	-0.434812
H	-1.730707	1.870586	-1.286728
H	2.878204	1.650320	0.604722
H	3.496558	-0.644069	0.079562
H	1.945805	-2.102005	-1.086405
H	-0.451514	-1.541939	-1.272953

Frequencies

-377.7876	183.2011	218.7834
267.0907	381.4539	440.6347
464.8811	538.0899	568.4530
639.6151	669.6052	694.2526
716.7832	753.6491	781.1492

827.0735	863.2214	889.6246
925.3080	946.8294	954.2739
984.7752	987.5521	1011.7587
1035.7178	1055.7958	1103.5248
1121.7691	1133.8056	1195.7948
1218.7376	1222.9060	1261.7624
1304.5751	1347.6812	1386.8515
1405.2081	1452.3538	1489.2216
1513.2758	1548.1580	1660.4287
3158.7544	3174.3374	3183.7654
3189.2193	3197.5628	3209.7267
3220.6933	3236.6918	3249.0848

i2 – i5

C	-1.318750	-1.177031	-0.000042
C	-2.688048	-1.008145	-0.000003
C	-3.124982	0.320529	0.000024
C	-2.227040	1.391978	0.000038
C	-0.848535	1.193493	0.000018
C	-0.414272	-0.127704	-0.000041
H	-0.151457	-1.977134	-0.000002
H	-3.390902	-1.831824	0.000013
H	-4.190085	0.526970	0.000062
H	-2.620532	2.402334	0.000087
H	-0.164630	2.034089	0.000081
C	0.796532	-0.930899	-0.000005
C	2.122893	-0.855323	0.000015
C	2.856643	0.406871	-0.000144
C	4.186734	0.493432	0.000088
H	2.705928	-1.772476	0.000151
H	2.263161	1.317594	-0.000470
H	4.690817	1.452445	-0.000022
H	4.810655	-0.395199	0.000414

Frequencies

-2346.2195	52.2371	86.2429
129.8992	157.4384	296.7406
355.5882	369.5781	411.3816
505.9523	530.3425	618.1089
658.1541	717.3402	720.3266
771.5854	780.7874	878.3577
893.1197	948.2168	956.0988
966.2931	1002.0732	1006.9570
1031.5220	1033.3161	1042.8014
1126.0544	1159.5155	1187.5741
1197.6943	1267.3154	1312.3736

1322.7465	1351.9324	1456.1357
1472.9702	1494.4049	1625.2966
1661.6260	1700.5694	1741.2532
1905.7777	3151.0450	3166.1979
3174.4414	3190.1903	3204.9178
3219.0841	3226.1189	3249.9042

i18 – i20

C	-1.439538	-1.307168	-0.000006
C	-2.638291	-0.614241	-0.000020
C	-2.648584	0.779394	-0.000012
C	-1.445491	1.476955	0.000013
C	-0.264435	0.761656	0.000028
C	-0.207789	-0.628487	0.000016
C	1.032123	-1.401721	0.000020
C	2.314225	-0.990029	0.000000
C	2.870508	0.360140	-0.000027
C	2.197631	1.505817	0.000000
H	-1.443914	-2.393107	-0.000014
H	-3.574803	-1.160251	-0.000039
H	-3.590376	1.317042	-0.000025
H	-1.435636	2.561618	0.000021
H	0.878169	-2.478062	0.000033
H	3.061962	-1.777674	-0.000001
H	3.959808	0.405578	-0.000072
H	0.908750	1.364053	0.000040
H	2.613878	2.506910	-0.000023

Frequencies

-1486.5577	59.0766	146.3029
244.2897	268.3763	395.1824
399.5608	424.6903	433.1159
543.3871	565.3568	651.2109
681.7067	725.7888	757.9618
762.7677	816.8253	844.8473
876.8801	948.8869	952.2180
961.4408	1007.2661	1014.8766
1025.3927	1030.2383	1059.9049
1090.3208	1150.4963	1186.4019
1225.9307	1254.0133	1299.0947
1328.0368	1349.6506	1455.1708
1467.1828	1486.7609	1541.1338
1624.8026	1659.8726	1671.8388
1717.5316	3128.4112	3163.8858
3184.7387	3191.3683	3193.1039
3205.2472	3215.6095	3218.5332

i5 – i11

C	-0.583638	-0.533093	0.000000
C	-1.979786	-0.601315	0.000000
C	-2.735604	0.565316	0.000000
C	-2.116655	1.810729	0.000000
C	-0.722888	1.899684	0.000000
C	0.000000	0.728681	0.000000
C	0.268236	-1.728943	0.000000
C	1.608958	-1.658321	0.000000
C	2.290137	-0.382483	0.000000
C	3.578478	-0.078955	0.000000
H	-2.471506	-1.569297	0.000000
H	-3.817887	0.502253	0.000000
H	-2.715634	2.714944	0.000000
H	-0.231767	2.866365	0.000000
H	-0.226195	-2.694972	0.000000
H	2.206729	-2.567544	0.000000
H	1.345988	0.528303	0.000000
H	3.925209	0.948791	0.000000
H	4.341626	-0.856646	0.000000

Frequencies

-1704.4097	72.7278	158.5075
210.4057	223.8330	328.7424
399.1467	423.6188	433.9298
499.0654	519.7078	610.4122
656.0347	723.9015	728.8261
767.5384	818.0888	833.4290
879.8186	927.1301	939.7767
960.5809	994.7768	1007.1534
1018.1307	1059.2992	1099.3651
1117.2750	1156.6560	1184.4464
1209.5823	1250.8485	1291.2538
1335.7361	1397.8763	1448.6373
1479.6766	1488.8165	1613.9403
1628.2572	1657.9407	1684.4473
1733.5587	3120.1371	3148.9970
3184.1553	3191.7743	3203.1762
3207.2085	3215.6903	3218.2328

i8 – p14

C	-0.507553	-0.437685	0.000091
C	-0.675531	0.951509	0.000180
C	-1.944473	1.505933	0.000087
C	-3.069139	0.684959	-0.000097

C	-2.914220	-0.695156	-0.000167
C	-1.642730	-1.252251	-0.000063
C	0.822239	-1.055995	0.000175
C	1.971440	-0.415432	0.000016
C	3.184974	-0.007111	-0.000055
C	4.263554	0.747138	-0.000161
H	0.200255	1.591832	0.000341
H	-2.061223	2.583746	0.000140
H	-4.060882	1.122374	-0.000192
H	-3.785066	-1.340769	-0.000306
H	-1.524104	-2.331003	-0.000091
H	0.856279	-2.145587	0.000382
H	5.258594	0.321495	-0.000039
H	4.165935	1.827877	-0.000397
H	4.018852	-1.785414	0.000123

Frequencies

-798.0084	40.2837	66.8720
105.2164	200.5465	233.1926
248.9511	364.9488	414.1469
437.3150	457.6002	501.2782
535.1616	629.2153	634.3692
637.7877	710.3783	775.6281
831.9971	856.3986	875.2765
890.5115	945.7861	959.0612
1000.6127	1018.6885	1024.4020
1033.4219	1061.5101	1117.6968
1189.0245	1208.7052	1227.7863
1301.1154	1347.5194	1364.3301
1452.3815	1499.8890	1541.3926
1653.8555	1678.2926	1712.3871
2133.1412	3137.2257	3159.9184
3186.2115	3188.8250	3201.3850
3207.7198	3222.8238	3257.2483

i9 – p12

C	-0.454102	-0.180729	-0.066897
C	-1.317376	-1.280627	-0.034300
C	-2.692405	-1.109505	0.042422
C	-3.231969	0.169199	0.082135
C	-2.386362	1.273957	0.040959
C	-1.013913	1.102446	-0.034644
C	0.989652	-0.424706	-0.132965
C	1.963185	0.491846	-0.012704
C	3.339025	0.165156	-0.085839
C	4.516371	-0.109006	-0.079670

H	-0.899669	-2.281741	-0.064677
H	-3.343105	-1.976051	0.070219
H	-4.305286	0.307746	0.142103
H	-2.802362	2.274770	0.064044
H	-0.374581	1.976824	-0.078074
H	1.285008	-1.459915	-0.281904
H	1.731216	1.538778	0.157766
H	5.544664	-0.314103	-0.259544
H	4.891473	-0.654491	1.939083

Frequencies

-567.9619	47.9884	77.3637
91.1572	122.6559	233.0394
239.3457	298.9330	382.7316
413.1036	447.4951	500.9769
542.4782	638.0201	641.6394
707.1289	709.4576	757.1459
774.5020	859.0630	867.1793
889.8244	942.3837	997.4154
1006.5833	1022.1715	1023.5034
1042.2046	1067.0807	1120.7384
1190.6916	1215.3653	1241.1140
1307.9550	1335.0530	1352.6426
1369.8424	1495.8067	1544.5889
1652.5271	1679.9095	1696.1641
2170.5814	3180.7457	3186.1430
3189.2266	3196.0596	3203.4756
3211.5844	3222.8341	3469.7263

i8 – i10

C	-0.474686	0.541036	-0.110670
C	-0.627121	-0.842258	-0.057001
C	-1.833588	-1.470705	0.082668
C	-2.972987	-0.650645	0.158107
C	-2.853422	0.729918	0.102946
C	-1.602187	1.341466	-0.029588
C	0.952792	0.892392	-0.245504
C	1.724250	-0.191033	-0.265332
C	3.136088	-0.463895	-0.304857
C	4.019642	0.063954	0.549139
H	0.755061	-1.126936	-0.183622
H	-1.925302	-2.550025	0.128384
H	-3.952543	-1.105045	0.259140
H	-3.744065	1.345093	0.164586
H	-1.520168	2.423019	-0.064063
H	1.316740	1.910693	-0.339514

H	3.477954	-1.167817	-1.060687
H	3.703548	0.738533	1.337606
H	5.076088	-0.168889	0.478718

Frequencies

-2042.7375	72.5853	94.2068
172.5551	219.2467	282.3334
364.5561	402.8363	412.8700
542.6316	556.5986	630.4904
651.4114	697.7217	725.5837
766.2874	859.1408	864.7097
895.4822	953.9026	954.2336
989.9541	1007.2006	1027.0421
1027.5565	1042.7540	1063.9775
1110.5866	1132.0062	1181.3332
1187.8447	1248.6077	1307.6739
1325.9828	1372.7717	1444.8153
1476.5140	1489.5171	1643.0157
1653.4189	1667.0468	1703.5324
1763.6946	3153.4993	3164.2785
3182.8425	3190.8419	3194.9253
3202.8190	3212.5659	3254.7377

i8 – i11

C	0.448677	-0.584503	-0.019779
C	1.706659	-1.205344	0.029915
C	2.871852	-0.455616	0.038530
C	2.811740	0.933667	0.001991
C	1.571980	1.563590	-0.047305
C	0.403960	0.818808	-0.057206
C	-0.754031	-1.402309	-0.032598
C	-2.004575	-0.904670	0.158912
C	-2.916076	0.025493	-0.057831
C	-3.834146	0.978284	0.065982
H	1.761438	-2.288856	0.061795
H	3.832790	-0.956624	0.075062
H	3.723287	1.520024	0.010129
H	1.515488	2.645983	-0.081931
H	-0.553513	1.325276	-0.106730
H	-0.626167	-2.477018	-0.109070
H	-3.094500	-1.152564	-0.564380
H	-3.721488	1.726632	0.842299
H	-4.673574	1.052750	-0.610842

Frequencies

-1509.2363	45.5923	66.1831
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169.1410	229.4319	266.8888
363.5351	387.3608	415.7540
494.1065	518.4159	542.7982
635.4473	643.8344	707.7973
735.4853	755.9131	793.0330
816.9043	851.9466	912.5520
920.5838	929.6543	989.5040
1011.4252	1017.0127	1062.1824
1066.9450	1122.2990	1186.5574
1209.8385	1238.2750	1312.0279
1343.8243	1362.9387	1414.0803
1485.8483	1520.0046	1536.4250
1642.9368	1664.0119	1859.7622
2269.2627	3159.4682	3182.7557
3185.5032	3191.2134	3201.7825
3211.5454	3219.2230	3263.0991

ill - p13

C	-0.337173	-0.594930	0.104365
C	-1.577035	-1.214242	-0.098264
C	-2.742461	-0.470126	-0.198372
C	-2.692903	0.913858	-0.082138
C	-1.472425	1.541602	0.137819
C	-0.304452	0.799387	0.230961
C	0.849275	-1.451413	0.191010
C	2.154105	-1.145191	0.075688
C	2.725700	0.121427	-0.196344
C	3.270010	1.185589	-0.380366
H	-1.621838	-2.295266	-0.185520
H	-3.690257	-0.969964	-0.362241
H	-3.602491	1.499136	-0.155214
H	-1.428480	2.619596	0.244002
H	0.634255	1.303440	0.415688
H	0.629648	-2.502795	0.357784
H	2.873299	-1.952201	0.178867
H	3.746807	2.072285	-0.724669
H	3.223213	2.109997	1.525147

Frequencies

-561.1935	30.3698	71.3972
124.2509	162.5766	216.6824
260.0823	352.1385	390.2893
417.6355	456.3237	522.5289
594.5624	636.4087	687.0320
715.6764	739.2295	749.9763
763.7922	805.7119	826.4668

873.8986	954.6740	983.3975
1008.1654	1017.9517	1024.6544
1030.1556	1065.7736	1124.1751
1188.8866	1217.1125	1223.1336
1277.4142	1348.0562	1372.4354
1450.2881	1494.8156	1545.7430
1647.3675	1680.4636	1688.9752
2165.1884	3167.4882	3184.2860
3188.0606	3195.0354	3206.2374
3218.6950	3245.2657	3470.0065

i4 – p12

C	0.426276	0.176389	-0.049615
C	1.280486	1.282896	-0.020065
C	2.658204	1.122305	0.030953
C	3.208668	-0.152185	0.046293
C	2.371437	-1.263239	0.006397
C	0.996318	-1.102146	-0.043485
C	-1.022362	0.408494	-0.087815
C	-1.980473	-0.512710	0.075715
C	-3.372607	-0.171182	0.028850
C	-4.419484	0.445678	0.057829
H	0.854240	2.280823	-0.032079
H	3.302141	1.993997	0.056848
H	4.284043	-0.282483	0.084748
H	2.795824	-2.260786	0.008286
H	0.362786	-1.980581	-0.089966
H	-1.329719	1.437617	-0.254017
H	-1.739715	-1.553261	0.258230
H	-5.400038	0.858452	0.051134
H	-4.008339	-1.899578	-0.353523

Frequencies

-857.8553	33.4002	56.8609
93.9732	129.6078	247.1947
267.3675	392.3642	413.1993
440.7418	504.3091	539.9512
554.5981	632.4056	639.6535
651.4173	691.4994	709.0792
772.6801	859.2537	868.5688
891.8466	941.6117	997.0780
1011.3786	1021.5958	1023.3592
1029.4113	1067.6356	1122.0305
1190.3771	1218.5306	1242.2608
1310.5837	1341.6974	1351.1863
1374.3901	1495.7015	1546.3093

1654.0859	1681.5634	1709.5900
2125.0050	3181.9991	3188.7571
3194.6761	3202.5739	3207.8435
3212.4416	3223.0561	3470.9256

i107 – p2

C	0.503019	-0.072387	0.024327
C	1.112713	1.184590	0.134192
C	2.493265	1.296002	0.083200
C	3.282213	0.161607	-0.076075
C	2.684649	-1.089427	-0.184758
C	1.304837	-1.210823	-0.135550
C	-0.912912	-0.193956	0.075790
C	-2.111676	-0.340554	0.219452
C	-3.533077	-0.400311	0.045337
C	-4.264906	0.635925	-0.359992
H	0.493193	2.064477	0.259662
H	2.956963	2.271799	0.170113
H	4.361493	0.253440	-0.116642
H	3.296801	-1.975449	-0.307539
H	0.832741	-2.182180	-0.219878
H	-2.134356	-1.040888	2.052953
H	-4.004910	-1.352802	0.264697
H	-3.814491	1.598971	-0.570340
H	-5.336191	0.538633	-0.488568

Frequencies

-768.7724	35.5479	69.8272
89.4358	99.4980	216.0172
258.3646	351.4590	412.7439
433.7685	458.0551	513.3103
556.8637	604.0019	643.4831
705.5163	709.1271	725.2150
781.2604	867.6418	946.5194
955.0455	973.3488	1003.5176
1021.2112	1022.1915	1024.8883
1059.1919	1108.4432	1113.3932
1189.2593	1208.4590	1303.1579
1318.5825	1334.5533	1356.5477
1452.4314	1487.7091	1539.3783
1643.1720	1672.8311	1702.2014
2261.9976	3166.4913	3191.3384
3193.9966	3204.4835	3212.7784
3223.0919	3227.4460	3263.5816

i8 – p2

C	0.506610	-0.147708	0.037235
C	1.388839	-1.231481	0.049920
C	2.758008	-1.016864	0.009124
C	3.263203	0.277528	-0.038909
C	2.391325	1.360017	-0.046272
C	1.020320	1.152520	-0.008717
C	-0.919089	-0.344407	0.041276
C	-2.112899	-0.262190	-0.174793
C	-3.517593	-0.282071	-0.363231
C	-4.364890	0.540968	0.260584
H	0.989285	-2.237441	0.096569
H	3.434693	-1.863597	0.017431
H	4.334163	0.442249	-0.069042
H	2.780610	2.371070	-0.082089
H	0.334946	1.991619	-0.016479
H	-1.015673	-1.726097	1.476736
H	-3.895973	-1.021600	-1.063783
H	-4.014137	1.285429	0.965787
H	-5.430917	0.480495	0.077562

Frequencies

-750.5686	45.3005	59.4829
105.7575	134.7419	200.2778
262.8503	352.7051	413.8117
420.5668	476.9474	519.8251
557.1295	592.2270	640.9791
706.7912	711.4540	727.7303
780.7429	868.7895	947.7474
960.3701	973.5931	1003.3458
1020.9031	1023.0876	1024.1256
1060.4188	1111.2385	1112.3814
1189.6792	1206.8209	1288.2959
1317.8940	1328.0324	1354.3930
1452.0307	1488.4503	1537.7888
1648.2664	1674.6129	1685.1521
2261.3118	3163.1545	3172.8745
3195.0856	3203.8662	3214.1062
3221.1246	3226.6387	3264.5987

i9 – p14

C	-0.480031	-0.469594	0.020271
C	-1.639630	-1.246546	-0.080988
C	-2.890697	-0.649377	-0.126281
C	-3.003603	0.734387	-0.064963
C	-1.857156	1.517479	0.041066
C	-0.606938	0.923922	0.084308

C	0.821899	-1.126145	0.058027
C	1.997208	-0.500132	0.148599
C	3.132330	0.030213	-0.044482
C	4.299326	0.588417	-0.256861
H	-1.552821	-2.327334	-0.128230
H	-3.779757	-1.264355	-0.206731
H	-3.980485	1.202906	-0.098113
H	-1.942755	2.596873	0.094253
H	0.286188	1.532825	0.171301
H	0.824491	-2.213997	0.066924
H	1.913625	0.005579	2.123578
H	4.391146	1.660014	-0.396404
H	5.204112	-0.008260	-0.298763

Frequencies

-750.7658	52.2111	61.6607
125.2021	198.8421	252.4244
263.5398	345.7332	398.8688
414.3850	426.1816	452.0446
544.7256	607.4502	633.0553
637.1751	708.3152	773.0964
834.3539	850.0382	865.1043
889.0165	944.0733	952.1825
998.5354	1018.1266	1022.6519
1026.1950	1060.5690	1118.8404
1189.7096	1205.7869	1232.0263
1307.6460	1349.7283	1363.5869
1439.7016	1500.0970	1537.5164
1643.2673	1661.9574	1674.0177
2166.1456	3150.4529	3163.3452
3186.7674	3194.4753	3204.9705
3212.3154	3223.1400	3236.7950

i75 – p26

C	-0.627968	0.015792	-0.043598
C	-1.497438	1.202948	-0.034233
C	-2.773506	0.784155	-0.068534
C	-2.791668	-0.693231	-0.097974
C	-1.514076	-1.145398	-0.096408
C	0.726102	0.003147	-0.014279
C	1.596478	-1.181154	-0.019751
C	2.871830	-0.754207	0.016187
C	2.884776	0.719598	0.045929
C	1.616869	1.170445	0.027732
H	-1.147562	2.223664	0.003529
H	-3.657694	1.406489	-0.066772

H	-3.683481	-1.294608	-0.208769
H	-3.347474	-0.838116	2.018814
H	-1.190079	-2.174450	-0.131424
H	1.250401	-2.203477	-0.047295
H	3.756907	-1.375947	0.022924
H	3.780851	1.324642	0.076967
H	1.289741	2.199236	0.041596

Frequencies

-592.7636	93.4311	119.8547
171.8241	197.4463	218.1504
280.9347	408.6249	448.0551
536.1224	584.2210	609.9220
660.0917	728.7338	730.8451
786.1046	801.2119	816.6979
822.0735	841.1051	908.5741
942.7684	950.9500	955.9447
960.9290	964.3309	1009.3769
1031.5048	1096.7065	1115.7615
1117.3429	1143.2597	1163.5747
1246.6562	1331.2383	1340.7339
1386.2217	1400.2046	1531.4437
1568.3874	1627.2038	1644.7289
1706.0625	3222.7650	3229.6524
3234.2005	3243.0982	3258.6511
3262.8857	3265.1935	3270.0063

$i2 - i3$

C	-1.016017	1.172779	0.268500
C	-2.355836	1.321854	-0.018569
C	-3.151052	0.212342	-0.316834
C	-2.581558	-1.063342	-0.324586
C	-1.244513	-1.240830	-0.040714
C	-0.415909	-0.121063	0.266126
C	0.912263	-0.284461	0.560739
C	2.187920	-0.426328	0.760033
H	-0.399743	2.033379	0.499543
H	-2.795716	2.312945	-0.012262
H	-4.203568	0.341249	-0.539079
H	-3.195772	-1.926194	-0.557322
H	-0.803190	-2.230282	-0.047029
H	2.561235	-0.594171	1.774273
C	3.209821	-0.390071	-0.331094
C	3.949979	0.672526	-0.614216
H	3.338804	-1.308615	-0.899437
H	4.686471	0.648655	-1.409780

H 3.840900 1.602596 -0.065213

Frequencies

-133.9077	28.2966	72.5060
159.5437	180.2909	340.3047
405.7242	431.9700	464.1825
480.3994	539.6272	631.4288
674.1229	686.7541	757.1039
791.3976	801.0189	831.2844
902.1852	933.1868	975.7360
985.9780	990.0550	1002.1014
1026.0067	1043.2620	1106.3420
1111.3122	1153.1081	1177.8910
1207.1909	1303.1505	1308.4834
1320.8191	1348.7541	1447.7512
1469.0305	1495.3569	1591.1106
1615.3295	1720.4470	1914.7021
3076.5494	3152.8960	3168.1610
3190.2895	3198.1856	3211.7464
3219.3700	3225.2884	3246.5759

i71 – p26

C	-0.667260	0.000000	0.107716
C	-1.550732	-1.177708	0.022061
C	-2.811407	-0.735152	-0.134792
C	-2.811408	0.735150	-0.134792
C	-1.550733	1.177708	0.022060
C	0.694303	0.000001	0.025014
C	1.569425	1.174873	-0.014419
C	2.841828	0.737092	-0.072716
C	2.841828	-0.737093	-0.072716
C	1.569425	-1.174873	-0.014419
H	-0.856669	0.000003	2.191861
H	-1.214539	-2.202768	0.058749
H	-3.695266	-1.348872	-0.243591
H	-3.695268	1.348870	-0.243592
H	-1.214541	2.202769	0.058747
H	1.231311	2.199999	0.003406
H	3.731025	1.351423	-0.113485
H	3.731024	-1.351424	-0.113486
H	1.231310	-2.199999	0.003406

Frequencies

-723.9131	103.3502	115.9322
154.8978	181.1046	256.7768

357.2117	406.4440	446.7412
533.5756	580.3967	601.1764
662.1067	734.9121	739.4356
776.6507	798.3630	811.3865
813.5614	842.6810	909.6093
946.1026	953.9423	959.6652
960.0073	964.8533	1013.3620
1035.6883	1106.4082	1114.0214
1118.5174	1150.1209	1151.7642
1249.4127	1329.9037	1336.9924
1387.9925	1405.5629	1559.6479
1564.4614	1631.8936	1645.4137
1647.2884	3224.9087	3225.5251
3235.4134	3236.9121	3257.0057
3261.3357	3261.8630	3266.4047

i20 – p13

C	1.478517	-1.227705	-0.255165
C	2.667465	-0.523124	-0.367893
C	2.699636	0.834115	-0.071222
C	1.537420	1.475054	0.341675
C	0.345240	0.773055	0.445124
C	0.295684	-0.590467	0.136081
C	-0.926937	-1.399561	0.228912
C	-2.210105	-1.026297	0.140891
C	-2.708814	0.294082	-0.123146
C	-3.028495	1.327844	-0.677173
H	1.459059	-2.289519	-0.479611
H	3.570590	-1.034020	-0.681698
H	3.628410	1.387258	-0.152638
H	1.559931	2.530308	0.589502
H	-0.548533	1.281591	0.781579
H	-0.754651	-2.463502	0.369953
H	-2.976823	-1.785170	0.257718
H	-3.468754	0.477633	1.555063
H	-3.366892	2.273448	-1.028369

Frequencies

-926.5389	29.4618	58.1013
122.2658	168.9515	235.4593
329.7838	392.6172	417.6399
460.5729	475.9742	524.8561
591.0710	628.5857	638.1533
694.0833	716.0402	734.4403
762.7382	803.3493	827.0842
867.5985	951.9129	972.0978

1000.9354	1017.9543	1023.7821
1024.8911	1063.5911	1121.3858
1187.7966	1215.8238	1220.9010
1277.0355	1345.8899	1366.6557
1445.0443	1494.1242	1543.0866
1650.3053	1680.8801	1712.4186
2120.2220	3167.8745	3185.0394
3190.0717	3193.5438	3205.9300
3219.6763	3238.0766	3470.0399

i66 – i67

C	-0.830586	1.390099	0.225297
C	-0.210997	-0.906072	-0.644497
C	-1.565184	-1.255560	-0.515212
C	-2.477605	-0.393574	0.047535
C	-2.101205	0.959063	0.356151
C	0.269303	0.446739	-0.104677
C	0.751402	-0.545186	0.916554
C	2.129840	-0.680890	0.771728
C	2.576278	0.202084	-0.256797
C	1.520936	0.893506	-0.770605
H	-0.571838	2.431471	0.376663
H	0.461488	-1.465292	-1.280634
H	-1.893559	-2.209428	-0.914033
H	-3.514047	-0.690820	0.152775
H	-2.877341	1.660753	0.642302
H	0.128013	-0.915687	1.715502
H	2.753018	-1.363003	1.333137
H	3.600646	0.281641	-0.597604
H	1.540527	1.609116	-1.580976

Frequencies

-637.4374	149.8381	222.0150
245.3623	405.2595	412.4571
454.2544	567.2177	582.0858
627.0676	669.1890	712.4477
726.3977	763.7113	789.1385
816.1411	837.1340	877.9777
905.7727	914.7735	951.6683
954.4707	979.8221	993.1903
998.6361	1044.9068	1079.5846
1097.4933	1118.6548	1161.3819
1180.9068	1214.7922	1249.6917
1292.6968	1308.4805	1368.7095
1420.0937	1453.4009	1473.7760
1502.3157	1553.3759	1659.0595

3188.5245	3194.3777	3213.9944
3221.7846	3222.5556	3232.9657
3239.4532	3251.0860	3267.7527

i21 – i68

C	-1.383078	1.356323	0.111144
C	1.410362	-1.063629	-0.260483
C	-1.113675	-1.436520	-0.112303
C	-2.363771	-0.854685	0.029765
C	-2.491152	0.538222	0.148868
C	-0.101059	0.784134	-0.039354
C	1.139558	1.442261	-0.209611
C	2.306082	0.605328	-0.347415
C	2.423408	-0.461881	0.705137
C	0.019903	-0.628792	-0.113866
H	-1.487703	2.433276	0.183028
H	1.899671	-0.335719	-1.238431
H	1.632230	-2.060283	-0.637483
H	-1.015541	-2.513383	-0.199864
H	-3.249978	-1.478223	0.052928
H	-3.477539	0.974796	0.259252
H	1.226380	2.516194	-0.324722
H	3.362950	-1.007544	0.745328
H	2.030064	-0.213673	1.688673

Frequencies

-1151.5827	159.8898	188.2403
361.7638	365.0289	440.4662
459.3919	514.8117	551.2722
567.8125	618.5793	703.7981
709.8437	761.7958	786.6021
788.4325	873.1395	889.4521
918.7597	945.8169	971.9043
1010.3781	1019.6649	1048.2938
1058.2836	1075.2371	1138.2135
1149.2755	1174.6509	1187.8754
1213.1279	1244.7058	1267.4603
1312.3266	1338.9893	1386.1971
1406.7772	1487.4354	1497.2575
1519.8992	1612.8791	1656.0789
2066.1685	3114.6177	3151.6894
3183.7264	3191.5763	3192.2857
3203.3574	3208.4200	3213.0524

i73 – i75

C	-0.669279	0.019312	-0.033117
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C	-1.521300	1.153873	0.014611
C	-2.845806	0.763609	0.014053
C	-2.896201	-0.650849	-0.043299
C	-1.504780	-1.124728	-0.082036
C	0.754336	0.008320	-0.010753
C	1.602326	-1.160858	0.025449
C	2.895528	-0.737388	0.029228
C	2.904656	0.725215	-0.008862
C	1.616687	1.165353	-0.031332
H	-1.172820	2.173486	0.107861
H	-3.707567	1.410357	0.084356
H	-3.758283	-1.281055	-0.209261
H	-1.214311	-2.151332	-0.250797
H	-2.278813	-1.107102	0.999019
H	1.258439	-2.184983	0.055376
H	3.777273	-1.363157	0.057179
H	3.794524	1.339953	-0.018628
H	1.284551	2.192664	-0.068758

Frequencies

-1247.7338	73.4293	112.7423
157.6113	293.2921	394.8184
438.4415	553.0572	590.6230
614.4615	655.9586	706.2945
741.7651	752.4842	779.7547
796.8309	849.4428	855.3545
895.7098	919.2037	928.1400
941.1414	990.4339	1001.5967
1020.4818	1053.5395	1075.3484
1086.1894	1104.4578	1143.9805
1146.3367	1235.5361	1251.8197
1297.0125	1336.2121	1394.3267
1423.2479	1448.8836	1504.0987
1525.9844	1562.4812	1565.7111
2140.2589	3218.8679	3229.4927
3237.8834	3247.5469	3249.4183
3255.1390	3260.7535	3268.5178

i76 – i77

C	0.605674	1.616976	0.029063
C	0.594597	-1.612727	-0.046597
C	1.916668	-1.275062	-0.072861
C	2.531881	-0.005409	-0.005302
C	1.931145	1.269121	0.038530
C	-0.534146	0.740823	-0.001693
C	-1.868663	1.153261	-0.089674

C	-2.726240	0.053093	-0.072205
C	-1.945159	-1.105305	0.026971
C	-0.525210	-0.691471	0.074113
H	0.373791	2.677976	0.027884
H	0.337631	-2.665116	-0.115163
H	2.606395	-2.110573	-0.163515
H	3.616721	-0.012864	-0.015737
H	2.631272	2.100240	0.062327
H	-2.182462	2.189304	-0.109730
H	-3.805648	0.078376	-0.080072
H	-2.259874	-2.138384	-0.026358
H	-1.201103	-0.978762	1.138293

Frequencies

-1197.8586	112.0360	189.3725
308.7713	334.0689	391.3519
422.8582	500.9432	578.7321
599.6416	663.5940	672.0275
707.1891	757.7914	771.0155
779.3533	819.3377	870.5762
903.6085	918.3796	927.7183
941.8084	988.9747	994.4116
1041.0991	1081.4511	1116.9127
1148.6308	1187.7511	1207.4820
1250.8748	1256.7437	1284.2743
1349.3746	1391.9319	1434.9349
1472.2191	1481.4624	1492.6525
1554.3877	1595.4907	1630.2499
2084.5494	3161.9324	3165.2145
3182.6934	3188.8264	3201.5816
3220.7849	3241.0521	3263.1956

i77 – i78

C	0.614115	1.608712	-0.000672
C	0.606769	-1.602957	-0.013321
C	1.935938	-1.275810	0.001956
C	2.549012	-0.006030	0.012138
C	1.937488	1.267213	0.014435
C	-0.529383	0.719348	-0.039890
C	-1.853603	1.167577	-0.026427
C	-2.717786	0.060302	-0.016642
C	-1.858955	-1.139719	-0.030197
C	-0.518959	-0.703804	-0.038033
H	0.376374	2.668203	0.006490
H	0.359427	-2.660662	-0.011660
H	2.625001	-2.116596	0.011109

H	3.633882	-0.006205	0.026113
H	2.633103	2.102889	0.031963
H	-2.164236	2.201795	0.015566
H	-3.790127	0.044548	-0.146932
H	-2.219391	-2.150766	-0.159696
H	-2.441848	-0.652207	1.046958

Frequencies

-1257.9488	111.6336	184.8054
298.8769	336.1089	393.9132
417.9704	500.5832	572.0611
611.0702	673.2953	678.0682
701.1404	759.5547	769.4410
780.0884	818.1032	841.1693
870.7925	917.6873	943.2482
989.2740	991.4221	1001.7200
1013.3864	1048.3427	1112.1170
1158.5233	1184.3452	1220.8839
1246.3767	1260.1938	1267.1594
1346.7080	1397.4955	1425.7270
1451.0532	1481.4146	1502.0914
1557.1575	1601.4583	1630.0586
2097.3812	3158.5834	3161.0635
3178.6150	3183.0148	3200.1735
3238.5059	3245.3703	3260.1981

i2 – p21

C	-1.174037	1.158110	0.364433
C	-2.472140	1.279616	-0.106553
C	-3.176979	0.153654	-0.518715
C	-2.576954	-1.099453	-0.457024
C	-1.279264	-1.230989	0.012218
C	-0.561875	-0.100846	0.427162
C	0.775243	-0.229161	0.899682
C	1.954421	-0.311965	1.170868
C	3.270659	0.078810	-0.796024
C	4.562742	0.206042	-0.636399
H	-0.620099	2.032020	0.685831
H	-2.936738	2.257816	-0.153698
H	-4.191209	0.253204	-0.888012
H	-3.122908	-1.979526	-0.777133
H	-0.806608	-2.204566	0.062323
H	2.872202	-0.440267	1.696504
H	2.606625	0.133071	-1.647776
H	5.230649	0.410685	-1.475057
H	5.037197	0.114656	0.339125

Frequencies

-343.2699	20.6016	41.0729
48.5235	152.3934	161.6795
173.1556	217.9793	377.7859
412.5237	479.9909	543.8671
547.5957	640.6102	696.1012
708.8771	719.4833	771.4586
779.2342	784.3656	864.8004
895.5158	940.9207	943.1595
1000.2877	1017.6900	1022.7325
1060.9611	1077.7397	1114.5420
1190.6556	1209.0000	1235.2168
1318.8801	1359.2981	1402.4441
1489.4685	1536.7595	1643.9998
1663.8991	1673.3494	2136.6632
3086.3383	3162.9482	3193.5333
3202.3506	3212.1388	3219.9965
3225.4007	3246.1196	3442.8187

i78 – p24

C	0.597764	-1.590753	-0.012299
C	0.597771	1.590751	-0.012269
C	1.946878	1.262103	0.022190
C	2.536020	-0.000005	0.038528
C	1.946866	-1.262117	0.022146
C	-0.507403	-0.745776	-0.040690
C	-1.840616	-1.149790	-0.080704
C	-2.654002	0.000027	-0.080605
C	-1.840609	1.149815	-0.080755
C	-0.507394	0.745784	-0.040694
H	0.367851	-2.653890	-0.018843
H	0.367863	2.653890	-0.018733
H	2.636281	2.100462	0.040057
H	3.622333	-0.000010	0.068575
H	2.636265	-2.100479	0.040009
H	-2.185948	-2.173790	-0.092147
H	-3.182943	-0.000267	1.880745
H	-3.727438	0.000025	-0.216567
H	-2.185915	2.173825	-0.092192

Frequencies

-703.1622	154.3168	156.8235
252.2620	273.5985	340.6528
360.1401	412.9262	428.3343
491.8631	584.9909	615.5395

688.5915	712.3973	722.8117
747.2139	792.6652	802.7546
839.2114	884.7278	917.1177
972.1010	972.7043	973.4860
981.4119	1005.3229	1024.5101
1067.9578	1068.4257	1176.7852
1222.4267	1257.0969	1309.5933
1320.5442	1332.3252	1434.7064
1448.0951	1485.0514	1495.6891
1517.2276	1592.6537	1649.0040
1659.3366	3161.0671	3162.8231
3172.7126	3190.9625	3200.4490
3226.5701	3243.4278	3251.6802

i20 – p15

C	1.421563	-1.194232	-0.445670
C	2.567683	-0.417391	-0.549154
C	2.589115	0.865276	-0.016225
C	1.458551	1.360495	0.625055
C	0.312929	0.584800	0.725944
C	0.273792	-0.700982	0.179691
C	-0.926750	-1.556299	0.256725
C	-2.187150	-1.185556	0.358036
C	-3.034689	0.875197	-0.083748
C	-2.452435	1.399245	-1.012084
H	1.410289	-2.196256	-0.863067
H	3.446573	-0.816859	-1.042714
H	3.484702	1.471751	-0.090359
H	1.472784	2.354352	1.058622
H	-0.561490	0.970137	1.234736
H	-0.728279	-2.631359	0.205301
H	-3.079212	-1.798756	0.390106
H	-3.764233	0.761212	0.686694
H	-1.816774	1.702460	-1.810735

Frequencies

-468.6758	26.9464	55.4072
108.7842	142.5243	205.1130
234.4958	314.7692	421.5974
439.4400	487.1970	579.5879
603.1664	637.4046	670.2824
689.3409	722.8975	772.2180
783.3434	788.8885	807.5579
875.0707	894.9559	950.9444
989.5608	1006.4491	1023.6532
1024.1758	1062.1760	1113.7616

1183.3787	1210.8019	1230.8590
1282.7689	1338.3589	1359.2145
1489.1521	1539.2646	1648.2946
1678.1834	1687.1630	1943.2857
3077.7328	3187.2206	3194.9757
3207.3571	3217.0422	3218.6451
3234.4705	3392.4216	3483.7649

i23 – i24

C	-1.270100	1.386276	0.024101
C	-2.481188	0.695968	0.009535
C	-2.478852	-0.690702	-0.023456
C	-1.275879	-1.388100	-0.031287
C	-0.052952	-0.711053	-0.002314
C	-0.054787	0.711509	0.013224
C	1.217779	1.429172	-0.009540
C	2.408578	0.780769	-0.051257
C	2.486020	-0.644667	-0.019926
C	1.206554	-1.416623	0.006188
H	-1.266725	2.471702	0.038205
H	-3.417425	1.241703	0.020392
H	-3.415893	-1.236042	-0.039491
H	-1.278273	-2.473071	-0.055681
H	1.187012	2.513075	-0.011176
H	3.334256	1.343442	-0.097387
H	1.977433	-1.118740	1.046727
H	3.404096	-1.170652	-0.243933
H	1.244472	-2.486713	-0.149259

Frequencies

-2110.2154	153.2582	164.4927
323.6589	361.9487	445.4745
471.4985	499.9282	511.5666
584.1660	610.7550	635.0393
722.9335	759.1512	764.2234
786.1045	795.0174	841.9538
876.7080	927.6653	942.7410
953.4022	968.0744	991.4969
1069.6246	1103.2901	1146.6758
1165.9241	1187.0007	1209.4684
1232.7324	1240.4488	1293.4400
1329.8077	1375.8360	1388.7736
1456.9109	1488.7475	1522.5696
1580.2578	1632.2245	1645.3111
2198.9788	3185.4035	3189.9513
3193.0176	3203.6877	3210.2924

3219.5625	3220.7477	3233.2552
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i8 – p23

C	0.672501	-0.565833	0.011452
C	0.572088	0.799865	-0.096226
C	1.760798	1.530170	-0.106921
C	2.984989	0.874726	-0.011166
C	3.036610	-0.511127	0.095866
C	1.856065	-1.257985	0.107853
C	-1.499349	-1.717060	0.019690
C	-2.331889	-0.859462	-0.176723
C	-3.194802	0.235391	-0.437667
C	-3.676955	1.047816	0.508124
H	-0.392580	1.291324	-0.169601
H	1.728898	2.611471	-0.191311
H	3.905451	1.447357	-0.020321
H	3.994372	-1.015434	0.170438
H	1.887369	-2.339597	0.190981
H	-0.982575	-2.628083	0.209716
H	-3.457375	0.398446	-1.479403
H	-3.432087	0.904357	1.554165
H	-4.331807	1.871155	0.249657

Frequencies

-244.0575	20.2201	45.0512
67.7306	91.2227	125.2509
230.5313	338.1813	405.2020
432.6869	566.5625	577.7063
612.6367	687.1734	690.6077
696.9123	717.3556	733.7165
845.4262	904.3887	912.5552
959.7362	982.8678	986.8331
1014.1595	1016.0893	1032.2794
1060.3943	1092.4888	1118.9394
1182.4754	1191.2185	1322.4278
1325.9009	1330.6796	1446.9267
1476.2552	1494.4502	1614.7146
1665.3101	1672.2962	2139.1233
3166.5596	3178.8674	3179.7377
3183.4406	3193.7295	3199.6599
3213.5197	3265.8068	3456.8170

i21 – i24

C	-1.344208	1.362239	0.156216
C	1.369689	-1.134086	-0.278888
C	-1.159871	-1.413638	-0.174092

C	-2.399873	-0.802945	0.004571
C	-2.489495	0.575477	0.179354
C	-0.097985	0.764205	-0.023755
C	1.175097	1.409845	-0.261643
C	2.293475	0.590772	-0.198739
C	2.321110	-0.610631	0.713529
C	-0.006944	-0.642625	-0.165598
H	-1.419453	2.439913	0.257281
H	1.662083	-1.877626	-1.010296
H	-1.095162	-2.488573	-0.306121
H	-3.300358	-1.406721	0.007106
H	-3.459443	1.039646	0.317109
H	1.226679	2.402749	-0.693039
H	3.204457	0.846199	-0.728993
H	3.288421	-1.105407	0.734038
H	1.926813	-0.441863	1.717188

Frequencies

-701.1185	159.6267	183.4490
369.1847	375.8840	420.5074
473.1866	518.0622	562.8030
595.9051	662.3199	676.3968
700.3314	775.0807	780.6766
803.6797	852.7783	890.7418
901.5672	954.2386	974.1803
1009.8575	1013.3730	1056.6651
1096.1937	1138.7324	1167.6802
1180.3260	1186.6105	1212.2745
1221.9184	1241.8617	1284.9438
1327.2846	1371.3737	1411.9920
1464.2445	1493.1915	1505.6729
1520.4649	1636.1414	1660.3670
3079.3436	3176.5890	3181.4804
3189.6973	3192.3351	3199.8454
3210.8968	3211.6382	3218.3832

i24 – p1

C	-1.301163	1.386920	0.032624
C	-2.474396	0.679193	0.046855
C	-2.454502	-0.732076	0.013793
C	-1.263355	-1.404594	-0.029626
C	-0.032502	-0.700352	-0.039405
C	-0.054386	0.721208	-0.011669
C	1.179655	1.430661	-0.046520
C	2.368569	0.769208	-0.072930
C	2.400041	-0.658183	-0.037914

C	1.213103	-1.367819	-0.087360
H	-1.314433	2.471835	0.055521
H	-3.423944	1.200864	0.082394
H	-3.389393	-1.280746	0.024181
H	-1.244498	-2.489309	-0.053748
H	1.155047	2.515518	-0.056991
H	3.303142	1.317139	-0.096187
H	2.858167	-0.857579	1.768435
H	3.340242	-1.171053	-0.203395
H	1.229294	-2.451664	-0.127285

Frequencies

-898.3490	160.8872	176.8299
318.5125	355.8948	383.5936
418.8907	485.1527	502.9738
520.1803	528.3060	634.1081
646.8918	746.1018	781.3993
784.0884	811.1667	822.4555
852.5743	900.8078	951.9697
976.6721	992.8018	1011.3852
1024.8929	1042.1979	1053.5551
1155.3347	1165.2028	1177.1882
1195.0025	1235.6521	1269.3038
1292.7465	1396.6779	1421.2121
1425.5743	1489.7092	1503.0472
1558.8011	1632.8301	1663.3053
1695.7993	3188.9744	3191.1039
3193.5478	3196.3976	3207.5524
3208.8258	3220.4386	3221.1410

i5 – i18

C	1.545330	-1.237929	0.173619
C	2.703760	-0.470274	0.181765
C	2.644185	0.905349	-0.012930
C	1.407464	1.523760	-0.220532
C	0.300235	0.718622	-0.223749
C	0.286740	-0.649993	-0.029395
C	-0.931628	-1.468956	-0.040994
H	1.607516	-2.311290	0.328172
H	3.662123	-0.950458	0.342156
H	3.552200	1.498670	-0.004179
H	1.336313	2.595023	-0.373966
H	-0.777987	-2.537409	0.084597
C	-2.179241	-1.021340	-0.197974
H	-2.986103	-1.750678	-0.214381

C	-2.571522	0.393714	-0.381720
C	-2.842675	1.230517	0.614255
H	-2.672041	0.739649	-1.409951
H	-2.754442	0.921305	1.650805
H	-3.143464	2.254372	0.422680

Frequencies

-101.5397	52.4766	102.0412
149.7989	262.5919	319.0334
421.1693	444.0584	460.8257
578.0473	594.2805	630.0185
713.2356	752.3307	766.0567
793.5394	828.9371	886.2833
946.9992	968.7040	969.7551
991.6267	1009.3280	1014.7499
1028.8061	1055.3236	1102.0011
1136.4836	1183.5751	1213.6725
1244.6994	1282.3240	1312.2826
1331.9335	1420.6535	1455.9913
1470.8875	1498.4150	1606.1193
1667.3863	1703.8190	1743.8787
3142.2013	3157.1060	3160.6770
3178.6869	3183.2261	3186.7499
3200.7366	3212.3813	3248.0207

i5 – i19

C	-2.673398	0.297630	0.118450
C	-2.412430	-1.063424	-0.011176
C	-1.095986	-1.519612	-0.135723
C	-0.104033	-0.573636	-0.114743
C	-0.313318	0.788142	0.010061
C	-1.636413	1.224595	0.126723
C	2.161057	-0.413840	-0.385814
C	2.060811	1.051440	-0.162675
C	0.874576	1.640268	0.005589
H	-3.697583	0.639669	0.214998
H	-3.231250	-1.774986	-0.011368
H	-0.880934	-2.577989	-0.236757
H	-1.849743	2.284700	0.224769
H	1.954458	-0.760875	-1.397911
H	2.981598	1.625796	-0.147689
H	0.777166	2.711112	0.148718
C	2.789371	-1.253323	0.470658
H	2.942649	-2.296973	0.222841
H	3.102221	-0.919889	1.454294

Frequencies

-330.3899	69.7801	152.4664
206.0108	301.1124	344.6391
410.1910	437.3539	476.4536
547.0346	586.5837	619.6239
715.8332	731.7382	758.2702
796.6811	845.3352	879.1675
884.2634	911.3500	944.8882
963.6215	1001.3902	1008.9055
1013.0554	1050.3772	1097.0847
1133.0784	1178.0461	1179.8932
1242.6508	1274.2681	1280.2662
1336.9244	1387.5166	1445.7740
1466.4131	1493.6550	1580.0862
1616.6503	1662.5021	1706.4249
3137.5429	3157.9388	3183.4477
3184.1184	3190.6649	3202.8499
3208.5753	3217.3409	3254.1832

i10 – i12

C	1.694624	-1.335887	-0.011923
C	-3.489020	0.066316	-0.857815
C	1.453589	1.509746	-0.066658
C	2.693545	0.875365	-0.199007
C	2.805754	-0.520529	-0.175544
C	0.448168	-0.711248	0.118196
C	-0.923225	-1.096566	0.259414
C	-1.589387	0.074816	0.710926
C	-2.944786	0.439022	0.302776
C	0.362084	0.681062	0.072812
H	1.795357	-2.415507	0.011810
H	-2.922617	-0.505596	-1.586294
H	-4.507514	0.331503	-1.116897
H	1.374469	2.590587	-0.088564
H	3.588074	1.475461	-0.330017
H	3.786411	-0.969972	-0.285796
H	-1.416451	-1.970186	-0.150868
H	-1.246119	0.509926	1.643838
H	-3.519692	1.061205	0.983723

Frequencies

-611.5393	82.5409	108.6400
189.3241	251.6468	300.7626
401.3009	417.5481	498.4235
560.3061	571.9582	611.8210
680.7554	695.7461	734.4590

758.1692	776.0463	866.4959
878.7801	952.9722	969.3515
986.2021	1005.7133	1007.8804
1033.3107	1041.4225	1063.9449
1134.0014	1170.4439	1190.8424
1233.1477	1256.9624	1314.8446
1336.3889	1363.4279	1445.2919
1456.3753	1482.3709	1494.0386
1609.0938	1637.6603	1690.9914
3154.4929	3167.1079	3182.1517
3183.5701	3195.5552	3205.2294
3212.4886	3213.3076	3248.8147

i6 – i13

C	0.865888	-1.208123	-0.085882
C	2.247987	-1.211442	0.026691
C	2.948099	-0.012594	0.107299
C	2.252981	1.192521	0.079609
C	0.871117	1.200238	-0.023181
C	0.155731	-0.001636	-0.108684
C	-1.291512	-0.014117	-0.226740
C	-2.323353	1.026137	-0.036027
C	-3.289861	-0.046913	0.260565
C	-2.355738	-1.019905	0.086139
H	0.324275	-2.145314	-0.150645
H	2.782189	-2.154593	0.051147
H	4.028413	-0.016552	0.194868
H	2.791370	2.131224	0.147211
H	0.336942	2.144588	-0.034173
H	-1.767060	0.678278	-1.244718
H	-2.227302	2.080003	0.185553
H	-4.364444	-0.046083	0.374047
H	-2.392405	-2.096544	-0.002026

Frequencies

-2016.6416	57.9935	115.7228
145.0418	290.9075	384.4071
413.5309	442.7383	509.6850
614.2413	634.3669	700.3128
710.0463	714.6651	757.4611
801.2091	846.2825	854.8250
931.7053	934.7702	962.2841
992.1178	1008.7891	1015.3430
1019.3726	1061.4068	1097.8682
1138.8622	1159.0959	1185.6423
1216.1384	1224.8162	1255.4989

1294.5150	1333.5107	1364.1188
1431.0858	1491.2238	1534.5693
1555.9970	1644.4814	1669.3380
1961.3592	3189.0794	3194.9599
3203.8234	3211.8999	3222.0928
3228.6392	3242.1225	3261.0068

i13 – i65

C	-1.217653	-1.384888	-0.040963
C	-2.466034	-0.736306	0.068923
C	-2.524638	0.659884	0.048623
C	-1.394470	1.426762	-0.172157
C	-0.123493	0.795929	-0.374342
C	-0.089476	-0.653591	-0.282858
C	1.292657	-0.927883	0.235492
C	1.386643	0.490126	0.864970
C	2.618989	0.696105	0.095478
C	2.520950	-0.485851	-0.547818
H	-1.137999	-2.450342	0.152224
H	-3.367838	-1.314473	0.231203
H	-3.483115	1.151107	0.180624
H	-1.474802	2.505617	-0.244819
H	0.547504	1.290189	-1.072238
H	1.397929	-1.817957	0.856481
H	1.136256	0.763648	1.884343
H	3.287731	1.543012	-0.006404
H	3.073486	-0.952528	-1.353510

Frequencies

-710.6154	126.1773	192.6793
294.6012	323.4353	387.6474
410.2916	553.2143	595.4868
625.4636	695.8776	726.9770
756.2822	815.6729	834.9970
849.1421	865.0684	897.7794
923.2531	932.2472	962.1981
974.8405	990.7380	1005.5251
1013.4956	1039.4454	1101.8986
1108.0261	1161.7843	1169.1059
1184.9349	1189.8803	1212.5479
1246.9888	1309.9372	1326.4313
1354.9577	1459.7150	1491.3565
1553.2081	1580.5283	1636.1621
3124.8129	3143.2432	3181.3371
3185.5499	3193.3698	3201.7726
3207.2194	3219.3177	3235.5824

i4 – i13

C	-1.144695	-1.266376	-0.203835
C	-2.504963	-1.044810	-0.053909
C	-2.979858	0.243934	0.166691
C	-2.085768	1.305789	0.245890
C	-0.724173	1.081464	0.104281
C	-0.233956	-0.206123	-0.139035
C	1.201726	-0.449381	-0.314037
C	2.914266	-0.434191	1.007599
C	3.335966	0.252490	-0.074600
C	2.123269	0.519593	-0.767952
H	-0.774953	-2.271610	-0.379728
H	-3.198774	-1.876037	-0.109602
H	-4.043038	0.418065	0.287382
H	-2.451608	2.309345	0.431673
H	-0.024412	1.904659	0.200756
H	1.486014	-1.490674	-0.416795
H	3.384372	-0.949432	1.840280
H	4.349062	0.530946	-0.350300
H	1.862444	1.410395	-1.330226

Frequencies

-635.6059	66.1314	106.2812
159.1241	308.4229	387.0663
401.1072	422.9425	539.0195
568.0137	637.1814	665.6463
705.1256	720.0865	745.3276
773.1638	806.1027	873.4866
890.5128	904.5899	930.4065
955.4545	1006.0441	1023.1605
1029.4109	1055.6756	1062.3766
1111.6634	1169.2034	1189.8687
1205.7952	1233.9752	1258.9085
1324.5917	1354.1422	1365.5576
1463.7558	1496.7825	1525.7792
1546.5167	1655.1926	1675.8332
3163.1075	3186.4522	3187.2255
3192.8480	3193.8177	3198.4686
3202.6081	3211.3393	3221.3869

i13 – i64

C	0.924200	-1.271784	0.107620
C	0.376631	1.122855	0.163226
C	1.706316	1.407420	0.002423
C	2.663552	0.385191	-0.115128

C	2.247922	-0.953353	-0.048509
C	-0.099249	-0.244977	0.169875
C	-1.463590	-0.683517	0.691083
C	-2.496429	0.426073	0.612411
C	-2.463763	0.443433	-0.732820
C	-1.454579	-0.646933	-0.804791
H	0.614405	-2.310697	0.169758
H	-0.348988	1.921918	0.252405
H	2.026615	2.443515	-0.025844
H	3.711673	0.626782	-0.241763
H	2.984436	-1.747273	-0.110240
H	-1.527212	-1.571352	1.309861
H	-2.921498	1.077277	1.365281
H	-2.873225	1.108094	-1.483407
H	-1.312267	-1.454722	-1.508392

Frequencies

-456.9880	121.5754	169.4149
218.3755	380.0207	394.7296
421.3908	472.1306	590.0925
616.8055	654.8634	707.4986
729.3559	764.2143	799.4714
813.3771	861.2854	873.7411
905.3929	941.6365	973.2795
984.6303	991.7144	996.1206
1016.9522	1028.8599	1045.2082
1102.0756	1120.5212	1165.7245
1191.3173	1207.9693	1208.5838
1271.7384	1319.5793	1333.6619
1346.0835	1457.1899	1483.1171
1570.1097	1593.3003	1612.8024
3178.4066	3187.6712	3188.5825
3200.1036	3207.5929	3217.8711
3224.7370	3235.4831	3244.0428

i65 – p9

C	-1.239707	1.447870	0.027397
C	-2.423102	0.720107	0.211858
C	-2.446931	-0.675735	0.132704
C	-1.287828	-1.417668	-0.076317
C	-0.090282	-0.696338	-0.108038
C	-0.094410	0.708374	-0.154620
C	1.360966	0.803732	-0.595776
C	1.368808	-0.777280	-0.598061
C	2.434928	-0.652543	0.475658
C	2.425398	0.682431	0.482562

H	-1.254732	2.531365	-0.015838
H	-3.356192	1.250477	0.366788
H	-3.398526	-1.188077	0.221031
H	-1.319131	-2.497474	-0.165018
H	0.261571	-1.014973	1.653717
H	1.577680	1.378370	-1.496610
H	1.567919	-1.346537	-1.505021
H	2.948441	-1.399072	1.068858
H	2.925936	1.428218	1.087897

Frequencies

-952.5314	154.2536	188.3109
297.8649	352.9701	369.5226
415.1056	453.6653	546.7364
571.7046	575.9626	657.3143
751.3007	765.2985	773.0723
841.9552	845.6634	870.8573
887.1563	928.9420	940.2453
963.8495	978.3955	1008.7716
1009.6062	1029.5837	1065.6186
1103.7200	1145.6684	1150.1509
1170.9802	1178.0378	1203.7202
1214.2526	1224.4630	1297.0383
1309.3415	1366.0053	1471.4905
1502.3856	1630.0069	1645.0305
1656.8105	3123.5429	3142.9240
3189.3838	3198.9564	3208.6676
3209.1197	3217.7941	3240.8447

i22 – i65

C	1.220812	1.428480	-0.042418
C	2.421046	0.748678	0.009490
C	2.445910	-0.688859	0.025331
C	1.320973	-1.424450	-0.092551
C	-0.003507	-0.775934	-0.351752
C	0.021197	0.731515	-0.208431
C	-1.260903	1.138430	0.259389
C	-1.161091	-0.891635	0.635952
C	-2.489619	-0.743164	-0.023804
C	-2.541659	0.560553	-0.265271
H	1.187763	2.499852	0.133344
H	3.351179	1.292423	0.124334
H	3.400595	-1.186589	0.160012
H	1.358350	-2.508818	-0.070548
H	-0.367122	-1.102337	-1.339962
H	-1.317132	2.082452	0.804229

H	-1.003023	-1.174871	1.670454
H	-3.149595	-1.535441	-0.362837
H	-3.299966	1.131642	-0.794646

Frequencies

-955.9450	128.8624	179.1317
279.3912	316.3695	358.6684
429.6487	490.1824	533.9195
578.5940	623.2962	684.8325
703.0605	752.7225	765.7883
789.2710	834.0383	901.7578
925.6687	942.5945	959.2817
987.8461	993.0681	1011.2372
1030.3576	1052.3702	1090.4888
1108.1043	1139.1466	1174.9413
1211.4558	1234.5864	1258.0749
1302.0570	1337.0523	1364.9444
1390.2747	1412.1475	1451.1079
1522.0760	1648.7245	1695.9998
2974.3967	3122.5669	3164.7840
3177.4263	3180.5805	3196.8282
3199.3931	3214.3513	3217.4594

i19 – p20

C	2.568794	0.146898	-0.044654
C	2.123870	-1.171629	0.015424
C	0.761711	-1.460892	0.058770
C	-0.137585	-0.410387	0.040219
C	0.307569	0.920246	-0.020940
C	1.664718	1.205607	-0.063977
C	-1.623254	-0.383766	0.053372
C	-1.984281	1.052649	0.026250
C	-0.868317	1.797170	-0.031129
C	-2.450565	-1.414914	-0.232965
H	3.633418	0.349506	-0.077615
H	2.846045	-1.979825	0.031025
H	0.420323	-2.489163	0.114437
H	2.017062	2.230128	-0.114291
H	-1.671495	-0.393942	1.957638
H	-3.004734	1.410031	0.030228
H	-0.823775	2.877284	-0.077623
H	-3.519537	-1.264535	-0.327138
H	-2.073259	-2.425378	-0.338878

Frequencies

-943.3606	138.6876	191.8425
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253.8085	320.6542	332.0473
415.8079	446.9836	460.1592
545.4692	556.1459	575.9459
641.4683	642.9998	728.5345
763.6226	772.2016	776.8400
813.0453	872.8644	895.8568
912.4202	944.5695	959.8842
968.0041	1007.5073	1051.0658
1088.5165	1108.2419	1152.6050
1186.4314	1222.8656	1246.1600
1326.1888	1342.2598	1394.8796
1443.9596	1500.2452	1511.3792
1613.6771	1644.0306	1668.4472
1687.8652	3163.6115	3189.9635
3195.4986	3207.4225	3220.9897
3227.0679	3251.0058	3259.6984

il2 - p10

C	-2.059220	1.074926	-0.113217
C	3.092736	-1.082457	-0.198364
C	-0.642990	-1.423882	0.099398
C	-2.066789	-1.368399	0.029901
C	-2.741524	-0.173833	-0.071914
C	-0.701391	1.004985	-0.042622
C	0.608008	1.732153	-0.034489
C	1.304978	0.557350	0.080006
C	2.691788	0.182145	-0.053079
C	-0.009019	-0.225025	0.060011
H	-2.606506	2.005940	-0.199930
H	2.381238	-1.901042	-0.197812
H	4.139184	-1.331448	-0.325425
H	-0.130752	-2.374870	0.182718
H	-2.629224	-2.294713	0.059979
H	-3.824554	-0.181868	-0.123469
H	0.906365	2.768468	-0.111789
H	1.488757	0.649769	2.237358
H	3.416027	0.991981	-0.055422

Frequencies

-659.7765	103.8385	133.3314
159.0145	218.4276	283.8619
342.7364	360.9078	373.5737
418.9893	507.4675	557.5646
582.1870	652.5165	694.3979
727.3355	753.4506	773.3235
822.3922	853.8110	900.9777

937.7420	957.6079	993.4268
994.4302	1000.4341	1030.7819
1066.0733	1105.1423	1112.5372
1164.1305	1193.1606	1267.4733
1309.3809	1319.4105	1411.2409
1443.0779	1464.4133	1478.2021
1567.7721	1669.5347	1699.4349
1728.3283	3168.1105	3186.6293
3192.0140	3205.6133	3215.0135
3221.5345	3247.9557	3263.1818

i9 – i11

C	-0.383911	-0.499876	0.146404
C	-1.511888	-1.250905	-0.274042
C	-2.745098	-0.653377	-0.437493
C	-2.907113	0.710633	-0.189340
C	-1.812286	1.469891	0.223983
C	-0.572217	0.884183	0.389517
C	0.868953	-1.129414	0.309460
H	-1.390870	-2.311760	-0.467854
H	-3.592378	-1.247881	-0.760875
H	-3.876633	1.177212	-0.318927
H	-1.934576	2.530237	0.415574
H	0.275558	1.482100	0.703768
H	0.942216	-2.194974	0.110298
C	2.086710	-0.437184	0.784518
C	2.962023	0.111058	-0.012737
C	3.831531	0.656523	-0.811710
H	2.267722	-0.387261	1.859818
H	4.671121	0.088830	-1.198984
H	3.737612	1.694306	-1.114178

Frequencies

-108.4046	69.2777	156.6131
170.0127	250.8801	314.1581
378.5233	416.7431	473.4108
494.8317	567.0111	630.6550
647.6273	695.9588	710.6346
785.9691	843.9883	855.0123
882.9412	885.3313	928.0663
995.9945	1000.2597	1013.8262
1017.8176	1019.2888	1052.5718
1119.8283	1151.5474	1182.4993
1190.9259	1235.2024	1323.7102
1339.6888	1357.5019	1414.1641
1474.9746	1498.3690	1513.3464

1613.9690	1629.4068	2083.6267
3110.5578	3151.7947	3174.4809
3184.0413	3191.5102	3200.1019
3208.1050	3217.0828	3234.9016

il1 – il5

C	0.331735	-0.607243	-0.144640
C	1.563472	-1.218719	0.139515
C	2.724108	-0.474094	0.263302
C	2.690417	0.907322	0.095833
C	1.486267	1.527763	-0.209705
C	0.320881	0.782959	-0.332917
C	-0.859892	-1.440673	-0.231493
C	-2.164646	-1.065812	-0.113070
C	-2.691195	0.190605	0.226858
C	-3.401411	1.271639	0.300967
H	1.598246	-2.295061	0.275025
H	3.660880	-0.970878	0.489772
H	3.598677	1.491069	0.191474
H	1.453188	2.600329	-0.366148
H	-0.594718	1.281996	-0.623298
H	-0.679011	-2.501415	-0.373006
H	-2.920728	-1.843385	-0.180463
H	-2.290736	1.028573	1.048424
H	-3.824220	1.966286	-0.429680

Frequencies

-1836.4407	45.0709	116.3497
157.5895	205.4909	274.8579
306.4261	359.4888	423.2293
431.4427	495.3154	548.1837
585.9852	635.4775	714.9612
726.2968	745.8687	793.2450
817.3347	866.8363	898.7783
937.9190	949.1833	961.0053
1002.8091	1019.7939	1022.8488
1063.2246	1122.6837	1185.5559
1205.7194	1217.1004	1259.9815
1342.1677	1364.9473	1433.7712
1480.5351	1537.4036	1568.5436
1647.4617	1672.3857	1898.7259
2379.3332	3060.7523	3168.7775
3185.9731	3192.3081	3195.4661
3206.1693	3219.9453	3233.9588

i4 – i9

C	0.435773	-0.188630	0.043130
C	1.312263	-1.282445	0.028363
C	2.686475	-1.102750	-0.021305
C	3.222349	0.178664	-0.053835
C	2.367272	1.276736	-0.032766
C	0.994618	1.097924	0.016306
C	-1.000748	-0.440458	0.084630
C	-1.984010	0.487579	-0.036375
C	-3.355138	0.184299	0.082782
C	-4.547247	-0.270597	-0.099060
H	0.901349	-2.286705	0.052869
H	3.341991	-1.966397	-0.033990
H	4.295816	0.323225	-0.092779
H	2.776595	2.280744	-0.051106
H	0.351907	1.970763	0.042866
H	-1.296655	-1.477692	0.215422
H	-1.746724	1.539346	-0.164235
H	-4.230404	0.599973	0.871062
H	-5.183522	-0.625187	-0.911331

Frequencies

-2065.8316	62.3828	75.2832
101.9524	179.6739	234.6683
241.1165	358.4450	376.6339
414.0550	455.0269	520.8580
579.8256	638.3372	660.4240
706.6068	765.5801	836.5784
849.0294	861.9738	868.1052
926.6994	956.0175	991.9278
997.0784	1013.5291	1020.8530
1063.1399	1116.6750	1187.8350
1208.9964	1237.1841	1302.5386
1313.3785	1346.5474	1361.6110
1489.3323	1538.4035	1589.5735
1650.4090	1671.9544	1932.3947
2389.7455	3092.9488	3180.2090
3185.8489	3186.5005	3192.8967
3200.8614	3207.8916	3220.7392

il1 – il7

C	-0.015861	-0.768023	0.286233
C	1.170208	-1.438953	-0.133352
C	2.328982	-0.753937	-0.354765
C	2.391738	0.651440	-0.127502
C	1.314036	1.323020	0.363687

C	0.055740	0.657689	0.579969
C	-1.254757	-1.396766	0.267610
C	-2.467486	-0.662924	-0.004011
C	-2.388690	0.623008	-0.357939
C	-1.371625	1.556183	-0.452634
H	1.118040	-2.506152	-0.324284
H	3.210043	-1.275181	-0.710701
H	3.324684	1.175700	-0.302610
H	1.392925	2.377139	0.609428
H	-0.486608	0.949979	1.475717
H	-1.302588	-2.479698	0.203006
H	-3.393861	-1.220954	-0.099547
H	-1.393662	2.417600	0.207879
H	-1.042681	1.817147	-1.462663

Frequencies

-774.9149	137.1420	143.4613
251.0519	314.0581	403.5196
423.2330	449.2159	514.7774
528.8218	610.6284	687.9370
726.4874	730.9058	769.8787
798.7709	826.5689	874.2945
901.4956	928.0313	983.0811
1002.2333	1012.3532	1019.6932
1025.6861	1063.8349	1084.2280
1090.0515	1119.9428	1186.8357
1205.0459	1232.1826	1309.3094
1339.9704	1370.8873	1420.9231
1465.7844	1480.8312	1492.3967
1561.0089	1661.6825	1685.9127
3086.2186	3132.1317	3175.3809
3184.5881	3186.5952	3188.8940
3191.0270	3204.5782	3219.1336

i64 – i66

C	-0.859224	-1.279904	-0.009103
C	-0.388611	1.163570	-0.093228
C	-1.725452	1.395899	-0.038520
C	-2.658100	0.334172	0.026107
C	-2.189586	-0.996949	0.033033
C	0.183998	-0.218733	-0.050782
C	1.332750	-0.509742	-1.007135
C	2.549305	0.251061	-0.629466
C	2.483817	0.347343	0.706174
C	1.248283	-0.410155	1.043738
H	-0.513429	-2.309321	-0.000766

H	0.317106	1.985027	-0.143069
H	-2.089047	2.418321	-0.051024
H	-3.720288	0.539981	0.070351
H	-2.905732	-1.810928	0.073064
H	1.366527	-1.457907	-1.535788
H	3.289198	0.642957	-1.316421
H	3.134488	0.863595	1.399987
H	1.258101	-1.331101	1.618761

Frequencies

-746.3042	77.9183	174.3523
197.5163	214.9314	363.6001
399.4330	415.3816	435.4460
545.3511	566.4773	603.7745
624.9741	700.2783	712.4696
741.3259	762.1847	783.5561
828.7066	894.5201	945.3922
970.6815	982.8017	986.6430
1001.0261	1004.1165	1036.3981
1091.9070	1110.1579	1129.9687
1148.7845	1204.2613	1217.4402
1242.0737	1321.6409	1338.2921
1341.7246	1411.2259	1461.7660
1547.4765	1562.8039	1622.0465
3176.9975	3184.8228	3185.6665
3188.0234	3199.8305	3204.7515
3211.7204	3224.0494	3234.1738

i19 – i21

C	-1.453936	1.319747	0.185997
C	1.528770	-0.768342	-0.409082
C	-0.993715	-1.428789	-0.234693
C	-2.282971	-0.947769	-0.015795
C	-2.505627	0.413174	0.194815
C	-0.161956	0.847731	-0.049473
C	1.107843	1.537643	-0.128160
C	2.101353	0.618355	-0.391322
C	2.246369	-0.907361	0.891135
C	0.057022	-0.530037	-0.252589
H	-1.635071	2.376254	0.350790
H	1.840284	-1.451122	-1.198251
H	-0.820638	-2.488739	-0.387716
H	-3.119928	-1.636705	-0.006085
H	-3.516260	0.767211	0.366174
H	1.252290	2.599010	0.019658
H	3.133551	0.834758	-0.623139

H	3.268993	-1.259588	0.919420
H	1.737861	-0.667193	1.814152

Frequencies

-576.6911	153.6075	180.6498
336.0849	376.8915	405.2344
483.7602	522.3720	549.7616
582.9314	607.2565	629.0687
732.3120	748.9529	781.6678
803.9571	821.8975	868.7639
882.6647	905.2282	958.7733
976.8808	1010.6354	1016.0863
1054.5551	1095.3371	1108.5359
1137.9294	1179.1560	1187.3448
1198.4300	1240.8927	1278.5739
1329.5974	1357.6115	1390.4330
1432.7242	1449.8166	1502.2581
1523.4883	1645.6844	1677.1350
3131.4125	3173.5739	3188.3067
3194.7937	3205.8087	3218.4481
3232.8570	3254.6151	3296.5621

i21 – i70

C	-1.390631	1.401623	0.053535
C	1.255900	-1.062821	-0.420396
C	-1.240087	-1.458528	-0.029493
C	-2.422790	-0.812736	0.147748
C	-2.494678	0.625810	0.190719
C	-0.115343	0.770651	-0.146290
C	1.137459	1.287813	-0.296768
C	2.117841	0.163764	-0.413955
C	2.805095	-0.132545	0.889943
C	-0.047188	-0.689324	-0.193069
H	-1.458566	2.483147	0.092475
H	1.642003	-2.066459	-0.528040
H	-1.193067	-2.541670	-0.057668
H	-3.339980	-1.379081	0.263655
H	-3.463937	1.088766	0.340489
H	1.415890	2.332435	-0.279294
H	2.823147	0.251257	-1.244226
H	3.667360	-0.789024	0.906984
H	2.273677	0.058384	1.813773

Frequencies

-274.5812	136.6246	191.3410
297.3041	380.0395	384.4818

451.9704	506.7609	528.1114
547.5177	572.6237	584.3116
693.2945	731.9600	738.1584
777.6816	822.5532	825.6422
859.3123	893.5706	915.5187
982.6315	987.8154	1000.3592
1011.7905	1052.4141	1076.9419
1150.5977	1164.8761	1190.1634
1204.4235	1238.7638	1254.5345
1312.4019	1376.5002	1405.2754
1411.6557	1444.7615	1470.9219
1578.0341	1606.3640	1685.9031
3092.8867	3154.3505	3184.8417
3195.9406	3207.0830	3217.9040
3236.6585	3247.2424	3275.0152

il2 - p11

C	-1.888522	1.296642	-0.053423
C	-1.055911	-1.459872	-0.008105
C	-2.433359	-1.089787	-0.086805
C	-2.829329	0.226318	-0.108588
C	-0.582175	0.927071	0.024726
C	0.857493	1.343586	0.103786
C	1.274612	0.039188	0.131758
C	-0.177861	-0.428997	0.046744
H	-2.219272	2.328194	-0.078287
H	-0.761655	-2.502653	0.007763
H	-3.184662	-1.870137	-0.129365
H	-3.886332	0.459278	-0.171481
H	1.374236	2.292824	0.131649
C	3.695311	-0.063404	-0.315552
C	2.548083	-0.648955	0.030419
H	3.744487	0.993910	-0.555019
H	4.619144	-0.626396	-0.371216
H	2.530066	-1.714400	0.240637
H	1.333933	-0.211365	2.335558

Frequencies

-640.1197	68.8491	140.8350
152.7631	215.1350	268.6850
308.5047	333.7974	363.6534
414.5304	490.0785	576.0392
607.2490	626.9701	683.1996
749.2470	752.5219	771.7644
816.5757	852.4243	895.5157
930.8437	958.1303	990.2994

992.6408	1025.7250	1036.9197
1057.8713	1100.8091	1113.2780
1149.0092	1199.1446	1217.0777
1304.9485	1325.8288	1403.2784
1443.7683	1463.2118	1483.0667
1569.8424	1676.9600	1690.8402
1733.5076	3159.3480	3183.2243
3192.3108	3202.1132	3210.6241
3220.4231	3248.4124	3253.2663

i68 – i74

C	1.470482	1.347194	0.033285
C	-1.360106	-0.986783	-0.454911
C	1.129594	-1.447504	-0.015183
C	2.393871	-0.894406	0.135557
C	2.555263	0.496519	0.150386
C	0.186588	0.797649	-0.092071
C	-1.094547	1.441949	-0.132861
C	-2.171033	0.596092	-0.153253
C	-2.905075	-0.329648	0.603767
C	0.038375	-0.599867	-0.161242
H	1.605769	2.422469	0.070697
H	-1.613950	-0.927782	-1.515226
H	-1.643792	-1.973960	-0.090963
H	1.000744	-2.524746	-0.047581
H	3.259798	-1.539090	0.229617
H	3.549249	0.913915	0.269894
H	-1.213402	2.515271	-0.227970
H	-3.851244	-0.732509	0.253971
H	-2.553642	-0.680743	1.576726

Frequencies

-1067.3649	134.7783	179.1152
261.6737	321.5765	356.1637
426.9519	493.8109	541.4478
545.8215	582.6006	627.2020
684.7578	722.5912	750.6237
774.6856	799.3464	813.2881
869.7462	877.9606	896.8930
958.9699	990.3014	1006.2354
1048.2129	1054.6358	1113.5014
1127.4937	1148.0210	1181.5456
1219.2695	1227.9997	1294.3474
1340.6513	1367.2294	1435.5640
1439.6532	1485.8255	1507.6489
1529.2327	1633.6761	1668.1560

3048.9251	3102.2179	3160.2649
3176.1571	3184.1734	3189.8487
3195.7681	3205.8848	3218.2481

i3 – i6

C	1.030103	-1.219018	0.170546
C	2.408911	-1.118672	0.234781
C	3.036354	0.114653	0.076644
C	2.267265	1.254814	-0.145640
C	0.887974	1.168911	-0.211541
C	0.238619	-0.073629	-0.065747
C	-1.174390	-0.168245	-0.095030
C	-2.893195	1.040086	0.384550
C	-3.327155	-0.261431	0.104103
C	-2.225642	-0.910003	-0.512467
H	0.542593	-2.177638	0.306034
H	3.001271	-2.009207	0.413784
H	4.116103	0.188579	0.133095
H	2.750215	2.218080	-0.266146
H	0.291118	2.058454	-0.377217
H	-2.493061	1.651268	-0.414474
H	-3.259557	1.598435	1.245872
H	-4.224861	-0.725718	0.497659
H	-2.216894	-1.767045	-1.179805

Frequencies

-741.2998	56.8702	86.5743
108.5567	251.0100	370.7463
408.9614	418.4186	475.3405
523.8589	633.0073	664.5959
701.6943	704.6816	770.8047
790.6647	856.4641	883.9105
887.0706	923.7887	941.4147
997.1149	1007.9357	1013.0706
1017.0592	1054.9040	1067.0755
1113.2333	1138.9600	1183.4050
1204.1357	1218.4792	1308.4967
1335.6674	1353.8717	1426.8990
1478.9523	1511.3398	1524.6828
1618.0285	1634.2382	1653.6839
3125.2221	3174.0616	3188.1578
3194.7788	3204.1272	3206.1866
3213.5497	3220.6510	3229.9259

i15 – i20

C	0.282519	0.545124	-0.072450
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C	1.467863	1.246854	0.177661
C	2.692111	0.598266	0.242684
C	2.759567	-0.775619	0.050916
C	1.593400	-1.487732	-0.204895
C	0.368559	-0.839346	-0.265273
C	-0.967777	1.321293	-0.129320
C	-2.239342	0.926158	-0.234506
C	-2.771886	-0.464822	-0.320381
C	-3.176346	-1.141878	0.723673
H	1.423459	2.321397	0.324971
H	3.594350	1.165798	0.440849
H	3.713511	-1.288240	0.099415
H	1.637352	-2.560220	-0.358422
H	-0.525521	-1.416149	-0.456538
H	-0.812586	2.396571	-0.071464
H	-2.999795	1.703012	-0.264365
H	-2.858833	-0.904138	-1.316682
H	-3.223941	-0.987813	1.793574

Frequencies

-72.5733	51.0958	139.0767
170.9582	266.2924	304.5508
417.2370	435.9355	470.2291
575.8100	627.2091	639.3801
711.8527	726.0571	767.0146
805.1941	813.6069	865.6282
874.0257	915.6817	952.2456
1001.3763	1007.3366	1018.8821
1024.9027	1027.4378	1064.6278
1122.1607	1189.2714	1213.7365
1218.0017	1250.1382	1277.5969
1346.6431	1363.8824	1440.7771
1494.9795	1541.8288	1650.8282
1672.9953	1681.5952	1730.5237
3098.6493	3151.2395	3174.3585
3185.5581	3195.6255	3205.9594
3219.3910	3246.6790	3248.0824

i17 – i22

C	0.022238	0.759184	0.148026
C	-1.178376	1.443563	-0.045170
C	-2.380012	0.771489	-0.160117
C	-2.414135	-0.661466	-0.137813
C	-1.300223	-1.379078	0.110883
C	-0.002116	-0.715651	0.446801
C	1.294142	1.388445	0.092536

C	2.452117	0.672249	-0.016987
C	2.492717	-0.782284	-0.225710
C	1.242666	-1.400802	-0.107143
H	-1.149076	2.522651	-0.162412
H	-3.296380	1.322191	-0.334765
H	-3.351722	-1.166791	-0.341578
H	-1.329032	-2.464385	0.122415
H	0.135071	-0.814065	1.546136
H	1.321900	2.475690	0.069392
H	3.396533	1.205618	-0.058467
H	1.178577	-2.485489	-0.209575
H	1.720030	-1.169318	-1.262971

Frequencies

-1128.8702	97.4526	144.3790
299.8551	350.7578	390.5932
458.5993	481.6027	510.8141
540.4765	611.0879	676.4263
700.7023	750.0227	765.3815
792.6726	814.2371	894.8876
924.7634	958.3925	972.7506
985.7142	994.2681	1006.7854
1064.7862	1081.1200	1114.7369
1179.4002	1183.2040	1217.7993
1240.4899	1250.5674	1285.9373
1334.1877	1370.9059	1388.1261
1424.1989	1452.5870	1470.5016
1515.2845	1551.9779	1653.5866
2200.4090	2853.4259	3117.3153
3163.0100	3183.2367	3185.9773
3188.8799	3204.8289	3222.1445

i17 – i23

C	-0.050633	0.756100	0.153657
C	1.207934	1.423197	0.164380
C	2.367771	0.734546	-0.011590
C	2.356902	-0.684553	-0.181140
C	1.193899	-1.377706	-0.150494
C	-0.080946	-0.691278	-0.035375
C	-1.278483	1.420268	0.105108
C	-2.378381	0.656879	-0.278374
C	-2.196473	-0.720914	-0.392838
C	-1.289316	-1.401562	0.586448
H	1.221159	2.499971	0.298401
H	3.315912	1.259854	-0.018780
H	3.298587	-1.208680	-0.300987

H	1.189225	-2.459651	-0.228496
H	-0.831133	-0.754496	-1.136241
H	-1.330355	2.501433	0.171655
H	-3.296942	1.129567	-0.612677
H	-1.203866	-2.476909	0.424841
H	-1.476230	-1.180945	1.643586

Frequencies

-1386.6978	175.5165	194.5839
332.7139	371.1247	434.3462
473.1517	501.2422	532.7396
584.2364	629.9564	706.7447
741.9196	759.9184	793.1169
801.2138	862.8543	912.6644
936.7748	951.4484	994.1077
995.6648	1016.1112	1028.4723
1079.3186	1114.0982	1170.7535
1173.3809	1196.5109	1216.9137
1248.1171	1261.1783	1288.0941
1327.3368	1421.6107	1432.4856
1465.2811	1492.4620	1498.6528
1557.8459	1597.7958	1695.6974
1762.3290	3049.4163	3132.8342
3181.4396	3187.8658	3192.8702
3202.7981	3207.3312	3219.9848

il6 – il9

C	-2.566476	0.109549	0.027030
C	-2.079170	-1.221613	0.033551
C	-0.738603	-1.495216	-0.007269
C	0.167063	-0.398037	-0.081523
C	-0.319022	0.950371	-0.007727
C	-1.703428	1.181471	0.012761
C	1.660109	-0.327014	-0.044356
C	1.957528	1.085732	0.013622
C	0.803717	1.821483	0.045841
C	2.555929	-1.405076	0.106370
H	-3.636679	0.278306	0.054032
H	-2.789043	-2.039688	0.083615
H	-0.371949	-2.515270	0.004015
H	-2.084087	2.196822	0.043227
H	0.918219	-0.459182	-1.159615
H	2.965998	1.475925	0.021232
H	0.746494	2.901738	0.061325
H	3.619417	-1.219963	0.169638
H	2.205739	-2.428587	0.132725

Frequencies

-1292.8282	150.5476	208.1000
239.9725	323.4701	375.3773
445.6828	455.4708	536.0725
563.9600	567.5640	575.6213
662.2463	716.0178	735.8721
742.4600	769.9658	804.8913
861.1982	881.7771	931.8607
953.4505	963.1663	995.1335
1031.4492	1079.2824	1091.5051
1111.0136	1156.3915	1185.9536
1229.3497	1249.5612	1310.2573
1354.7208	1382.7479	1440.5185
1458.1640	1496.2198	1517.1434
1536.4299	1603.2785	1667.1188
1933.6389	3177.4138	3191.6738
3198.2889	3210.7127	3221.1204
3228.9469	3249.4037	3281.8840

i22 – i23

C	-1.255932	1.402824	0.021300
C	-2.461906	0.706968	-0.010313
C	-2.444218	-0.694286	-0.072077
C	-1.266875	-1.400087	-0.055915
C	-0.014162	-0.707469	0.090703
C	-0.034846	0.743613	0.036877
C	1.239392	1.423245	0.015370
C	2.414470	0.743136	-0.068804
C	2.463433	-0.680865	-0.096363
C	1.277522	-1.384217	0.014423
H	-1.256746	2.488480	0.012529
H	-3.403380	1.241223	-0.026844
H	-3.380702	-1.234600	-0.162530
H	-1.264153	-2.482387	-0.123821
H	0.553532	-1.061224	1.256845
H	1.238505	2.508143	0.020173
H	3.346031	1.297281	-0.112948
H	3.408963	-1.204884	-0.112716
H	1.256687	-2.469192	-0.001891

Frequencies

-1824.8180	141.1761	190.1920
342.2988	374.4432	437.6985
480.8843	500.4701	518.3394
600.6791	621.8271	680.4412

726.6848	736.9819	774.1425
783.4501	804.4250	847.5295
917.0051	934.1612	939.4684
986.4005	998.3395	1013.9317
1040.5960	1056.2737	1132.1657
1141.4164	1180.9369	1187.6022
1225.3254	1249.4961	1257.5083
1290.6775	1375.4384	1422.6123
1449.9175	1477.5029	1480.5003
1525.9708	1572.4058	1631.6829
1689.4016	3186.3661	3188.4545
3190.0475	3199.4657	3204.9448
3208.3180	3225.5739	3237.7855

i3 – p21

C	-0.971883	-0.303317	1.208607
C	-2.236417	0.264226	1.204093
C	-2.872223	0.551930	0.000876
C	-2.236059	0.269028	-1.203289
C	-0.971524	-0.298494	-1.209689
C	-0.324028	-0.590824	-0.001022
C	0.980206	-1.159355	-0.001977
C	2.148581	-1.486000	-0.002537
H	-0.470408	-0.527198	2.142464
H	-2.728768	0.484169	2.144415
H	-3.861122	0.995634	0.001615
H	-2.728128	0.492723	-2.142873
H	-0.469767	-0.518646	-2.144280
H	3.039966	-2.068536	-0.003560
C	3.431061	0.545373	0.000974
C	2.708509	1.634816	0.002967
H	4.498043	0.357341	0.000528
H	3.162002	2.626761	0.004666
H	1.620841	1.593448	0.003007

Frequencies

-358.7982	23.4038	40.3355
47.2229	151.4675	163.4325
222.8437	284.4336	387.0274
413.5989	480.1608	545.2693
547.5871	640.4380	695.6329
696.9936	712.6852	779.1568
783.1622	790.7286	868.1913
882.7741	947.3151	947.9847
1003.6584	1022.0505	1023.2289
1059.3975	1086.7884	1112.4410

1188.3693	1205.9107	1236.0405
1318.6004	1355.9064	1393.9262
1487.1736	1533.4354	1642.2272
1669.9329	1671.5211	2130.9311
3088.8082	3171.9655	3189.0175
3197.8667	3208.4072	3215.8006
3218.3330	3220.8849	3450.9868

i77 – p24

C	0.618757	-1.593971	0.038020
C	0.541860	1.578485	-0.067307
C	1.902197	1.286340	-0.044230
C	2.521450	0.040266	0.011013
C	1.964367	-1.233246	0.050373
C	-0.498614	-0.777686	-0.013474
C	-1.835234	-1.213947	-0.042240
C	-2.665576	-0.102273	-0.088007
C	-1.893409	1.077339	-0.057730
C	-0.533750	0.706759	-0.052189
H	0.414053	-2.661857	0.068980
H	0.283660	2.634727	-0.094483
H	2.569615	2.141999	-0.064657
H	3.607789	0.067788	0.027455
H	2.672703	-2.054578	0.092297
H	-2.149279	-2.248366	-0.026696
H	-3.746600	-0.130509	-0.122312
H	-2.123406	1.560532	1.924158
H	-2.260816	2.081872	-0.210108

Frequencies

-542.2206	150.5942	163.1349
272.0921	294.4783	321.7547
343.1600	413.3164	432.3408
494.1478	580.2148	615.0741
689.4318	707.6296	726.7809
755.1577	794.7185	839.5652
854.4705	895.3954	916.9346
952.2458	969.2189	974.7831
984.2000	1006.8023	1026.2225
1068.0042	1082.0589	1175.0815
1220.3597	1256.6110	1300.8300
1326.1801	1334.4802	1425.4285
1445.2829	1490.5658	1494.2561
1536.4651	1601.0787	1656.1021
1668.3799	3161.2805	3165.0707

3172.9084	3191.2528	3200.7988
3227.3512	3241.8721	3253.6390

i74 – p25

C	-1.404463	1.443481	-0.056650
C	1.169393	-1.143435	0.088382
C	-1.372200	-1.427448	0.094520
C	-2.528694	-0.728973	0.050177
C	-2.544917	0.718985	-0.028575
C	-0.139034	0.759413	-0.007060
C	1.141864	1.216138	-0.011530
C	2.026240	0.049175	0.055507
C	3.364011	0.066621	0.092884
C	-0.123698	-0.715067	0.064123
H	-1.429591	2.525922	-0.116538
H	1.527672	-2.159286	0.174388
H	-1.373074	-2.510334	0.150872
H	-3.478873	-1.251016	0.072069
H	-3.506330	1.219078	-0.065769
H	1.476772	2.242696	-0.060104
H	1.398895	-1.648159	-2.420943
H	3.937793	-0.852597	0.142241
H	3.915729	1.000354	0.073120

Frequencies

-300.1094	109.9418	115.9599
144.5188	211.4224	262.0788
264.5256	445.3478	459.4557
503.2781	506.8840	573.5475
652.1507	670.5597	673.5807
730.3878	744.3395	793.5321
806.0509	840.6097	861.7701
912.5150	943.9187	972.3954
985.9681	988.1146	992.3167
1009.5422	1152.9488	1173.3937
1182.1806	1197.2902	1228.7456
1323.9822	1400.0398	1402.6110
1422.3428	1461.8496	1490.9878
1600.4653	1628.9226	1714.6601
1731.1218	3159.2361	3190.6687
3197.6435	3210.7771	3220.2493
3244.1105	3248.5298	3253.0464

il1 – il6

C	2.496800	0.245803	-0.481993
C	2.235743	-1.091349	-0.166840

C	1.051261	-1.450590	0.448884
C	0.066018	-0.474395	0.716056
C	0.313962	0.875920	0.323225
C	1.533413	1.221830	-0.241631
C	-1.888493	-0.395980	-0.196707
C	-2.010075	1.031937	-0.038456
C	-0.879820	1.707673	0.243061
C	-2.679351	-1.407363	-0.489409
H	3.440686	0.518985	-0.939084
H	2.988080	-1.845686	-0.369162
H	0.889615	-2.474343	0.766856
H	-0.616711	-0.658232	1.540514
H	1.707568	2.247085	-0.552056
H	-2.966793	1.525334	-0.193215
H	-0.835302	2.789333	0.299327
H	-3.736904	-1.257094	-0.711650
H	-2.306993	-2.426310	-0.538667

Frequencies

-549.3297	82.9566	163.3981
220.9684	271.6302	312.9987
409.7159	467.6559	481.6289
526.7060	611.3131	617.5540
691.2456	735.9069	764.6550
799.0854	820.5307	848.2869
877.9797	891.5270	920.4841
952.4218	983.4429	997.5541
1020.7236	1048.7458	1069.9531
1112.0866	1159.3992	1179.1639
1196.6552	1226.1127	1325.3549
1328.0808	1379.4253	1430.8199
1465.3777	1520.9649	1591.8230
1629.0685	1638.4796	1732.7660
3097.0859	3158.9507	3161.3642
3188.8298	3194.3726	3195.2920
3210.7831	3213.6134	3221.3159

il6 – p20

C	2.547493	0.153236	-0.053219
C	2.102276	-1.171424	-0.065960
C	0.749196	-1.467242	-0.013359
C	-0.162328	-0.412437	0.120104
C	0.289386	0.931197	0.022528
C	1.643951	1.213424	-0.029804
C	-1.646875	-0.381424	-0.003429
C	-2.001218	1.044306	-0.041182

C	-0.885484	1.797307	-0.027782
C	-2.475454	-1.419834	-0.106778
H	3.611492	0.356577	-0.095771
H	2.826346	-1.975804	-0.125994
H	0.406376	-2.495854	-0.029875
H	-0.287132	-0.413460	1.961317
H	1.996875	2.237831	-0.076727
H	-3.019963	1.405389	-0.081682
H	-0.844484	2.878170	-0.058468
H	-3.543540	-1.274617	-0.221662
H	-2.111628	-2.440882	-0.077852

Frequencies

-978.9155	126.4841	200.6498
251.0499	314.1363	400.4556
420.6426	465.1780	472.0923
543.2897	561.1472	574.2131
659.8670	674.7373	726.7510
755.6980	768.1162	801.6132
817.3823	870.8815	890.7318
950.1494	951.1054	958.6852
969.6546	1002.0175	1047.6493
1090.0224	1107.6198	1152.8786
1181.8080	1220.8363	1246.8940
1326.7804	1339.1419	1395.1255
1451.5130	1477.0951	1508.6725
1603.3623	1640.7050	1663.4275
1745.9361	3163.0883	3191.4163
3197.7747	3208.3085	3220.4755
3226.6246	3248.8128	3253.2188

i70 – i74

C	1.393068	1.430776	-0.005346
C	-1.138501	-1.183620	0.017622
C	1.412864	-1.419851	-0.013228
C	2.570451	-0.703478	-0.041985
C	2.557729	0.728648	-0.035901
C	0.153008	0.721157	0.002973
C	-1.155856	1.163464	0.057018
C	-2.028730	0.013224	0.098578
C	-3.444773	0.032158	-0.183874
C	0.171820	-0.723139	-0.002970
H	1.395830	2.515293	0.004361
H	-1.501201	-2.201676	0.008712
H	-1.823203	-0.480807	1.182150
H	1.428009	-2.504449	-0.013868

H	3.525215	-1.216544	-0.067130
H	3.505474	1.255628	-0.053361
H	-1.498214	2.188117	0.083637
H	-4.010076	-0.887773	-0.255382
H	-3.968315	0.976177	-0.246436

Frequencies

-1112.7327	135.1703	217.7456
251.1468	277.2642	313.7984
439.8898	453.9641	500.4860
515.7658	555.1753	595.9261
646.4791	685.3266	709.0125
748.8164	785.0477	817.7956
839.0460	861.2266	910.3348
942.3809	973.7826	977.2363
1003.9527	1015.0583	1089.5654
1158.3385	1161.6298	1179.8501
1190.5453	1246.1092	1317.1904
1366.8687	1396.9802	1418.2263
1453.0067	1483.8621	1510.1242
1583.1607	1597.3564	1703.8468
2254.9499	3175.5244	3189.4670
3196.8065	3209.3747	3219.5990
3244.6997	3252.2211	3286.4319

il3 – i20

C	-0.088013	-0.344595	-0.308686
C	-1.069890	-1.288267	0.002964
C	-2.378403	-0.900696	0.258555
C	-2.735547	0.439857	0.192914
C	-1.770805	1.385859	-0.138629
C	-0.463730	1.000215	-0.391332
C	1.287280	-0.812694	-0.621423
C	2.093828	-0.179469	1.321051
C	2.681594	0.644611	0.434081
C	2.429960	-0.009445	-0.809457
H	-0.799861	-2.338333	0.056471
H	-3.121590	-1.650290	0.506738
H	-3.757647	0.744410	0.386250
H	-2.041407	2.433522	-0.212301
H	0.277827	1.743205	-0.661502
H	1.276342	-1.790755	-1.109223
H	1.878861	-0.171418	2.385875
H	3.226933	1.564948	0.623898
H	3.142895	-0.147543	-1.616438

Frequencies

-707.2963	52.0587	121.1300
178.9012	242.6465	355.4628
415.9189	434.4163	503.7459
556.0352	637.1088	656.8351
715.9053	747.5377	762.3067
774.0553	833.7312	860.1809
881.3230	911.9612	931.3224
970.5516	994.8627	1017.0763
1021.6418	1058.6637	1061.8413
1110.4218	1117.8280	1184.5366
1212.0722	1235.2603	1247.0145
1326.4555	1357.2087	1417.0297
1444.1761	1496.4192	1525.0763
1540.2665	1651.3204	1675.2234
3106.4659	3163.3558	3182.4393
3183.8912	3191.6746	3198.4103
3203.4039	3213.2886	3221.5663

i14 – i18

C	1.127473	-1.281966	0.041662
C	2.433558	-0.842140	0.236880
C	2.756455	0.503486	0.126609
C	1.751341	1.426919	-0.190052
C	0.487724	0.938599	-0.362773
C	0.092735	-0.383429	-0.255757
C	-1.284175	-0.870796	-0.508408
C	-2.368650	-0.032085	-0.894944
C	-2.628652	0.747624	0.204396
C	-2.113020	0.018811	1.302245
H	0.898548	-2.340934	0.122558
H	3.206602	-1.564411	0.473517
H	3.776142	0.840721	0.275829
H	1.976071	2.482588	-0.298534
H	-1.279408	-1.915067	-0.838401
H	-2.911183	-0.101410	-1.832666
H	-3.065703	1.740260	0.253770
H	-2.462534	-0.990539	1.470241
H	-1.667265	0.498661	2.174543

Frequencies

-711.4237	52.2727	120.8384
154.0562	251.7150	356.5129
417.9908	435.6481	520.0963
586.9509	630.7230	675.6881
708.1444	755.1153	768.0137

835.4278	850.8741	867.9784
906.6273	940.4045	951.3757
965.1886	989.7318	998.7092
1039.8629	1055.4349	1108.4452
1128.4613	1135.1921	1182.6623
1226.0090	1238.4713	1264.9616
1327.7742	1376.9731	1448.2384
1484.7751	1493.3138	1538.5449
1556.6744	1601.3567	1666.8385
3075.3479	3118.9351	3175.4528
3177.1123	3190.8072	3195.3860
3203.3423	3218.5373	3244.4273

i10 – i14

C	1.155795	1.230055	0.285906
C	2.509953	1.021777	0.066223
C	2.995191	-0.250823	-0.223719
C	2.113396	-1.332690	-0.301460
C	0.788704	-1.064649	-0.081654
C	0.237875	0.167026	0.220558
C	-1.199562	0.361697	0.432750
C	-2.112619	-0.701719	0.706725
C	-3.247599	-0.357326	0.021511
C	-2.805186	0.570382	-0.958035
H	0.785884	2.226649	0.508930
H	3.197616	1.857732	0.121916
H	4.055202	-0.406394	-0.392200
H	2.470908	-2.330807	-0.528621
H	-1.484887	1.357055	0.750979
H	-1.881307	-1.599728	1.270806
H	-4.278491	-0.632785	0.221540
H	-3.415572	1.414422	-1.286358
H	-2.065049	0.251485	-1.679822

Frequencies

-676.0484	62.6265	100.4580
139.2531	285.0111	385.2871
402.3226	424.3335	535.0213
590.0425	633.9234	680.7636
707.8093	723.4437	763.0581
816.8269	864.5008	874.9327
900.6009	937.8547	964.3608
971.3863	995.4219	1013.2476
1034.6474	1050.5466	1115.5969
1133.9027	1165.7378	1180.0303
1224.1963	1235.8396	1275.8366

1328.5725	1353.4652	1441.8280
1482.4980	1495.6771	1532.6878
1563.5104	1606.2918	1662.2945
3101.1649	3174.1394	3183.8853
3193.5804	3195.3103	3205.6968
3206.9990	3218.4749	3232.5234

i4 – i7

C	-0.342928	-0.248352	0.072804
C	-1.287536	-1.284094	-0.026651
C	-2.644495	-1.016116	-0.108034
C	-3.100188	0.297705	-0.096383
C	-2.179728	1.338200	-0.005369
C	-0.823335	1.073418	0.077278
C	1.064170	-0.583648	0.159865
C	2.103949	0.300166	0.373364
C	3.535105	-0.113558	0.412513
C	3.610212	0.219155	-0.827803
H	-0.940111	-2.312437	-0.037355
H	-3.351579	-1.834882	-0.182225
H	-4.161020	0.509593	-0.163252
H	-2.525065	2.366265	-0.003912
H	-0.126793	1.901912	0.131210
H	1.317793	-1.631566	0.019634
H	1.889363	1.336737	0.612138
H	4.156208	-0.524235	1.201844
H	4.129853	0.291355	-1.767584

Frequencies

-721.3913	52.6010	84.1842
171.2006	207.0022	298.1803
341.5721	412.6171	416.5477
504.3699	572.0709	633.5651
639.0926	654.8385	704.2547
758.9510	821.4963	847.2053
853.2247	875.7702	924.1577
940.2194	989.4041	1009.9456
1015.9417	1048.8266	1062.0683
1113.7534	1166.8424	1185.9449
1201.4735	1247.1307	1282.0995
1318.7664	1350.8912	1355.8956
1479.0154	1523.7124	1535.7144
1639.7807	1659.5042	1727.1205
3169.9911	3175.8775	3178.9699
3183.5930	3191.4788	3202.6506
3213.4682	3221.3430	3308.4618

i7 – i20

C	0.238272	-0.510782	0.120096
C	1.392762	-1.278233	-0.124264
C	2.642897	-0.693744	-0.232197
C	2.783815	0.683673	-0.096847
C	1.657677	1.461456	0.150516
C	0.404493	0.879331	0.258352
C	-1.030379	-1.204252	0.219525
H	1.292655	-2.353470	-0.233262
H	3.512175	-1.313261	-0.422868
H	3.760430	1.146068	-0.181876
H	1.757900	2.535371	0.263287
H	-0.451390	1.511029	0.450535
H	-0.957870	-2.287566	0.168287
C	-2.320540	-0.706283	0.319282
C	-2.751727	0.719265	0.343399
C	-2.978183	0.605343	-0.917746
H	-3.104385	-1.442712	0.465126
H	-2.801135	1.464496	1.131010
H	-3.242907	1.005403	-1.880936

Frequencies

-703.9555	38.4118	111.4038
180.3318	209.5244	306.3356
369.5757	417.0264	474.6813
517.2855	562.5146	636.1814
653.0643	707.5184	714.2599
744.0787	805.9104	814.5782
857.0325	866.7664	930.6980
935.5429	995.5988	997.3290
1017.7532	1018.1379	1062.4248
1122.1597	1145.5554	1187.9588
1208.6165	1226.8246	1273.8012
1341.3104	1358.7985	1427.2443
1456.8357	1515.8310	1534.2942
1640.5016	1661.6709	1725.4220
3158.7252	3167.8773	3178.7390
3183.2261	3190.9333	3202.6855
3216.0392	3245.9751	3314.4083

il2 – il8

C	1.543491	-1.163217	-0.629406
C	-2.184104	1.468654	-0.769580
C	1.053898	1.268040	0.779152
C	2.282247	1.014555	0.161638

C	2.517282	-0.179363	-0.530226
C	0.312899	-0.919355	-0.010717
C	-0.895643	-1.637740	0.272613
C	-1.875146	-0.673699	0.612308
C	-2.532560	0.264015	-0.342101
C	0.099067	0.278176	0.668130
H	1.738157	-2.088540	-1.160113
H	-1.285477	1.961201	-0.420309
H	-2.802973	1.995125	-1.487932
H	0.879340	2.196498	1.310908
H	3.071871	1.756137	0.223271
H	3.484697	-0.335354	-0.994447
H	-0.949545	-2.676686	0.580239
H	-2.588508	-0.981229	1.384538
H	-3.476148	-0.147544	-0.707014

Frequencies

-679.2618	63.7396	102.7424
168.0833	255.6958	324.9524
421.2242	457.2814	470.3830
504.6956	588.1486	614.8332
654.9048	722.0119	753.3363
785.1208	831.4571	887.5114
915.8798	955.9502	965.0415
972.6427	999.8733	1017.6668
1019.3229	1036.1370	1081.3473
1137.6668	1157.6186	1181.5835
1240.3599	1267.8232	1325.4018
1334.3147	1401.9862	1431.5031
1452.7739	1467.3664	1499.0164
1613.9482	1639.8806	1736.1124
3075.2743	3108.1140	3172.9624
3183.3777	3192.8168	3195.9446
3206.9242	3213.2100	3268.1162

il3 – il4

C	-1.141344	1.324212	0.182588
C	-2.433892	0.888164	-0.097657
C	-2.710752	-0.466201	-0.266262
C	-1.694243	-1.417298	-0.153228
C	-0.426807	-0.952988	0.125928
C	-0.121714	0.384987	0.295062
C	1.345606	0.613392	0.556157
C	2.223999	0.812256	-0.676956
C	2.796755	-0.398172	-0.578968
C	2.003996	-0.796401	0.607904

H	-0.937771	2.382339	0.316191
H	-3.236293	1.612367	-0.184280
H	-3.724883	-0.785230	-0.482562
H	-1.906106	-2.473035	-0.280915
H	0.925826	-1.453828	0.308650
H	1.550276	1.283811	1.394253
H	2.309712	1.631778	-1.380180
H	3.539799	-0.919261	-1.170147
H	2.429824	-1.230644	1.511578

Frequencies

-1849.1793	104.5986	141.2065
270.6682	298.8265	393.9497
422.6061	489.3430	541.6827
629.6715	675.8857	725.7780
733.6619	771.9999	857.9451
879.4593	891.7910	913.9782
931.7270	960.6961	972.8469
996.3442	1014.7908	1016.1201
1017.7272	1051.8766	1117.4806
1141.6353	1180.0756	1184.7557
1194.9647	1219.8350	1260.8583
1292.6751	1315.3980	1336.4735
1345.4782	1479.4227	1493.5245
1605.4068	1638.5413	1661.0434
1668.5087	3099.4565	3146.1287
3181.1400	3189.9617	3202.7825
3206.9894	3213.3274	3238.0849

i3 – i8

C	0.487293	0.072477	-0.242873
C	1.258811	1.218838	0.018673
C	2.611519	1.101469	0.291139
C	3.224050	-0.148330	0.308684
C	2.467186	-1.287728	0.048158
C	1.115089	-1.185600	-0.231787
C	-0.896263	0.189896	-0.579602
C	-2.157329	0.345378	-0.416115
C	-3.446449	0.434775	0.162421
C	-4.192067	-0.627019	0.532172
H	0.782162	2.192125	0.009879
H	3.192764	1.993350	0.497406
H	4.283028	-0.234772	0.521617
H	2.936842	-2.264867	0.064488
H	0.528681	-2.073511	-0.437771
H	-1.685020	0.394280	-1.601524

H	-3.862531	1.436404	0.228096
H	-3.809277	-1.638433	0.463592
H	-5.197696	-0.489514	0.908998

Frequencies

-2140.4517	32.9947	48.7189
94.6898	180.0487	207.6095
297.0609	357.3289	394.3994
413.8001	473.8676	513.2413
581.0811	638.5499	639.0870
706.4203	714.0298	769.2717
850.9012	859.8293	922.4389
931.9877	962.0949	990.9433
1012.8088	1014.7320	1055.9690
1084.2127	1112.0219	1184.7366
1203.1025	1254.6020	1297.2094
1311.5259	1355.6886	1427.3104
1483.0841	1523.3731	1588.5437
1626.2956	1655.3301	2079.4225
2371.2945	3164.6803	3174.9493
3191.7518	3198.5697	3210.0545
3217.0332	3224.5312	3264.4516

il – i107

C	-1.382334	-1.223997	0.002225
C	-2.760427	-1.074514	-0.006641
C	-3.330286	0.194027	-0.009950
C	-2.510380	1.317339	-0.002377
C	-1.131278	1.177418	0.009621
C	-0.548093	-0.097320	0.010919
C	0.868394	-0.245589	0.019391
C	2.072250	-0.375874	0.032550
C	3.473120	-0.511800	0.001888
C	4.392544	0.657962	0.033791
H	-0.935769	-2.211182	0.002618
H	-3.394436	-1.954049	-0.012379
H	-4.408248	0.307354	-0.018476
H	-2.948956	2.308814	-0.004365
H	-0.490331	2.051146	0.018151
H	4.001869	-0.078582	-1.047320
H	3.901334	-1.479245	0.239483
H	5.435506	0.494432	0.262246
H	3.977970	1.655410	0.011537

Frequencies

-1915.9509	21.8504	69.1080
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83.9165	187.8082	236.0417
367.5871	380.2718	413.2611
483.5634	499.6003	540.6443
582.8309	638.7490	642.8753
709.1041	717.8481	775.0658
796.3490	862.9442	928.0602
936.0558	997.6970	1013.9023
1021.6797	1057.9114	1080.6956
1111.6646	1161.8758	1187.6446
1206.6911	1245.5681	1299.3585
1314.1424	1355.2984	1414.7978
1441.5437	1486.8894	1542.0515
1641.7491	1673.6598	2229.1347
2293.5655	3181.4720	3188.8904
3194.2811	3198.1770	3208.4276
3219.6393	3224.5049	3311.3398

il07 - p2

C	1.383549	-1.222387	0.031682
C	2.762559	-1.079820	0.045275
C	3.336126	0.186509	0.018662
C	2.523615	1.314239	-0.021167
C	1.143691	1.179961	-0.035638
C	0.558652	-0.091696	-0.009216
C	-0.861713	-0.234789	-0.025312
C	-2.062794	-0.349553	-0.041664
C	-3.471478	-0.513816	-0.058654
C	-4.345498	0.499064	-0.161994
H	0.930834	-2.206448	0.052731
H	3.393025	-1.961085	0.076329
H	4.414607	0.295059	0.029789
H	2.967820	2.302732	-0.041841
H	0.505302	2.054877	-0.066322
H	-3.838107	-1.532519	0.031742
H	-4.752717	1.091117	1.964114
H	-5.410516	0.308245	-0.209342
H	-4.010498	1.521755	-0.289048

Frequencies

-478.3773	40.7619	64.9410
80.0016	163.7567	200.7321
251.4979	281.0995	378.3610
409.2349	413.0225	511.5013
554.6008	591.9716	642.0304
709.5512	721.3971	728.3039
780.7808	866.4627	945.6754
956.5738	964.0215	1001.6644

1012.2047	1018.6725	1023.3670
1060.0970	1105.9181	1112.4754
1189.4449	1207.9369	1301.5794
1311.3806	1317.3855	1356.1610
1446.8362	1488.1155	1540.9999
1646.0693	1649.6047	1680.3235
2340.1297	3169.7510	3179.9605
3192.0104	3201.7059	3210.6930
3221.5846	3226.1558	3269.7550

il – i25

C	-1.032520	1.236201	0.087314
C	-2.405394	1.137297	0.258367
C	-3.033239	-0.099071	0.158287
C	-2.286630	-1.239597	-0.119826
C	-0.915853	-1.145305	-0.301867
C	-0.275882	0.094785	-0.201277
C	1.145361	0.196994	-0.377564
C	2.254966	0.525198	-0.879224
C	2.657576	-0.571714	1.007021
C	3.457664	0.113912	-0.095961
H	-0.531670	2.193390	0.168615
H	-2.986104	2.026664	0.474413
H	-4.105504	-0.175580	0.298275
H	-2.776211	-2.203279	-0.199199
H	-0.325973	-2.027224	-0.522070
H	2.616709	-1.655908	1.019430
H	2.542070	-0.060317	1.956701
H	4.052097	0.964765	0.245376
H	4.118293	-0.554697	-0.653158

Frequencies

-787.8299	30.6386	93.3553
105.3588	220.0016	267.9184
390.4366	409.8474	415.8436
512.8903	562.3435	641.1170
658.5185	715.3125	757.4193
772.0045	795.1220	804.0122
872.9503	962.1284	994.2546
1008.1962	1024.7480	1032.4384
1043.4964	1062.6985	1064.3841
1112.3827	1189.5301	1207.0133
1212.9891	1240.9332	1270.2644
1321.2173	1355.0826	1431.2615
1486.3287	1488.3011	1534.6844
1647.2414	1674.4521	1925.9571

3073.8313	3117.7459	3139.1724
3192.7070	3201.1249	3210.8005
3218.6974	3224.3518	3255.3972

i25 – i26

C	0.939269	1.186410	0.101927
C	2.323998	1.130477	0.006358
C	2.966861	-0.097167	-0.083264
C	2.217795	-1.270673	-0.081489
C	0.835766	-1.214891	-0.002981
C	0.177411	0.015827	0.089568
C	-1.282269	0.073188	0.155851
C	-2.219682	-0.888155	0.334451
C	-2.137187	1.218146	-0.112317
C	-3.449904	-0.513765	-0.193900
H	0.442206	2.145793	0.201949
H	2.901758	2.047946	0.013461
H	4.047840	-0.142454	-0.152122
H	2.715251	-2.231445	-0.151626
H	0.247761	-2.126415	-0.019130
H	-1.901189	1.915784	-0.920980
H	-2.749159	1.616315	0.685720
H	-4.394544	-0.679976	0.326221
H	-3.542267	-0.381927	-1.268722

Frequencies

-705.1304	75.6417	110.8419
150.1841	260.9339	365.8530
419.3470	435.4189	472.3740
583.9005	635.9497	640.0973
673.7540	692.2552	720.6957
792.5715	816.1827	871.9075
888.8618	948.8551	978.0029
1003.9346	1021.5541	1023.8240
1027.3970	1054.2127	1062.5667
1111.6079	1139.1743	1186.8954
1212.1852	1223.8074	1332.3841
1356.0230	1367.2395	1466.9789
1493.7824	1511.9769	1541.7663
1617.9333	1655.0013	1683.8210
3083.8729	3106.6295	3184.4058
3189.2722	3192.0377	3198.0294
3206.7751	3218.1224	3242.5286

i26 – p16

C	-1.091499	1.172410	-0.287786
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C	-2.428620	0.801733	-0.307162
C	-2.794251	-0.508908	-0.024007
C	-1.813382	-1.447371	0.271079
C	-0.475380	-1.078279	0.288384
C	-0.100288	0.239396	0.022101
C	1.332762	0.641184	0.081150
C	2.304284	-0.343616	-0.277667
C	1.736350	1.857955	0.472980
C	3.111170	-1.214513	-0.503488
H	-0.813181	2.190176	-0.537438
H	-3.185910	1.536242	-0.556413
H	-3.838643	-0.798732	-0.043279
H	-2.088815	-2.473368	0.486942
H	0.287531	-1.814194	0.516413
H	1.022799	2.607842	0.792786
H	2.787480	2.115535	0.496018
H	3.822631	-1.903399	-0.893120
H	3.319235	-2.180040	1.324592

Frequencies

-614.7664	49.0104	67.2690
122.2331	162.1400	225.5078
257.3743	356.9793	411.4504
420.6289	431.0481	494.8746
625.4242	636.3967	648.2826
708.2005	714.1729	736.0444
748.3681	775.8275	801.1830
871.9798	927.8085	946.2429
954.1430	1004.6076	1022.7154
1024.3008	1062.6383	1117.6255
1137.7831	1189.3759	1219.6359
1311.1166	1344.7824	1364.3876
1439.6018	1492.3020	1546.1556
1650.9028	1679.7073	1684.7165
2170.5687	3173.4422	3189.4494
3197.7505	3204.6702	3214.4379
3221.3384	3270.4658	3465.9851

i26 – p18

C	1.124219	1.231920	0.000239
C	2.490640	0.947256	0.000213
C	2.928656	-0.372986	-0.000013
C	2.011569	-1.419548	-0.000204
C	0.641477	-1.153162	-0.000175
C	0.258716	0.165402	0.000046
C	-2.054148	0.732524	-0.000102

C	-2.477666	-0.466069	0.000094
C	-2.027347	2.067765	-0.000298
C	-2.911343	-1.702107	0.000222
H	0.763965	2.255190	0.000410
H	3.210254	1.759185	0.000366
H	3.991090	-0.588043	-0.000041
H	2.359532	-2.447174	-0.000382
H	-0.089348	-1.955273	-0.000310
H	-1.968332	2.622581	-0.930651
H	-1.969157	2.622874	0.929932
H	-3.103597	-2.227456	0.929979
H	-3.103033	-2.227847	-0.929434

Frequencies

-340.0622	24.0762	75.6411
100.6978	135.6110	140.3407
224.4053	233.4864	377.2135
409.1725	437.7054	466.8617
612.8399	614.6694	696.1631
704.4338	739.4006	822.5966
847.7381	878.5104	888.0443
917.5608	979.4801	988.9024
1014.8871	1023.0923	1032.8779
1041.8334	1056.9587	1085.9554
1181.8751	1183.3826	1309.2152
1331.8994	1394.1094	1461.4706
1477.4517	1488.7681	1613.2267
1624.5075	1666.1267	2162.3926
3140.1993	3142.7532	3177.0996
3180.7789	3191.8385	3195.9146
3211.5450	3228.1058	3233.0272

i26 – i27

C	1.203017	1.276842	0.000030
C	2.509601	0.802422	0.000030
C	2.777899	-0.565833	0.000002
C	1.735210	-1.493345	-0.000026
C	0.451252	-0.994027	-0.000026
C	0.153918	0.360750	0.000000
C	-1.308338	0.598261	-0.000016
C	-1.957176	-0.724540	-0.000016
C	-1.931410	1.776811	-0.000039
C	-3.198748	-1.164799	0.000050
H	1.011248	2.344759	0.000052
H	3.333521	1.507049	0.000051
H	3.805879	-0.912044	0.000002

H	1.938261	-2.558154	-0.000047
H	-0.836064	-1.466143	-0.000045
H	-1.379028	2.709909	-0.000037
H	-3.013144	1.845067	-0.000066
H	-4.046622	-0.480062	0.000105
H	-3.425390	-2.225628	0.000052

Frequencies

-1920.3793	42.4363	131.4690
218.0565	227.2870	280.6012
380.7680	411.5274	447.8488
482.3832	525.8624	591.9813
660.8746	662.0282	717.4379
737.4377	764.9686	793.4479
874.9841	881.2949	918.1303
924.4229	958.7180	1005.9489
1010.6377	1051.0724	1077.2513
1096.6248	1130.0352	1143.1986
1185.8475	1254.1532	1314.6842
1344.9692	1422.1278	1455.2812
1480.5392	1494.8359	1642.1913
1660.4724	1712.0552	1745.1140
1786.7436	3115.0113	3163.9952
3188.2208	3196.0098	3207.9589
3212.8018	3218.5174	3250.6046

i27 – i28

C	-1.089008	1.220476	0.132004
C	-2.424237	0.841717	0.093836
C	-2.783657	-0.497378	-0.029962
C	-1.790720	-1.475577	-0.108754
C	-0.491548	-1.041848	-0.063666
C	-0.062843	0.266096	0.037550
C	1.379283	0.620628	0.046285
C	1.829346	1.813490	-0.343313
H	-0.832203	2.266811	0.260367
H	-3.194886	1.599821	0.172341
H	-3.829640	-0.782934	-0.057277
H	-2.042363	-2.526309	-0.200442
H	1.164576	2.583810	-0.718074
H	2.888458	2.042466	-0.316767
C	2.326271	-0.432455	0.513203
C	2.682634	-1.483839	-0.212942
H	2.725214	-0.308733	1.517780
H	2.298178	-1.634250	-1.216799
H	3.369534	-2.228533	0.173428

Frequencies

-117.6843	44.2113	137.8613
163.4524	292.1165	311.5654
392.6585	424.5958	476.5309
515.5360	629.9162	654.4871
691.4608	706.8377	743.1242
762.8473	782.9579	875.0769
913.3911	945.2031	965.4101
971.6073	992.7370	1006.6006
1025.8427	1054.7220	1080.1005
1137.1221	1146.6260	1189.1442
1250.6655	1322.6348	1326.8201
1339.4231	1437.1965	1451.7853
1468.6155	1496.8017	1605.3191
1667.5449	1697.0315	1742.8868
3147.2595	3159.6038	3162.3145
3186.2331	3196.5896	3205.7433
3216.0109	3241.2624	3249.8716

i28 – i29

C	0.912166	-1.354164	-0.127252
C	2.258926	-1.013438	-0.091974
C	2.655555	0.312909	0.058576
C	1.697150	1.322461	0.167754
C	0.377169	0.940006	0.159170
C	-0.064655	-0.363658	0.004906
C	-1.536709	-0.573242	0.027705
C	-2.229061	0.710884	0.158715
C	-2.148667	-1.763535	0.048049
C	-1.650046	1.841438	-0.336966
H	0.625426	-2.391471	-0.266606
H	3.009639	-1.789413	-0.188743
H	3.710824	0.562724	0.089860
H	1.991986	2.360936	0.271559
H	-3.069838	0.776457	0.841757
H	-3.229401	-1.832498	0.093202
H	-1.597168	-2.696021	0.022591
H	-2.003007	2.819263	-0.023544
H	-1.069431	1.832052	-1.252176

Frequencies

-559.5576	78.4619	147.9546
212.8049	285.5957	386.6227
412.4614	463.5265	494.4624
521.3638	576.4380	617.3187

657.2945	726.8391	740.0165
762.9895	788.9642	839.8278
882.3374	905.8139	913.2984
951.9731	965.6737	993.6308
1006.3943	1041.1157	1057.2771
1137.2984	1154.1062	1192.2144
1256.8250	1267.4839	1325.8664
1341.9246	1414.7443	1452.0464
1467.4447	1495.7156	1569.4063
1622.2744	1661.1057	1691.7424
3148.6139	3166.4345	3183.5529
3189.9259	3193.7603	3203.6251
3213.0508	3232.1098	3253.9997

i29 – i91

C	-1.002354	1.345867	-0.301046
C	-2.227349	0.735048	-0.306714
C	-2.372155	-0.617962	0.052507
C	-1.222222	-1.379928	0.279388
C	0.029058	-0.807076	0.318304
C	0.175963	0.642533	0.170669
C	1.742095	0.738009	-0.445855
C	2.224989	-0.497904	-0.541944
C	1.300896	1.565514	0.668273
C	1.290921	-1.561381	-0.019236
H	-0.916599	2.395804	-0.560219
H	-3.102649	1.308310	-0.593100
H	-3.349230	-1.084740	0.052042
H	-1.304823	-2.462167	0.333596
H	3.265479	-0.720273	-0.763740
H	1.796363	1.356869	1.612538
H	1.073951	2.616555	0.517999
H	1.803643	-1.990998	0.855649
H	1.094809	-2.395676	-0.700839

Frequencies

-742.1018	137.4243	176.8087
235.5654	365.6102	417.5328
450.9604	469.0631	516.6216
549.2197	656.3064	695.3316
702.9199	734.3179	788.0498
804.2423	834.2736	901.6648
915.1276	935.6678	950.8804
974.3671	1003.9973	1043.6151
1046.7384	1121.8918	1126.6493
1137.1798	1162.9098	1180.4735

1188.3846	1246.9228	1296.0229
1313.3166	1340.0007	1439.1270
1451.8283	1453.8124	1487.7523
1550.8156	1617.9549	1686.5961
3006.6221	3073.8942	3115.6597
3163.8125	3168.8183	3180.7057
3199.2476	3203.0839	3224.6140

i91 – i23

C	1.279472	1.377261	0.000784
C	2.456902	0.654579	-0.112145
C	2.411298	-0.735762	-0.118012
C	1.193724	-1.394885	-0.002789
C	0.004220	-0.683604	0.118067
C	0.053642	0.720715	0.112159
C	-2.418444	0.747641	-0.101466
C	-2.429552	-0.575722	-0.353512
C	-1.227203	1.448015	0.218362
C	-1.331472	-1.393258	0.292523
H	1.302423	2.462557	-0.000648
H	3.406434	1.169770	-0.199867
H	3.327798	-1.307426	-0.211522
H	1.166630	-2.480111	-0.002250
H	-3.138716	-1.046583	-1.023744
H	-1.952114	1.744431	-0.847406
H	-1.268854	2.399148	0.742549
H	-1.282994	-2.393004	-0.146837
H	-1.516136	-1.538664	1.365900

Frequencies

-1826.3955	128.4567	175.3354
287.6241	355.6205	424.1332
430.0494	490.8649	513.9708
548.9482	612.0303	672.5729
716.5828	744.7029	769.3739
779.6635	831.8911	873.5140
912.9080	931.5110	971.6391
1006.3187	1012.8610	1069.7354
1090.4976	1135.4044	1180.9001
1187.8447	1202.7886	1207.2546
1232.4605	1272.1841	1282.1659
1324.4515	1349.4800	1405.4385
1477.3588	1502.1232	1519.0554
1545.9729	1644.4576	1675.0120
2125.7027	3014.7307	3096.0039
3172.5673	3185.8143	3190.5731

3203.2572	3204.5075	3219.3941
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i29 – i94

C	-0.940007	-1.462521	-0.224876
C	-2.250630	-1.044619	-0.023718
C	-2.547789	0.302594	0.171010
C	-1.533566	1.258298	0.177884
C	-0.227850	0.848503	-0.029296
C	0.072679	-0.508500	-0.240760
C	1.516808	-0.658866	-0.423928
C	2.095058	0.597873	-0.285873
C	2.448787	-1.195418	0.574401
C	1.050050	1.654052	-0.008432
H	-0.709461	-2.511094	-0.375095
H	-3.051695	-1.775407	-0.017080
H	-3.576436	0.608248	0.325525
H	-1.767494	2.303556	0.352150
H	3.131456	0.832503	-0.489874
H	3.450285	-1.516125	0.313805
H	2.128428	-1.278046	1.606842
H	1.087658	2.427075	-0.785041
H	1.206014	2.160911	0.950291

Frequencies

-819.2665	139.1860	189.0462
300.3879	313.3433	399.7383
440.0941	530.6747	541.6771
563.5814	599.9967	611.8790
739.3521	747.1981	763.4180
789.3402	807.5102	852.2119
897.9607	923.4422	966.1621
985.0586	1012.3681	1017.7929
1055.9352	1095.3974	1152.0847
1157.0115	1176.0036	1185.8207
1224.6362	1252.2475	1323.2225
1343.5650	1384.0374	1415.9677
1450.1047	1468.1524	1509.5415
1513.2906	1646.2585	1679.4441
3049.6987	3085.8457	3146.7342
3186.6897	3197.3880	3209.4145
3221.1379	3222.8027	3258.1568

i94 – i95

C	-1.154397	-1.432619	-0.186281
C	-2.391124	-0.816665	0.000879
C	-2.478604	0.559567	0.166788

C	-1.327893	1.348919	0.144593
C	-0.097644	0.749101	-0.055066
C	-0.017790	-0.643906	-0.206489
C	1.410330	-0.980891	-0.331687
C	2.263210	0.254857	-0.330235
C	2.354496	-0.706326	0.793026
C	1.267121	1.408822	-0.149382
H	-1.083157	-2.506507	-0.314522
H	-3.292903	-1.418451	0.016872
H	-3.447198	1.025530	0.307295
H	-1.402038	2.424376	0.270779
H	3.091339	0.399714	-1.015253
H	2.290180	-1.804092	0.106331
H	2.080214	-0.657364	1.838954
H	1.313281	2.070211	-1.019033
H	1.484046	2.021424	0.731708

Frequencies

-1864.8024	126.6167	183.9914
307.0784	338.9316	374.2762
433.5103	524.6979	553.4825
579.4655	649.7347	708.8686
743.8097	783.7846	796.6081
809.4921	851.9013	898.9323
910.8128	921.5942	974.8997
993.4641	1015.8249	1040.0385
1056.0818	1077.8052	1115.0571
1133.8935	1181.0807	1189.8178
1201.6337	1229.7716	1259.2201
1305.8355	1341.3073	1363.1706
1413.5389	1472.0516	1506.9332
1511.8992	1654.6098	1684.6067
2309.1808	3058.2198	3099.0553
3171.3475	3182.1658	3191.3958
3204.8067	3210.6603	3214.3428

i95 – i23

C	-1.153861	-1.420255	-0.128201
C	-2.398605	-0.814272	-0.025490
C	-2.493250	0.566835	0.111605
C	-1.341433	1.346667	0.128210
C	-0.098425	0.747420	-0.005105
C	0.003896	-0.642996	-0.096428
C	1.345366	-1.250740	-0.073635
C	2.322774	0.500881	-0.278403
C	2.420932	-0.671979	0.598865

C	1.218780	1.487637	-0.094569
H	-1.076731	-2.499564	-0.212109
H	-3.297716	-1.419501	-0.047830
H	-3.466202	1.038933	0.186657
H	-1.415856	2.426430	0.211518
H	1.415206	-2.258628	-0.492535
H	2.972718	0.568805	-1.145279
H	3.348197	-1.210440	0.750261
H	1.193070	2.211587	-0.912682
H	1.370275	2.047189	0.840902

Frequencies

-908.5812	142.7286	179.9349
297.6093	357.5735	415.0205
462.4472	507.2060	547.9345
579.0365	603.5996	635.5818
737.3972	740.3925	779.0485
785.2225	873.3961	887.9262
922.6595	948.7552	971.9271
1005.1405	1011.4207	1065.0036
1127.3169	1135.5553	1170.2807
1182.9229	1191.2403	1217.0219
1235.7310	1271.7000	1283.5807
1337.4598	1340.0251	1363.3879
1446.7069	1463.3512	1507.6020
1533.7118	1656.9275	1675.2114
3007.5481	3089.2813	3103.1561
3173.3199	3180.8405	3185.6529
3198.8321	3209.7011	3213.8305

i29 – p20

C	-0.775917	-1.482347	0.038910
C	-2.133929	-1.168857	0.030583
C	-2.556772	0.156571	-0.021315
C	-1.633819	1.199259	-0.062891
C	-0.284073	0.887214	-0.055177
C	0.143407	-0.449165	-0.006347
C	1.623174	-0.449858	-0.023178
C	2.018423	0.958991	-0.099445
C	2.440765	-1.506385	0.015894
C	0.913281	1.746169	-0.086981
H	-0.453453	-2.517525	0.077675
H	-2.869446	-1.964399	0.063487
H	-3.618037	0.378301	-0.027852
H	-1.967594	2.230516	-0.097025
H	3.044786	1.295938	-0.146608

H	3.517718	-1.383107	-0.004273
H	2.056052	-2.518830	0.068734
H	0.893084	2.817733	-0.233063
H	0.869655	2.311818	1.918603

Frequencies

-648.0352	126.6137	189.1090
231.7067	258.4816	282.7895
373.8172	414.1265	460.7091
542.9763	568.2809	574.2860
650.8236	666.6262	726.8016
767.6038	774.2082	803.1961
825.2629	871.9258	894.9325
939.7318	951.4797	962.6925
976.9216	1006.1103	1052.0880
1080.1123	1110.9644	1153.5665
1187.4437	1218.4637	1250.0166
1330.9105	1342.9584	1396.4515
1451.0788	1501.4737	1507.2922
1558.7671	1663.6713	1688.5237
1718.7257	3162.6582	3188.3535
3194.0239	3206.3189	3219.7246
3229.8345	3249.6212	3253.8374

i26 – i89

C	0.994761	1.148045	0.387685
C	2.348977	0.859738	0.481897
C	2.825947	-0.391089	0.109026
C	1.936571	-1.352629	-0.354177
C	0.582189	-1.064281	-0.448716
C	0.093614	0.192735	-0.087766
C	-1.353654	0.517904	-0.200248
C	-2.289381	-0.543101	0.056758
C	-1.796345	1.729058	-0.588810
C	-3.225123	-1.188213	0.660525
H	0.625000	2.115690	0.707672
H	3.033357	1.611911	0.857855
H	3.883328	-0.616696	0.186806
H	2.298652	-2.332205	-0.645492
H	-0.104007	-1.818662	-0.817311
H	-1.101654	2.511207	-0.871681
H	-2.855822	1.941998	-0.655409
H	-3.804275	-1.222174	1.583390
H	-2.679917	-1.640076	-0.442876

Frequencies

-2144.7361	28.3978	79.6131
135.0520	166.3386	210.4664
249.3929	364.7798	382.1439
418.3371	488.0882	518.8808
627.6928	643.4456	663.0912
707.2126	721.9096	746.5011
798.9591	835.4578	867.4943
895.1216	905.4916	947.9819
999.7058	1021.7064	1024.2820
1060.8444	1112.9524	1131.1544
1189.5044	1211.7188	1291.8256
1333.6309	1356.4583	1426.2339
1490.8160	1541.0735	1616.3189
1657.7713	1681.5655	1922.5383
2411.7808	3100.7212	3170.6140
3189.2520	3194.7953	3205.2147
3211.5388	3221.7396	3267.6925

i89 – p16

C	1.049622	-1.177225	-0.277440
C	2.397555	-0.848866	-0.293329
C	2.804093	0.448930	-0.006476
C	1.852454	1.417036	0.288269
C	0.503845	1.089567	0.302641
C	0.086900	-0.215024	0.033393
C	-1.356009	-0.569433	0.089280
C	-2.315134	0.464243	-0.239076
C	-1.803635	-1.774062	0.456631
C	-3.224371	1.266172	-0.174362
H	0.739841	-2.184409	-0.532531
H	3.131993	-1.605823	-0.543839
H	3.857123	0.705744	-0.023718
H	2.159749	2.433774	0.505150
H	-0.236156	1.848861	0.529176
H	-1.655532	0.742161	-1.980029
H	-1.117745	-2.554983	0.762850
H	-2.863181	-1.994769	0.472258
H	-3.988012	2.001413	-0.266501

Frequencies

-889.2181	47.4935	96.0791
132.2803	189.5845	271.5617
322.5547	395.0147	417.6980
422.2774	490.9004	503.9177
620.0910	638.0877	642.0426
658.2245	712.7853	732.7696

741.0621	754.9100	801.4487
869.5826	921.8321	945.1754
954.5018	1002.9510	1021.6879
1025.9650	1062.5034	1117.5068
1135.8901	1189.6492	1217.7339
1309.0164	1343.3437	1363.1319
1440.4234	1492.0224	1545.4907
1653.2657	1682.1691	1698.2065
2127.8578	3174.4214	3190.7779
3200.3771	3206.4614	3215.8257
3222.6452	3270.7669	3469.9868

i89 – i90

C	0.940496	1.166584	0.366394
C	2.298371	0.899875	0.461242
C	2.795327	-0.344699	0.092070
C	1.919820	-1.322807	-0.361553
C	0.560356	-1.056898	-0.451061
C	0.050377	0.196850	-0.104439
C	-1.400352	0.487374	-0.240628
C	-1.874523	1.706121	-0.497517
H	0.560636	2.130142	0.686519
H	2.971016	1.663402	0.835717
H	3.856115	-0.553614	0.170696
H	2.295816	-2.300059	-0.643085
H	-0.114762	-1.832550	-0.794200
H	-1.216260	2.555377	-0.642853
H	-2.940247	1.882796	-0.583549
C	-2.353020	-0.666005	-0.131982
C	-2.810381	-1.149585	0.991690
H	-2.681453	-1.115496	-1.076227
H	-3.489696	-1.930860	1.301685

Frequencies

-122.4825	46.4237	127.9884
210.6708	266.8764	326.3251
417.2259	426.3979	488.8203
494.4628	630.2973	641.2079
689.6498	710.5089	728.9413
745.1923	805.4284	839.3894
860.1270	867.4983	944.3658
950.6179	976.8159	1000.4591
1021.2120	1024.4979	1062.8037
1117.8272	1138.4359	1190.6859
1218.6299	1245.5977	1307.9771
1338.5735	1363.8224	1442.7736

1491.6235	1543.9195	1651.8523
1681.2162	1686.6278	1719.2853
3050.9938	3166.6982	3189.8974
3197.7186	3207.0524	3213.1961
3222.5454	3256.0015	3258.6177

i90 – i93

C	0.667002	-1.369667	-0.278281
C	2.036900	-1.151776	-0.435537
C	2.592389	0.080896	-0.091895
C	1.802090	1.075271	0.455967
C	0.413933	0.873299	0.626546
C	-0.147039	-0.384338	0.247784
C	-1.618836	-0.397430	0.113711
C	-2.038922	0.906948	-0.440647
C	-2.434499	-1.417032	0.385513
C	-1.100305	1.828094	-0.559660
H	0.218899	-2.294366	-0.626266
H	2.663105	-1.931857	-0.852647
H	3.654803	0.249296	-0.228986
H	2.248971	2.006508	0.785066
H	-0.088481	1.468406	1.383072
H	-3.077708	1.063922	-0.727046
H	-2.058919	-2.340660	0.810669
H	-3.499971	-1.347687	0.195533
H	-1.096980	2.860853	-0.880396

Frequencies

-583.3639	106.1163	167.4896
240.7762	268.7202	357.1664
409.1120	485.9138	538.9215
549.9192	616.4988	628.9478
690.1800	734.6566	754.8973
771.1472	784.6860	801.9183
864.8468	894.2493	911.8821
933.1480	961.0408	977.3780
1004.2732	1021.4116	1050.1441
1100.1221	1137.4204	1182.5118
1199.0660	1225.4388	1302.4680
1330.5755	1351.3424	1444.6713
1465.9594	1524.0797	1601.4918
1632.8943	1637.5692	1733.3816
3147.2955	3158.9964	3166.7896
3190.4255	3196.5848	3209.5080
3220.8708	3245.3881	3249.4182

i93 – p20

C	0.724151	-1.483723	0.025955
C	2.088359	-1.200299	-0.021871
C	2.542596	0.119610	-0.096444
C	1.654625	1.181630	-0.071748
C	0.285416	0.908354	0.094763
C	-0.174975	-0.435059	0.047654
C	-1.645937	-0.400436	-0.022795
C	-2.005401	1.025494	-0.109618
C	-2.488744	-1.436659	-0.009477
C	-0.901079	1.782957	-0.047643
H	0.379869	-2.512499	0.013080
H	2.805493	-2.012691	-0.040956
H	3.605791	0.311732	-0.185626
H	2.008001	2.204771	-0.130445
H	0.297072	1.139307	1.882916
H	-3.023553	1.381332	-0.191426
H	-2.130973	-2.457161	0.070908
H	-3.560466	-1.289309	-0.079239
H	-0.855294	2.863299	-0.071866

Frequencies

-1044.6063	123.4922	201.7711
251.6676	299.5623	379.7048
406.0330	466.3691	496.0086
543.4091	557.7994	577.5410
658.4572	670.8063	722.9238
760.9780	776.2860	794.5127
816.3653	865.3629	893.5842
944.0468	948.4392	963.0239
968.8623	1005.5089	1047.6894
1088.6617	1110.6841	1154.4457
1180.2612	1214.7883	1249.3035
1329.2827	1334.6949	1385.9246
1451.6618	1479.0043	1507.7006
1613.2362	1648.1257	1662.6754
1728.8327	3163.2564	3190.9214
3197.8974	3210.7906	3222.6967
3229.1171	3251.6599	3253.7391

i25 – i80

C	-1.147387	1.342400	-0.000012
C	-2.508428	1.011894	0.000052
C	-2.923822	-0.309452	0.000054
C	-1.982800	-1.356209	-0.000040
C	-0.663541	-1.004152	-0.000080

C	-0.212599	0.322764	-0.000085
C	1.251298	0.281101	-0.000040
C	1.766834	-0.940979	0.000031
C	2.607776	0.957926	-0.000026
C	3.222124	-0.499144	0.000071
H	-0.833645	2.380744	-0.000021
H	-3.248741	1.803813	0.000112
H	-3.982847	-0.543073	0.000146
H	-2.306050	-2.391056	-0.000042
H	0.624879	-1.665097	0.000093
H	2.845519	1.540243	0.893752
H	2.845596	1.540169	-0.893828
H	3.799338	-0.751350	-0.892083
H	3.799223	-0.751279	0.892320

Frequencies

-2175.7697	89.3594	141.0078
221.4178	223.5586	381.7920
400.8997	416.0826	510.1745
570.1747	637.5648	690.0683
724.2215	757.0235	808.3753
842.5138	873.7289	881.2997
944.6025	995.5269	997.5344
1002.3014	1034.7305	1037.7041
1065.8096	1079.4062	1089.2623
1134.2209	1163.7119	1188.8906
1192.9160	1232.7341	1283.7828
1315.5915	1404.7843	1458.6950
1464.4111	1485.3986	1489.9889
1641.7684	1656.2884	1696.6217
1754.6108	3061.5727	3073.6375
3116.8284	3132.1013	3186.8453
3192.8442	3204.0889	3219.0422

i80 – i82

C	-1.296806	1.384717	0.180892
C	-2.546251	0.820396	-0.059061
C	-2.704207	-0.557050	-0.230426
C	-1.612123	-1.430918	-0.176425
C	-0.379022	-0.856058	0.056818
C	-0.209396	0.518061	0.245031
C	1.229526	0.556500	0.401911
C	1.666087	-0.765052	0.624656
C	2.414502	0.915161	-0.470851
C	2.865757	-0.582383	-0.294000
H	-1.183950	2.454381	0.316985

H	-3.420083	1.460391	-0.113065
H	-3.695611	-0.957341	-0.416418
H	-1.746299	-2.496848	-0.320225
H	1.542326	-1.437067	1.464858
H	3.116133	1.629421	-0.032261
H	2.178950	1.227363	-1.491878
H	2.788711	-1.145911	-1.226337
H	3.851426	-0.754628	0.147072

Frequencies

-650.3127	103.0563	127.2214
250.8822	283.6420	383.4035
416.2494	525.8157	539.4249
591.6883	699.5994	728.1739
749.9611	775.2231	797.1143
857.9774	895.8725	898.0254
943.2083	972.1594	980.6441
1009.4194	1014.2214	1034.6472
1065.4470	1084.7966	1126.5716
1161.1745	1169.4402	1180.4738
1217.7679	1250.8629	1283.5961
1304.1406	1368.1183	1404.3472
1459.1949	1462.0145	1486.9509
1497.8032	1622.4086	1644.2430
3060.2797	3066.4348	3109.3754
3129.0736	3181.5922	3195.5299
3206.5548	3212.9345	3219.3413

i82 – i84

C	1.300365	1.431144	-0.044477
C	2.471100	0.709898	0.199122
C	2.462907	-0.681355	0.222022
C	1.282067	-1.402852	0.005351
C	0.124557	-0.691498	-0.246005
C	0.133471	0.712657	-0.268486
C	-1.232722	1.097528	-0.561587
C	-1.277060	-1.096795	-0.510557
C	-2.428999	0.843221	0.295258
C	-2.311841	-0.685288	0.526461
H	1.309858	2.514264	-0.090857
H	3.404056	1.238738	0.358191
H	3.390495	-1.214503	0.398413
H	1.286756	-2.487704	0.014507
H	-1.501946	-1.875064	-1.232386
H	-3.341710	1.058912	-0.266240
H	-2.447397	1.456879	1.205985

H	-1.977217	-0.921576	1.543917
H	-3.265964	-1.189912	0.365858

Frequencies

-724.2927	115.4042	140.7017
191.9261	359.9139	363.5109
455.1995	501.6791	533.7939
564.2063	604.4103	703.8448
751.5375	767.9624	785.0296
802.0439	847.6627	888.3187
937.6985	958.9977	1002.8117
1007.4602	1026.4523	1036.5522
1058.9527	1127.1550	1153.6045
1181.3446	1206.9024	1222.4149
1251.1225	1261.1280	1281.1646
1316.2259	1337.6052	1381.3847
1469.5825	1481.9364	1492.8473
1499.5932	1633.4134	1642.8240
3015.5390	3040.2711	3093.0185
3121.4664	3190.4040	3192.3793
3199.5844	3209.2037	3219.9210

i84 – i24

C	1.287920	-1.394711	0.035665
C	2.492537	-0.700466	0.019099
C	2.482619	0.699126	-0.018330
C	1.291573	1.391024	-0.032858
C	0.050307	0.702338	-0.003037
C	0.064157	-0.732352	0.025615
C	-1.164028	-1.548607	0.061215
C	-2.349463	-0.805962	-0.024367
C	-2.477318	0.701688	0.073470
C	-1.163714	1.397093	-0.015899
H	1.268229	-2.478563	0.058295
H	3.434009	-1.236921	0.030494
H	3.420698	1.243336	-0.035774
H	1.289760	2.476184	-0.061417
H	-3.292843	-1.351472	0.038844
H	-2.960671	0.921844	1.039136
H	-3.180599	1.077715	-0.680512
H	-1.911196	-1.388862	-1.058702
H	-1.154932	2.481709	-0.053803

Frequencies

-1044.1864	104.3944	165.8179
244.9623	367.2322	407.1680

461.5272	494.1206	504.6498
545.3829	609.2484	671.1039
695.5878	751.6171	770.2271
782.3991	817.0882	877.5267
897.7940	923.8260	946.4720
983.5105	1004.7353	1045.4380
1060.7364	1129.0340	1161.8985
1181.7084	1191.7968	1215.6521
1285.5304	1287.7023	1331.3911
1360.4620	1403.1411	1428.6098
1458.3694	1459.1952	1478.8204
1524.0860	1589.0053	1625.3234
2216.7199	2983.9644	3036.5212
3117.4812	3185.0303	3190.5675
3200.5083	3209.7544	3223.1213

i84 – i87

C	-1.307322	-1.426212	-0.121349
C	-2.480416	-0.743099	-0.067998
C	-2.486440	0.674850	0.059813
C	-1.311616	1.370097	0.103103
C	-0.049022	0.727558	-0.015046
C	-0.038163	-0.744447	-0.081768
C	1.135683	-1.393860	0.117371
C	2.455930	-1.061892	0.278716
C	2.363393	0.892862	-0.362166
C	1.156526	1.433815	0.100158
H	-1.296443	-2.507039	-0.195346
H	-3.422404	-1.277909	-0.112406
H	-3.431764	1.202231	0.115020
H	-1.325449	2.452774	0.178476
H	3.166873	-1.276948	-0.512851
H	2.885459	-1.201833	1.275145
H	2.343505	0.465300	-1.359673
H	3.291051	1.404879	-0.120900
H	1.157860	2.360513	0.667539

Frequencies

-786.6917	130.1688	160.4427
272.4386	310.8335	339.7837
418.7624	461.6029	488.6133
524.8533	584.5353	602.0572
702.5736	719.8573	749.7176
755.0576	777.3290	846.7988
860.0408	907.9724	935.6306
979.1911	998.9472	1001.6626

1026.8135	1042.0286	1073.8008
1112.0453	1169.0437	1197.6302
1235.2106	1253.6008	1265.1717
1341.3864	1408.7943	1436.8577
1464.6109	1481.5723	1511.6219
1567.2749	1661.2779	1672.4204
3075.0587	3129.5286	3168.8877
3183.4120	3185.9425	3197.6784
3212.3595	3217.1899	3222.7141

i87 – p17

C	-1.026983	-1.458553	-0.166642
C	-2.319348	-0.966491	-0.126423
C	-2.527390	0.397740	0.038688
C	-1.441860	1.251228	0.150783
C	-0.124361	0.787233	0.089845
C	0.078044	-0.602384	-0.055156
C	1.370317	-1.206452	-0.048882
C	2.418727	-1.801094	0.044272
C	2.163775	1.737480	-0.352121
C	0.951893	1.790148	0.192956
H	-0.847695	-2.521376	-0.275347
H	-3.159123	-1.645933	-0.211624
H	-3.534109	0.796968	0.082983
H	-1.609843	2.315138	0.280711
H	3.369718	-2.261726	-0.081623
H	2.491502	-2.396474	2.021804
H	2.500936	0.895032	-0.942461
H	2.858263	2.559629	-0.222737
H	0.673468	2.685616	0.744359

Frequencies

-633.6234	67.1828	68.5021
122.9857	165.9425	188.3918
243.7352	286.0858	388.6591
415.2357	453.6172	518.5138
538.5672	574.6884	619.1590
664.6263	716.9927	725.8883
775.8461	784.2166	798.2111
839.4069	910.9346	967.2280
989.5546	1017.0099	1036.2231
1053.8229	1081.0596	1148.2375
1192.6758	1227.7410	1229.9862
1304.5009	1326.2486	1358.0499
1449.1078	1485.5268	1537.0441
1632.3750	1671.7930	1726.8258

2173.2825	3154.6184	3175.0529
3191.9502	3204.6153	3215.9477
3227.3036	3263.4858	3466.5112

i29 – i30

C	-0.736900	1.476275	0.016890
C	-2.089983	1.211680	0.015770
C	-2.568682	-0.113471	-0.004568
C	-1.698329	-1.179857	-0.014960
C	-0.316672	-0.924524	-0.026537
C	0.168145	0.407045	-0.017958
C	1.622466	0.404943	-0.018216
C	2.015317	-0.976056	-0.015745
C	2.463707	1.493329	-0.015727
C	0.797175	-1.820455	-0.028441
H	-0.377502	2.499481	0.036986
H	-2.800188	2.030689	0.031253
H	-3.638359	-0.290875	-0.007999
H	-2.070098	-2.198764	-0.022496
H	3.013287	-1.357433	-0.180257
H	3.539392	1.368662	-0.011273
H	2.073355	2.502990	-0.035496
H	1.528559	-1.540609	1.040216
H	0.794089	-2.887600	-0.193983

Frequencies

-1557.8927	146.0855	196.0007
270.0348	323.4212	418.1852
465.5932	512.4835	543.4807
562.4252	571.3490	620.1539
693.5293	715.1814	721.4113
764.2869	767.2269	791.3861
873.7624	879.0938	913.0828
949.7710	966.6850	1002.0632
1023.9165	1047.0644	1118.4698
1160.9681	1167.4665	1219.4603
1226.6540	1251.9563	1271.8908
1353.6723	1370.8004	1385.3576
1443.5942	1487.9395	1532.0678
1545.0097	1620.0783	1681.6611
2153.4590	3170.1622	3189.6791
3196.6399	3207.8612	3219.7177
3242.3650	3258.6543	3266.0452

i30 – i19

C	0.730581	-1.475746	0.054371
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C	2.084751	-1.220804	0.019669
C	2.568165	0.102668	-0.025991
C	1.707553	1.175784	-0.044894
C	0.319511	0.936243	-0.033845
C	-0.158461	-0.396061	0.027908
C	-1.613444	-0.372125	0.049402
C	-1.957461	1.082477	0.020247
C	-2.492371	-1.460747	-0.141006
C	-0.788188	1.831109	-0.038508
H	0.361615	-2.494937	0.097580
H	2.790738	-2.043327	0.029690
H	3.639093	0.272422	-0.047588
H	2.088567	2.190652	-0.078920
H	-2.976334	1.438288	-0.049397
H	-1.903422	0.292859	1.128246
H	-3.562127	-1.311885	-0.206179
H	-2.107322	-2.470691	-0.170179
H	-0.734614	2.909834	-0.027371

Frequencies

-1427.6621	154.8096	195.8103
251.0363	341.5298	364.3954
439.2189	458.2512	542.3068
563.2301	567.9122	575.7140
652.4515	721.6283	730.2230
762.8834	773.6494	798.0306
877.0308	885.1948	903.4271
924.8347	968.6735	1004.0842
1044.3778	1063.3247	1107.7677
1154.9068	1162.1133	1178.4162
1235.8093	1243.6567	1322.1424
1333.8301	1371.8400	1423.0573
1466.4100	1494.8266	1513.1565
1539.8574	1625.3923	1684.6021
1964.0547	3178.4038	3189.2822
3196.0658	3207.7761	3219.7533
3237.8346	3256.8256	3283.1045

il – i79

C	1.139973	-1.210423	-0.081024
C	2.515302	-1.203072	0.076970
C	3.211290	0.000008	0.157013
C	2.515289	1.203081	0.076977
C	1.139960	1.210418	-0.081016
C	0.425244	-0.000006	-0.161837
C	-0.973955	-0.000012	-0.325533

C	-2.205698	0.000003	-0.348176
C	-3.643074	0.000016	-0.514392
H	0.598707	-2.147002	-0.143712
H	3.050950	-2.143787	0.138750
H	4.287995	0.000013	0.280231
H	3.050927	2.143801	0.138761
H	0.598684	2.146991	-0.143700
H	-4.055255	-0.901262	-0.965891
H	-4.055245	0.901318	-0.965851
C	-3.525384	-0.000015	0.972542
H	-3.535218	0.933302	1.516154
H	-3.535225	-0.933353	1.516118

Frequencies

-690.2661	63.2889	65.7971
98.6425	209.3435	273.0572
349.3094	401.5735	413.8235
513.8790	534.4932	583.9504
641.0247	673.7873	706.9053
719.0631	771.6853	812.0559
857.5037	927.6832	974.7079
995.6378	1012.9643	1015.3931
1055.2842	1058.0139	1107.2824
1112.0809	1184.8941	1204.0477
1209.0953	1216.0044	1312.9590
1322.4265	1354.7627	1446.8461
1478.2319	1483.7186	1530.8055
1627.7115	1654.3172	2108.2071
3090.2419	3158.9068	3180.5015
3185.8357	3193.2258	3205.6432
3211.5768	3218.1191	3301.5114

i79 – i83

C	0.965853	1.167211	-0.194525
C	2.336957	1.248557	-0.046860
C	3.102383	0.093404	0.112751
C	2.477437	-1.153667	0.121652
C	1.107997	-1.254469	-0.027414
C	0.310072	-0.091255	-0.180960
C	-1.065699	-0.185504	-0.366733
C	-2.342030	-0.125330	-0.041202
C	-3.511707	-0.081981	-0.870475
C	-2.871685	0.241234	1.281441
H	0.371543	2.064872	-0.319542
H	2.819728	2.219483	-0.053698
H	4.177425	0.165329	0.228988

H	3.069000	-2.053945	0.245609
H	0.621676	-2.222770	-0.024607
H	-3.542008	0.476688	-1.800294
H	-4.415244	-0.577828	-0.536593
H	-3.453869	-0.460439	1.868652
H	-2.705724	1.239409	1.665432

Frequencies

-536.5765	39.1428	61.2474
97.0519	197.0189	295.8863
343.2385	374.0118	399.5218
410.4630	487.5975	512.2759
518.9024	569.0329	634.6276
678.8744	694.5041	728.0681
765.5674	840.1139	917.6213
920.3430	975.6365	988.1135
1006.6733	1007.7604	1043.4133
1053.1406	1109.7810	1179.9602
1188.9482	1217.9511	1269.0720
1302.1145	1349.2708	1430.5416
1463.4449	1473.8974	1502.0690
1603.5267	1626.0977	1798.3289
3148.7699	3156.0751	3193.5448
3202.0455	3212.2022	3220.3708
3226.0198	3259.8029	3273.7144

i83 – i26

C	1.083912	1.203367	0.035760
C	2.453691	0.982568	-0.014269
C	2.949706	-0.314970	-0.044710
C	2.069782	-1.394086	-0.024101
C	0.702431	-1.177249	0.025762
C	0.197658	0.126197	0.055179
C	-1.236919	0.370859	0.106070
C	-2.342855	-0.305843	-0.004554
C	-2.090603	1.553523	-0.034075
C	-3.422364	-1.107188	-0.047339
H	0.687309	2.212953	0.062988
H	3.136585	1.824527	-0.028068
H	4.019198	-0.487449	-0.084753
H	2.455165	-2.407216	-0.048073
H	0.011164	-2.013264	0.039621
H	-2.565393	2.008248	0.827458
H	-2.161162	2.063300	-0.989997
H	-3.706868	-1.693078	0.819516
H	-4.062631	-1.131092	-0.921032

Frequencies

-682.5559	60.4104	104.8112
114.1552	212.3323	261.2907
288.2474	415.6986	419.1626
423.4772	471.1270	547.7476
635.8273	662.1385	692.7302
713.8840	731.0891	764.8868
783.8099	870.3910	944.6808
1003.6646	1007.4336	1019.8361
1023.3256	1041.0222	1052.9122
1075.3622	1107.9068	1159.4363
1188.9541	1202.9541	1329.9318
1353.9718	1366.4970	1443.9701
1472.5546	1494.5266	1542.6487
1653.9212	1677.8726	1934.9324
3129.6256	3146.7185	3190.3340
3195.5224	3203.7212	3211.7528
3222.0579	3239.0667	3241.0316

i79 – i25

C	0.809201	-1.125128	-0.115881
C	2.167879	-1.298897	0.092795
C	3.005689	-0.190303	0.184140
C	2.484104	1.091921	0.059305
C	1.124937	1.265566	-0.161864
C	0.269684	0.162715	-0.245589
C	-1.154604	0.388742	-0.491087
C	-2.152826	-0.509418	-0.467847
C	-2.594162	0.230297	0.936689
C	-3.542963	-0.075325	-0.188670
H	0.138471	-1.974206	-0.184215
H	2.579551	-2.297457	0.188192
H	4.068404	-0.328943	0.349662
H	3.138590	1.953509	0.125824
H	0.702907	2.257598	-0.277539
H	-2.507243	-0.446315	1.778802
H	-2.424035	1.278385	1.145810
H	-3.941488	0.792518	-0.710779
H	-4.256777	-0.876113	-0.027701

Frequencies

-313.6613	54.2559	90.9748
136.9628	264.7474	320.7934
410.1552	422.3154	498.2413
611.6152	636.5088	687.0110

721.0978	791.5697	802.6324
826.2613	881.9693	887.9958
924.5441	978.9927	1007.4949
1018.2436	1025.3828	1037.7527
1045.9167	1058.8136	1101.8561
1107.8699	1146.2491	1178.4827
1189.7644	1199.1203	1247.8910
1322.6523	1349.0047	1454.3751
1488.2102	1496.7949	1523.9239
1607.1713	1646.9442	1671.0803
3111.7379	3155.2800	3187.9668
3195.7559	3204.8230	3205.4906
3213.7260	3219.5277	3255.5132

i83 – i25

C	0.995474	1.199059	0.009352
C	2.381380	1.140606	-0.030440
C	3.031482	-0.087715	-0.029231
C	2.283219	-1.261605	0.010635
C	0.900037	-1.209982	0.049957
C	0.236980	0.023937	0.043824
C	-1.202935	0.078076	0.090533
C	-2.238655	-0.735373	-0.147638
C	-3.630283	-0.488627	0.013937
C	-2.275127	1.040432	-0.027199
H	0.490361	2.159454	0.012775
H	2.956226	2.059574	-0.060890
H	4.114126	-0.132421	-0.057627
H	2.784610	-2.223089	0.011781
H	0.313698	-2.121983	0.079685
H	-4.075660	-0.107133	0.928264
H	-4.321699	-0.902282	-0.714387
H	-2.672891	1.524677	0.863768
H	-2.478204	1.550356	-0.965750

Frequencies

-881.8848	84.8341	95.4282
130.8939	244.4578	314.8141
366.9183	417.1479	466.0858
510.8515	576.8929	636.0280
670.1677	711.0264	727.6124
759.6325	777.9037	857.5444
875.4028	927.0670	994.0754
1004.7950	1010.8782	1019.6300
1051.8105	1055.9768	1067.4958
1087.2178	1113.4060	1151.5397

1185.1406	1209.0668	1328.1372
1348.6257	1360.1373	1473.7943
1490.9723	1496.6688	1539.4434
1642.4809	1652.7383	1675.5009
3087.1642	3109.4853	3184.7491
3186.6200	3192.1843	3197.2510
3201.0630	3208.8849	3220.6508

i27 – i80

C	0.993937	1.170760	-0.149818
C	2.376496	1.072933	-0.049263
C	2.992634	-0.165269	0.096163
C	2.216554	-1.328118	0.146471
C	0.860632	-1.168855	0.052847
C	0.181803	0.026753	-0.086514
C	-1.279022	0.102470	-0.151421
C	-2.203112	-0.901391	-0.373517
C	-2.082822	1.239351	0.139747
C	-3.370804	-0.458671	0.284162
H	0.523950	2.139200	-0.291474
H	2.980257	1.971955	-0.095888
H	4.072650	-0.235065	0.167218
H	2.677064	-2.303082	0.260535
H	-2.111559	-1.777122	-1.007962
H	-2.787276	1.587406	-0.602726
H	-1.770125	1.998690	0.861469
H	-3.328286	-0.246771	1.344287
H	-4.374451	-0.674987	-0.088601

Frequencies

-751.9745	74.7958	109.2659
143.3896	277.8062	362.0586
423.2966	437.1757	496.1934
573.5762	631.8477	674.5046
708.3472	723.6991	755.7728
788.5755	823.2453	880.2056
893.9653	954.8232	967.7631
980.5830	996.9416	1008.8482
1025.2857	1054.4724	1059.7874
1131.5962	1134.6630	1179.6753
1209.4146	1258.7703	1328.1298
1354.3171	1392.3104	1458.5042
1492.6669	1524.3016	1527.6671
1584.8684	1611.5529	1667.0352
3094.0802	3104.6523	3178.5631
3187.1275	3193.4953	3199.1701

3212.9429	3230.7735	3237.6211
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i83 – p19

C	1.142072	1.230818	-0.062268
C	2.503162	0.975689	-0.035200
C	2.964998	-0.336650	0.022247
C	2.063473	-1.394389	0.054317
C	0.699438	-1.143788	0.030337
C	0.229591	0.170992	-0.030216
C	-1.189518	0.419239	-0.054397
C	-2.518800	-0.121845	-0.051425
C	-2.202726	1.280139	-0.127359
C	-3.373820	-1.136245	-0.017184
H	0.772789	2.249408	-0.105755
H	3.209085	1.797743	-0.058042
H	4.030902	-0.533084	0.043888
H	2.425519	-2.414838	0.100863
H	-0.015029	-1.958395	0.057257
H	-2.338193	2.033885	1.935310
H	-2.530500	2.283151	-0.341410
H	-3.020415	-2.156422	0.063492
H	-4.441387	-0.965209	-0.068716

Frequencies

-564.2730	56.7741	93.7089
109.1162	167.2508	253.2482
284.0831	363.7024	415.7422
418.0996	474.5177	524.4829
582.4433	634.9792	707.3463
717.3315	722.2611	778.0659
784.3299	830.6302	867.4522
869.5416	952.3012	991.7106
1005.7992	1024.4271	1025.0191
1041.2698	1057.9645	1112.5246
1128.3291	1191.0234	1203.6303
1247.9442	1331.0139	1356.8061
1453.2475	1493.1862	1529.9770
1648.2688	1658.2784	1677.9827
1879.1256	3168.1859	3196.1155
3203.3447	3211.4536	3220.4581
3226.8719	3258.8907	3292.5393

i30 – p20

C	0.805465	-1.461919	0.041012
C	2.161294	-1.139285	0.051741
C	2.576836	0.189820	0.012515

C	1.649172	1.226458	-0.037090
C	0.297847	0.907667	-0.048490
C	-0.120511	-0.435395	-0.012438
C	-1.597731	-0.447256	-0.041135
C	-2.001291	0.975540	-0.042126
C	-2.407402	-1.504515	-0.091017
C	-0.891300	1.754822	-0.094368
H	0.489639	-2.499251	0.074956
H	2.901469	-1.930163	0.091354
H	3.636817	0.417450	0.022813
H	1.977572	2.259662	-0.065536
H	-3.022937	1.307353	-0.164390
H	-2.440639	1.115925	1.978976
H	-3.484874	-1.385973	-0.110446
H	-2.016625	-2.515831	-0.112654
H	-0.874698	2.835208	-0.146686

Frequencies

-628.7725	125.1772	177.5385
257.1496	274.6552	285.7430
355.3402	416.8487	461.4567
543.7225	553.7975	574.9469
661.3418	691.3234	724.5204
767.1819	771.9193	797.5029
829.7329	874.8395	896.8377
944.3628	945.5892	962.2091
969.4871	1005.5428	1051.9381
1080.0714	1113.0125	1152.0872
1187.4289	1223.2235	1249.7267
1329.7108	1343.8907	1397.0478
1449.4312	1493.8817	1509.0516
1561.9625	1660.1719	1683.3391
1745.9264	3163.4712	3187.9710
3193.3682	3205.6185	3219.3135
3231.7967	3252.2763	3254.0632

i29 – i93

C	0.708796	-1.490637	0.047214
C	2.059684	-1.239415	0.002523
C	2.553604	0.091340	-0.070717
C	1.716372	1.168837	-0.058323
C	0.308705	0.931850	0.079433
C	-0.196875	-0.418667	0.043384
C	-1.629584	-0.370774	-0.034611
C	-2.004335	1.005362	-0.071940
C	-2.497131	-1.459673	-0.026531

C	-0.879468	1.817033	-0.022489
H	0.341780	-2.511575	0.051652
H	2.764323	-2.062582	-0.004890
H	3.623025	0.250144	-0.154189
H	2.099495	2.181033	-0.120808
H	-0.124381	1.463426	1.134950
H	-3.023902	1.364883	-0.085556
H	-2.124859	-2.475252	0.024232
H	-3.568663	-1.315928	-0.085945
H	-0.825434	2.894314	-0.087104

Frequencies

-1377.6027	149.0016	201.0322
263.5401	322.8984	412.9203
457.4393	486.0918	542.2367
561.6684	570.0541	637.2205
704.9644	719.9226	742.1298
758.4027	761.1596	797.9902
848.6447	868.6292	897.1570
965.3031	967.6601	998.4842
1030.2987	1060.1692	1105.6883
1131.0137	1170.1324	1181.1308
1222.0308	1238.8934	1314.1457
1327.8333	1400.4326	1430.9648
1470.4858	1481.1670	1506.3646
1523.0627	1581.0572	1668.3893
2020.5875	3169.0321	3191.1889
3197.1471	3210.3502	3222.0955
3235.2817	3256.0018	3267.7755

il6 – i93

C	0.716155	-1.509713	0.006127
C	2.044193	-1.250207	-0.043141
C	2.553128	0.104551	-0.060706
C	1.727818	1.175723	-0.022768
C	0.299993	0.980595	0.095611
C	-0.227491	-0.425807	0.089545
C	-1.656139	-0.346400	-0.016467
C	-1.969117	1.052170	-0.087769
C	-2.544623	-1.414695	-0.024810
C	-0.837995	1.832471	-0.026823
H	0.343238	-2.526304	-0.044788
H	2.751720	-2.068892	-0.100928
H	3.623688	0.254390	-0.137082
H	2.116979	2.185090	-0.091823
H	0.117762	0.304449	1.154562

H	-2.981938	1.432378	-0.127598
H	-2.199061	-2.438015	0.053378
H	-3.608839	-1.247411	-0.129242
H	-0.799078	2.912190	-0.029276

Frequencies

-1375.0963	149.3058	193.6394
240.5381	312.5926	400.9843
454.7048	495.2526	535.3594
552.4362	557.6628	625.8424
671.2222	712.6718	722.4990
728.5803	756.1616	778.7970
847.3262	872.9831	913.8131
952.6888	987.3895	990.8796
1001.6778	1067.8767	1089.3389
1156.6907	1173.3419	1188.7442
1220.2328	1249.0405	1285.8305
1339.4576	1393.9445	1435.7823
1483.5834	1501.6028	1502.3314
1523.3494	1595.0415	1676.7255
2146.6928	3169.7046	3196.7540
3204.0448	3216.3812	3224.9068
3225.1037	3252.4806	3266.5329

i26 – i81

C	-0.747172	-1.229418	0.005459
C	-2.085099	-1.211366	0.316930
C	-2.776288	-0.000862	0.462948
C	-2.085525	1.210217	0.319758
C	-0.747591	1.229463	0.008406
C	-0.036382	0.000415	-0.221673
C	1.428273	0.000865	-0.412675
C	2.497779	-0.000309	0.311006
C	0.936174	0.002629	-1.777262
C	3.565892	-0.001585	1.055605
H	-0.208825	-2.166160	-0.085843
H	-2.607315	-2.149846	0.468495
H	-3.831212	-0.001352	0.708476
H	-2.608093	2.148177	0.473336
H	-0.209520	2.166575	-0.080702
H	0.856941	-0.928346	-2.325045
H	0.856388	0.934987	-2.322594
H	4.025602	-0.931178	1.374823
H	4.025676	0.926855	1.378040

Frequencies

-573.7334	68.8581	82.8501
187.2476	230.1348	303.8573
395.3703	406.0258	415.3508
455.3847	601.1272	611.7507
622.8644	652.1984	660.9439
705.7608	732.7037	806.5671
811.2973	863.5089	883.0597
912.1104	986.5347	996.5940
1002.5154	1014.4165	1026.4832
1033.6962	1109.6883	1156.7286
1168.9709	1211.9743	1311.4601
1343.1896	1372.7533	1437.5389
1461.1981	1482.9954	1544.4882
1570.8012	1613.5849	2130.8190
3149.1349	3151.0900	3188.4222
3192.9137	3205.8350	3210.3573
3220.7191	3232.7125	3264.9210

i92 – i26

C	1.075289	-1.209822	0.269989
C	2.419941	-0.874980	0.320722
C	2.825665	0.426607	0.044797
C	1.879610	1.389767	-0.282388
C	0.532590	1.056381	-0.331325
C	0.116444	-0.248410	-0.058922
C	-1.305731	-0.604431	-0.128098
C	-2.501259	0.210654	0.066294
C	-1.945389	-1.754073	-0.377906
C	-2.905913	1.419123	0.412360
H	0.758131	-2.221349	0.499766
H	3.153843	-1.628585	0.582452
H	3.876737	0.688274	0.088486
H	2.190531	2.405171	-0.500258
H	-0.201777	1.805938	-0.602798
H	-1.667192	-2.778457	-0.611141
H	-3.111804	-1.002623	-0.207248
H	-2.187854	2.201571	0.650016
H	-3.958101	1.665156	0.487585

Frequencies

-2220.7150	43.3549	113.0695
154.4101	193.8059	268.1997
375.1649	412.4657	416.5486
491.5406	531.1197	637.8476
657.9197	695.6505	710.0296
728.4177	752.3756	804.6832

874.6202	877.6558	920.9510
952.0604	1005.9155	1008.6035
1019.3986	1024.8344	1025.5902
1061.9210	1113.6011	1142.4686
1189.1885	1213.6947	1295.8310
1333.2945	1360.7056	1429.1506
1490.5158	1540.9395	1642.7694
1663.6506	1687.2090	1745.4522
1959.6108	3130.6736	3180.9349
3191.9907	3198.9053	3208.1114
3218.7198	3224.7554	3234.9349

i92 – p21

C	0.632129	-0.370736	1.205990
C	1.960579	0.030816	1.202671
C	2.628078	0.232405	-0.000003
C	1.960567	0.030876	-1.202680
C	0.632117	-0.370675	-1.206005
C	-0.038728	-0.581132	-0.000009
C	-1.426051	-0.995581	-0.000012
C	-2.347734	1.068088	-0.000011
C	-2.346500	-1.799298	-0.000012
C	-1.587736	2.134779	0.000058
H	0.102964	-0.519676	2.139504
H	2.475578	0.188766	2.143364
H	3.665158	0.547767	0.000000
H	2.475556	0.188873	-2.143370
H	0.102941	-0.519566	-2.139521
H	-3.422730	0.943627	-0.000064
H	-3.278859	-2.313014	-0.000012
H	-0.502040	2.069142	0.000106
H	-2.018899	3.136836	0.000069

Frequencies

-505.0340	30.8935	51.4202
83.6759	163.4546	203.0304
263.1820	295.1767	311.1093
413.8766	481.3660	510.3055
538.7132	550.5044	641.6429
713.5255	716.4612	776.1134
785.9143	824.8475	870.4600
905.0217	948.8794	948.9740
1003.4090	1023.0035	1025.9305
1061.0036	1102.4179	1111.4331
1188.3843	1206.9093	1219.9108
1320.1251	1355.5135	1394.3195

1488.4752	1536.4487	1651.6631
1659.4421	1678.1391	2055.8490
3089.3495	3179.7195	3188.1833
3197.6480	3207.8936	3215.7530
3220.5824	3229.8433	3459.7372

i81 – i85

C	-0.792691	0.357684	-1.232189
C	-1.899773	-0.448829	-1.215191
C	-2.461189	-0.884401	-0.003074
C	-1.897896	-0.460553	1.212326
C	-0.790886	0.345921	1.235350
C	-0.140500	0.738830	0.002956
H	-0.364523	0.696417	-2.169411
H	-2.357261	-0.743865	-2.153238
H	-3.335792	-1.523033	-0.005464
H	-2.353736	-0.765014	2.148155
H	-0.361136	0.675358	2.175158
C	1.510990	0.518450	0.001040
C	2.350341	-0.430848	-0.002535
C	0.918455	1.833181	0.007231
C	3.162041	-1.465530	-0.005963
H	0.998240	2.423535	-0.902240
H	0.999598	2.415236	0.921918
H	3.510987	-1.897890	-0.936869
H	3.510267	-1.904184	0.922276

Frequencies

-513.8990	71.6333	81.0344
169.1094	267.8455	318.2336
383.0470	392.0998	441.9210
479.3421	518.1903	544.2897
622.6745	650.8043	701.4684
747.2803	783.2767	791.0046
823.0168	842.5655	935.5939
972.6291	978.9003	995.2017
1025.3584	1025.4180	1039.7359
1117.7773	1121.6256	1153.7107
1167.7120	1213.6334	1334.4864
1346.5738	1368.1618	1456.8626
1459.6194	1483.2487	1532.2312
1569.9199	1610.8228	2087.9713
3109.2565	3154.5776	3187.9740
3190.0388	3193.5305	3201.8390
3208.7803	3220.5232	3241.2281

i85 – p14

C	1.635775	1.220502	0.094671
C	2.880804	0.607868	0.097291
C	2.975210	-0.775764	0.015190
C	1.816512	-1.542420	-0.068580
C	0.572900	-0.931897	-0.070812
C	0.467495	0.459428	0.012160
H	1.563658	2.301713	0.155257
H	3.778975	1.211399	0.161986
H	3.946658	-1.256570	0.016204
H	1.885943	-2.622317	-0.134337
H	-0.330111	-1.529062	-0.135907
C	-2.015939	0.524149	0.057561
C	-3.128844	-0.063599	0.060111
C	-0.837046	1.140268	0.021088
C	-4.297375	-0.670125	0.063749
H	-0.821077	2.219623	0.152630
H	-0.852089	1.719973	-2.039305
H	-5.220657	-0.104784	0.129732
H	-4.368248	-1.750448	-0.000836

Frequencies

-663.3793	42.4681	77.4864
168.8943	183.9107	256.1443
294.0040	330.3159	348.4192
413.9963	423.7631	435.0617
532.2955	588.1965	633.1979
638.2338	711.1924	781.4543
829.7838	863.4224	872.0065
907.8172	945.6192	948.6813
1000.2673	1019.2121	1024.5406
1030.9147	1061.4802	1118.0872
1189.6605	1205.5266	1226.8949
1301.0425	1347.9323	1362.7766
1444.1212	1501.0306	1539.3621
1651.3116	1675.6090	1676.4997
2118.6284	3151.3321	3164.4772
3185.7334	3192.8059	3203.3832
3209.6392	3223.2297	3238.5755

i85 – i11

C	-1.703846	-1.221790	0.024559
C	-2.912452	-0.547707	0.016566
C	-2.940034	0.844721	-0.003695
C	-1.743552	1.553489	-0.009045
C	-0.528779	0.885394	0.007148

C	-0.489548	-0.516402	0.023043
C	2.053229	-0.635909	-0.054110
C	3.101565	0.050604	0.023862
C	0.763704	-1.250876	0.036780
C	4.240391	0.738885	0.047525
H	-1.688608	-2.307096	0.037081
H	-3.840654	-1.108127	0.024383
H	-3.887264	1.371199	-0.013246
H	-1.757224	2.637759	-0.020044
H	0.401630	1.442209	0.012425
H	0.750034	-2.315599	0.242693
H	1.551342	-1.177359	-1.088740
H	5.162290	0.272461	0.372696
H	4.264385	1.782110	-0.243047

Frequencies

-1948.5648	48.1006	63.6554
172.2091	214.5378	253.9099
312.2392	347.3224	417.4374
426.4650	487.7531	506.3037
618.7579	634.4365	687.3064
708.1623	725.9264	783.6131
816.0695	851.3079	904.3536
924.6881	989.8581	1010.4319
1010.6881	1016.5399	1025.3421
1058.7396	1120.1320	1186.3929
1202.8537	1228.5201	1298.0245
1338.5129	1361.4557	1405.4080
1491.8721	1504.2954	1537.6665
1640.1458	1662.1031	2111.3297
2185.6526	3162.3106	3186.2488
3195.1562	3196.2186	3204.2188
3212.1104	3223.1908	3254.0627

i85 – i86

C	1.761442	1.262798	-0.000016
C	2.926788	0.501085	-0.000029
C	2.874446	-0.890907	-0.000014
C	1.644693	-1.551410	0.000014
C	0.516521	-0.762788	0.000026
C	0.528354	0.618544	0.000012
C	-1.776254	0.048387	0.000028
C	-3.037440	-0.163719	-0.000002
C	-0.851972	1.237138	0.000029
C	-4.320078	-0.453258	-0.000038
H	1.818894	2.346966	-0.000028

H	3.890169	0.998357	-0.000052
H	3.794502	-1.465371	-0.000024
H	1.591906	-2.634168	0.000026
H	-0.937436	-0.905671	0.000043
H	-1.012334	1.864263	0.882455
H	-1.012352	1.864282	-0.882379
H	-4.866205	-0.571933	0.929733
H	-4.866146	-0.571947	-0.929842

Frequencies

-1807.6666	42.6501	123.3176
189.7994	203.0517	332.8168
371.4721	394.1441	416.9276
468.9065	519.8456	572.2591
601.3292	659.1165	709.6774
749.1627	824.4005	859.4895
867.7331	937.7388	957.9912
961.2793	1006.3783	1009.6078
1015.1756	1032.0919	1048.5947
1140.4754	1180.0084	1181.3511
1212.6314	1239.5546	1291.2707
1329.7722	1342.0516	1460.4064
1480.4710	1492.1332	1497.2541
1635.7407	1667.2229	1737.6372
2042.9715	3060.2305	3099.3892
3150.9551	3184.1352	3190.9462
3207.7286	3218.0973	3237.8136

i86 – i88

C	1.388104	-1.199312	-0.298765
C	2.540955	-0.475280	-0.587744
C	2.649406	0.860743	-0.221527
C	1.590519	1.485604	0.444418
C	0.484346	0.719272	0.699823
C	0.310126	-0.605339	0.366169
C	-2.123409	-0.976432	-0.228264
C	-2.607242	0.229112	-0.314271
C	-0.960807	-1.363779	0.674286
C	-3.068394	1.443347	-0.397387
H	1.318203	-2.243935	-0.588740
H	3.362697	-0.961001	-1.101384
H	3.551214	1.419385	-0.447547
H	1.652789	2.526476	0.742137
H	-2.565209	-1.755203	-0.843977
H	-0.773523	-2.434288	0.567615
H	-1.237673	-1.192082	1.718046

H	-3.870773	1.785600	0.248301
H	-2.659346	2.147433	-1.114866

Frequencies

-69.7345	13.6769	93.1184
177.5677	267.4377	320.0661
334.9356	419.5998	492.9262
515.4112	570.0825	633.2862
660.0801	725.1258	754.2936
819.6284	867.1833	880.3344
889.0806	897.1426	954.0701
989.2576	999.8597	1004.1422
1024.8788	1055.1326	1133.2740
1153.1140	1180.2398	1199.5597
1234.7599	1285.8621	1326.2488
1340.7209	1370.8001	1466.6412
1482.4399	1491.3895	1499.4833
1611.2578	1669.7859	2084.4723
3072.1778	3121.8868	3141.6556
3172.7877	3176.2252	3187.9676
3199.9830	3211.6159	3224.6980

i88 – i91

C	-1.356668	-1.327390	0.047547
C	-2.546046	-0.612052	0.077322
C	-2.533750	0.777926	0.016399
C	-1.315816	1.447886	-0.073599
C	-0.159864	0.699300	-0.106437
C	-0.116519	-0.680538	-0.046896
C	1.141500	-1.531274	-0.096810
C	2.465156	-0.807936	0.045035
C	2.503175	0.491324	0.079495
C	1.969978	1.703370	0.054254
H	-1.383279	-2.412918	0.099799
H	-3.488782	-1.141919	0.153210
H	-3.464038	1.335419	0.042110
H	-1.284190	2.532045	-0.117848
H	1.075287	-2.297091	0.684360
H	1.152772	-2.079643	-1.047359
H	3.362058	-1.418278	0.101674
H	1.936181	2.271966	-0.870085
H	1.787110	2.246731	0.976272

Frequencies

-415.6176	38.5399	121.1494
209.3924	243.6900	354.7173

392.5164	419.6152	481.8594
484.9377	606.5878	614.9396
697.0626	713.4273	752.3824
789.9179	865.5305	880.4734
890.7085	947.1099	960.2018
982.8029	990.2269	1004.9098
1031.4113	1061.4131	1116.7111
1136.9778	1182.0904	1211.8111
1234.9296	1253.6011	1317.3863
1331.1956	1375.0895	1461.6635
1478.5273	1488.0719	1497.8900
1615.2019	1666.5891	1988.0381
3035.5912	3068.1460	3141.8756
3166.4083	3168.9709	3179.6067
3195.9728	3213.6252	3227.0916

Products

pI + H

C	0.000000	-0.710183	0.000000
C	0.000000	0.710183	0.000000
C	1.240907	1.396272	0.000000
C	2.421887	0.706735	0.000000
C	2.421887	-0.706735	0.000000
C	1.240908	-1.396272	0.000000
C	-1.240907	-1.396272	0.000000
C	-2.421887	-0.706734	0.000000
C	-2.421886	0.706734	0.000000
C	-1.240907	1.396272	0.000000
H	1.237769	2.481481	0.000000
H	3.364789	1.241538	0.000000
H	3.364790	-1.241538	0.000000
H	1.237770	-2.481481	0.000000
H	-1.237770	-2.481481	0.000000
H	-3.364794	-1.241538	0.000000
H	-3.364800	1.241541	0.000000
H	-1.237769	2.481481	0.000000

Frequencies

171.5891	183.9252	367.4296
394.8906	481.3061	485.9152
521.6916	523.1722	637.8144
641.6353	727.5514	785.3336
791.1627	804.1738	811.8000
850.9893	902.7167	954.8211
972.0033	989.1822	1008.7409

1014.3510	1042.9674	1056.7628
1162.3137	1162.7224	1182.5444
1197.4560	1240.5369	1271.7387
1292.4368	1400.4451	1424.5318
1430.5037	1499.3545	1507.2749
1569.3899	1653.8108	1674.8670
1714.8066	3188.8241	3189.5136
3193.0047	3195.1937	3207.7492
3208.4595	3220.8476	3221.7931

p20 + H

C	-0.283258	0.916700	0.000000
C	-1.638560	1.206877	0.000001
C	-2.546009	0.149096	0.000001
C	-2.103668	-1.170580	0.000000
C	-0.740371	-1.463695	-0.000002
C	0.163069	-0.416549	-0.000001
C	0.898299	1.790337	-0.000001
C	2.010334	1.035938	-0.000002
C	1.642422	-0.390664	-0.000001
C	2.477235	-1.430707	0.000003
H	-1.989376	2.233230	0.000005
H	-3.610533	0.355163	0.000003
H	-2.827279	-1.977693	0.000001
H	-0.402384	-2.494749	-0.000005
H	0.857665	2.871771	0.000003
H	3.031848	1.391509	0.000000
H	2.110951	-2.451567	0.000002
H	3.552149	-1.288179	0.000006

Frequencies

126.3582	196.3357	255.8370
313.8011	412.8448	458.3690
542.6148	554.4088	574.9900
658.3506	666.3424	725.7150
767.1655	773.9117	794.1780
817.7328	873.0931	895.0496
943.1760	948.9898	958.1894
966.3736	1004.5593	1051.1091
1088.7123	1111.2229	1153.0305
1186.7821	1220.3516	1252.6485
1330.5703	1344.3044	1400.8573
1453.2807	1500.9889	1510.8398
1619.4568	1667.6097	1688.2438
1745.1369	3161.5054	3187.7651
3193.1102	3205.8447	3220.0934

3225.5656 3248.2399 3251.5142

p2 + H

C	-1.090759	1.182941	0.018610
C	-2.472605	1.298989	0.012909
C	-3.270509	0.160463	-0.007568
C	-2.679933	-1.098099	-0.022595
C	-1.298927	-1.222126	-0.016316
C	-0.488769	-0.080618	0.004326
C	0.934409	-0.204802	0.012689
C	2.136120	-0.302714	0.021121
C	3.551709	-0.451036	0.037504
C	4.412494	0.563382	-0.050172
H	-0.464163	2.066764	0.034805
H	-2.929417	2.281897	0.025127
H	-4.350407	0.254598	-0.012103
H	-3.298434	-1.988253	-0.038887
H	-0.833580	-2.200446	-0.027981
H	3.923893	-1.467830	0.130110
H	5.481221	0.387012	-0.029658
H	4.071504	1.587976	-0.144469

Frequencies

37.8603	68.6306	86.0582
198.9542	234.3570	377.0909
396.1748	413.3466	511.2448
552.7850	592.4810	641.9058
700.4556	710.3587	721.8212
780.9459	866.4835	945.3717
955.9788	961.6923	1001.3475
1018.2981	1022.1640	1023.1395
1060.9032	1106.5774	1112.5288
1189.1342	1208.8206	1300.9315
1317.6602	1321.9348	1356.4636
1451.4968	1488.6456	1542.5602
1646.3072	1678.0686	1704.5522
2356.7409	3165.7967	3177.4723
3190.6170	3200.3570	3209.4294
3221.5049	3225.9779	3264.4163

p2I + C₂H₃

C	-0.119265	-1.207158	-0.000008
C	-1.506312	-1.203117	0.000006
C	-2.202502	0.000060	0.000011
C	-1.506211	1.203182	0.000007
C	-0.119165	1.207102	-0.000007

C	0.586875	-0.000056	-0.000019
C	2.019307	-0.000067	-0.000028
C	3.220066	0.000024	0.000020
H	0.428408	-2.141975	-0.000014
H	-2.045371	-2.143504	0.000017
H	-3.286551	0.000110	0.000015
H	-2.045202	2.143607	0.000012
H	0.428587	2.141875	-0.000016
H	4.283376	0.000073	0.000090

Frequencies

137.3843	155.5253	366.7567
413.0872	474.7755	541.5276
555.6593	639.3942	663.8182
703.3969	711.5628	781.6038
782.0728	868.2478	948.3097
1002.3031	1019.5345	1023.1707
1060.8202	1112.1349	1187.9976
1211.5549	1234.3248	1319.7864
1357.2781	1487.8739	1539.4179
1648.1242	1679.1080	2244.4052
3196.3573	3205.2715	3214.7833
3222.1286	3227.8177	3483.0168

p23 + C₄H₄ (vinylacetylene)

C	0.000036	-1.393683	-0.000024
C	1.221183	-0.768037	-0.000003
C	1.208498	0.629507	-0.000007
C	-0.000038	1.318554	-0.000013
C	-1.208546	0.629447	-0.000006
C	-1.221124	-0.768091	0.000015
H	2.155159	-1.318490	0.000040
H	2.146618	1.174278	0.000112
H	-0.000067	2.402510	-0.000017
H	-2.146682	1.174127	0.000033
H	-2.155080	-1.318605	0.000053

Frequencies

402.8095	428.5394	603.4433
623.5234	680.7388	726.3883
828.4957	903.3153	984.3491
992.5270	1008.1169	1030.6246
1058.7046	1083.8002	1179.9680
1186.8622	1310.5168	1327.9948
1471.4512	1486.8142	1608.9858

1661.9810	3188.2868	3193.9318
3205.5201	3208.8910	3220.9839

p24 + H

C	-0.549840	-1.588468	-0.000033
C	-0.549795	1.588341	-0.000250
C	-1.901415	1.261057	-0.000462
C	-2.489635	0.000007	0.000085
C	-1.901410	-1.261091	0.000366
C	0.551733	-0.745912	-0.000005
C	1.892973	-1.145191	-0.000453
C	2.694009	0.000089	-0.000082
C	1.892606	1.145245	0.000439
C	0.551516	0.745899	0.000722
H	-0.320133	-2.651956	-0.000422
H	-0.319909	2.651794	-0.000746
H	-2.590381	2.099926	-0.000949
H	-3.576550	0.000003	0.000184
H	-2.590417	-2.099930	0.000653
H	2.238450	-2.169658	-0.000888
H	3.776635	0.000185	-0.000379
H	2.237858	2.169772	0.000578

Frequencies

160.1419	166.8464	313.7243
338.4977	413.0205	431.5177
490.2147	578.5053	618.2064
690.0086	705.9157	723.2833
745.1868	786.1846	801.5647
839.2332	889.6726	918.2785
950.1130	965.1676	975.9681
981.2478	1008.0224	1027.2979
1069.3528	1084.5959	1180.4875
1225.2817	1258.4151	1317.8113
1326.4497	1334.3316	1435.0951
1445.8296	1497.8318	1506.2834
1555.0200	1605.0273	1672.2963
1680.2266	3158.9902	3160.2564
3171.3327	3190.7807	3200.2526
3222.5879	3238.4157	3249.1686

p25 + H

C	1.368720	-1.438963	-0.000064
C	-1.174906	1.181607	-0.000326
C	1.368667	1.438961	0.000089
C	2.515043	0.726562	0.000169

C	2.515067	-0.726511	0.000004
C	0.108156	-0.740202	-0.000016
C	-1.174911	-1.181639	0.000050
C	-2.045138	-0.000009	-0.000137
C	-3.383549	0.000015	0.000220
C	0.108127	0.740163	-0.000135
H	1.382618	-2.523346	-0.000262
H	-1.523050	2.204889	-0.000121
H	1.382530	2.523344	0.000257
H	3.471556	1.237468	0.000368
H	3.471601	-1.237382	-0.000125
H	-1.523064	-2.204943	0.000060
H	-3.946884	0.927132	0.000156
H	-3.946958	-0.927060	0.000550

Frequencies

112.9413	208.6692	258.8721
263.8973	446.9062	456.3335
504.9374	506.7965	573.2028
652.5914	664.9678	670.5127
728.6933	743.0744	799.3884
805.4463	842.7225	860.1723
913.6290	948.9241	974.8988
986.6420	986.7421	991.3168
1008.1092	1153.1348	1183.2021
1186.9157	1196.1147	1228.9327
1327.3115	1399.4439	1403.4049
1445.1587	1467.8497	1584.8901
1611.8905	1642.9861	1730.1173
1734.1936	3157.7569	3191.3591
3198.5665	3211.8832	3221.1554
3242.7489	3245.0627	3251.1977

p26 + H

C	0.675267	0.000011	-0.000015
C	1.557737	-1.176589	-0.000042
C	2.828938	-0.737184	-0.000028
C	2.828942	0.737172	0.000040
C	1.557750	1.176596	0.000019
C	-0.675249	0.000008	0.000001
C	-1.557744	1.176592	-0.000044
C	-2.828959	0.737173	-0.000031
C	-2.828950	-0.737186	0.000037
C	-1.557730	-1.176588	0.000049
H	1.220994	-2.202377	-0.000120
H	3.720007	-1.350434	-0.000066

H	3.720015	1.350416	0.000108
H	1.221021	2.202381	0.000168
H	-1.221021	2.202387	-0.000106
H	-3.720031	1.350419	-0.000072
H	-3.720014	-1.350444	0.000073
H	-1.220987	-2.202376	0.000099

Frequencies

100.2327	127.0299	179.5557
240.1959	408.9368	449.0342
529.7346	584.0231	610.1098
657.1361	728.1221	729.9878
783.4086	802.5190	817.5190
821.1652	842.6378	911.3889
948.5573	955.3562	957.9724
965.0474	966.6229	1012.6060
1030.1686	1100.1493	1118.1471
1121.5823	1144.7375	1165.5816
1246.8725	1332.9711	1344.5644
1389.2291	1402.1720	1568.3679
1575.7948	1649.5112	1651.7213
1751.7008	3221.0370	3221.6616
3232.1621	3233.6236	3257.5483
3261.2072	3264.0724	3268.2675

$p^9 + H$

C	1.229948	1.433319	0.020887
C	2.391372	0.697407	-0.238832
C	2.391350	-0.697446	-0.238837
C	1.229909	-1.433316	0.020903
C	0.092476	-0.694575	0.274444
C	0.092485	0.694618	0.274432
C	-1.398189	0.791127	0.588673
C	-1.398176	-0.791077	0.588720
C	-2.329718	-0.666959	-0.608658
C	-2.329721	0.666917	-0.608701
H	1.246158	2.517599	0.026912
H	3.319558	1.220528	-0.441895
H	3.319512	-1.220613	-0.441890
H	1.246089	-2.517597	0.026884
H	-1.717815	1.363216	1.459216
H	-1.717783	-1.363131	1.459296
H	-2.763053	-1.413404	-1.263316
H	-2.763082	1.413314	-1.263396

Frequencies

135.5524	178.2289	324.4173
366.6458	432.9525	440.1173
562.5154	571.8333	650.3906
755.7588	767.2823	774.6052
838.8095	839.4315	874.1329
888.2009	927.8626	942.8081
962.6592	979.0489	1005.8460
1010.5739	1030.3582	1067.2964
1104.3264	1144.6222	1156.7247
1171.6750	1182.1234	1214.1492
1222.1605	1222.2096	1301.1056
1311.8633	1377.4209	1494.8095
1507.8534	1651.5629	1668.4446
1680.0829	3127.3028	3134.2360
3186.8370	3198.2628	3201.9267
3208.1130	3216.1510	3234.5434

p10 + H

C	-2.045481	1.078207	0.000004
C	3.131358	-1.057299	0.000008
C	-0.615273	-1.419935	-0.000005
C	-2.043958	-1.369983	0.000000
C	-2.724481	-0.177949	0.000003
C	-0.689746	1.011320	0.000000
C	0.632211	1.740849	-0.000001
C	1.319943	0.575369	-0.000005
C	2.712186	0.209926	-0.000002
C	0.012564	-0.218724	-0.000004
H	-2.599803	2.009227	0.000007
H	2.425917	-1.881295	0.000012
H	4.186018	-1.304912	0.000009
H	-0.097389	-2.371747	-0.000010
H	-2.600527	-2.300371	0.000000
H	-3.808812	-0.187372	0.000007
H	0.927062	2.781339	0.000005
H	3.431594	1.024442	-0.000006

Frequencies

92.0496	144.8948	161.1593
275.3319	355.6184	370.2248
403.1333	505.5320	560.9278
583.1667	653.0477	700.0709
726.6406	750.1731	779.4045
848.0836	851.0610	900.0950
930.9470	956.6924	989.1807
990.5641	1003.0701	1032.5630

1064.2809	1106.5707	1115.1167
1162.1893	1196.1759	1279.4949
1309.5238	1322.7171	1443.1187
1461.0058	1474.5293	1516.8668
1638.6180	1682.7407	1719.6552
1742.5617	3164.3177	3183.5550
3192.0322	3205.4172	3214.6538
3221.7112	3240.0872	3258.1812

p11 + H

C	-1.874321	1.296105	0.006919
C	3.748869	-0.078489	0.098614
C	-1.039098	-1.458909	0.004295
C	-2.422145	-1.090925	0.028029
C	-2.818688	0.222068	0.029703
C	-0.569387	0.927931	-0.015538
C	0.885255	1.338331	-0.049428
C	1.290490	0.045735	-0.044372
C	2.558144	-0.656317	-0.065317
C	-0.161336	-0.428192	-0.016422
H	-2.207934	2.327093	0.007602
H	3.844551	0.987807	0.276930
H	4.664396	-0.656676	0.063921
H	-0.743667	-2.501703	0.003601
H	-3.172851	-1.872838	0.045488
H	-3.877356	0.455590	0.049124
H	1.403755	2.286615	-0.083588
H	2.502402	-1.729929	-0.221972

Frequencies

56.4955	140.1690	152.2507
251.7179	328.5784	357.3396
402.1265	486.9080	580.6416
607.9924	630.4038	692.2240
748.7273	750.8324	779.9948
848.0252	850.3283	898.6325
926.7160	970.1151	984.2825
988.8929	1028.2536	1044.3198
1067.6253	1099.0046	1114.5154
1156.1059	1202.5589	1221.9564
1303.2666	1333.3880	1447.6140
1458.6666	1478.7306	1521.4102
1653.7194	1687.6984	1701.0514
1743.1808	3158.7849	3181.8452
3189.9952	3199.3548	3209.2273
3219.5740	3247.0143	3251.6684

p12 + H

C	-0.384297	-0.190059	-0.045926
C	-1.259069	-1.279759	0.000427
C	-2.633643	-1.093323	0.046070
C	-3.161095	0.190990	0.038817
C	-2.303516	1.285494	-0.018107
C	-0.931436	1.098375	-0.062780
C	1.060074	-0.448737	-0.078700
C	2.035540	0.454457	0.084076
C	3.417858	0.120785	0.036023
C	4.590993	-0.138391	-0.000355
H	-0.851167	-2.285415	0.006428
H	-3.293625	-1.952447	0.085077
H	-4.234021	0.341328	0.072568
H	-2.709458	2.290636	-0.034667
H	-0.281611	1.964004	-0.123904
H	1.348202	-1.484448	-0.238456
H	1.805560	1.499225	0.270933
H	5.627659	-0.371869	-0.035249

Frequencies

57.0608	87.4571	115.4707
238.3551	256.0875	380.5228
412.5334	425.8785	499.4675
539.5718	637.3549	640.3078
659.3076	708.6874	714.4161
772.6862	858.8017	865.9556
890.9311	940.4111	996.1817
1009.8427	1020.4484	1023.5455
1039.3214	1066.5360	1119.7192
1190.1102	1214.3414	1242.2776
1310.0926	1344.7257	1352.4452
1369.7311	1495.4786	1543.6473
1653.9044	1680.5750	1719.4138
2237.0075	3178.4760	3183.8402
3189.6663	3196.7770	3204.6587
3212.5641	3223.1632	3485.2649

p13 + H

C	0.279769	-0.572595	-0.076138
C	1.505818	-1.224565	0.106253
C	2.694276	-0.513963	0.176120
C	2.682167	0.870005	0.052626
C	1.474926	1.530803	-0.142386
C	0.284587	0.821757	-0.206214

C	-0.930784	-1.399727	-0.131701
C	-2.227470	-1.057806	-0.072166
C	-2.785589	0.241863	0.080256
C	-3.326019	1.307716	0.214088
H	1.521655	-2.305870	0.200441
H	3.630712	-1.039754	0.323626
H	3.609291	1.429596	0.103341
H	1.459369	2.609597	-0.249592
H	-0.644696	1.350992	-0.365589
H	-0.734295	-2.464983	-0.222348
H	-2.960895	-1.856509	-0.130272
H	-3.791226	2.256010	0.335965

Frequencies

29.3432	122.7239	161.4914
230.3966	304.5390	384.1217
417.2545	444.5779	521.3079
595.7042	636.2190	693.7237
715.5393	726.2848	740.3354
759.5244	804.5471	823.1936
873.1558	953.6113	978.0064
1006.2616	1015.4956	1023.9229
1028.6345	1063.3806	1119.8280
1188.8008	1213.4152	1221.1503
1280.7781	1348.4695	1365.9764
1451.9447	1495.4035	1542.0455
1648.8352	1680.2781	1710.3822
2230.8690	3167.7847	3185.2801
3188.9204	3194.7989	3206.9671
3219.5128	3244.1369	3484.3042

p14 + H

C	-0.452813	-0.476617	0.000037
C	-0.562117	0.918357	0.000061
C	-1.806634	1.525734	0.000025
C	-2.965410	0.753775	-0.000036
C	-2.869082	-0.631708	-0.000058
C	-1.622190	-1.241647	-0.000019
C	0.848983	-1.154070	0.000058
C	2.023089	-0.555153	0.000028
C	3.145947	0.025181	-0.000013
C	4.315481	0.619495	-0.000064
H	0.340627	1.519672	0.000107
H	-1.877550	2.607622	0.000048
H	-3.937890	1.232546	-0.000063
H	-3.766864	-1.239418	-0.000105

H	-1.549373	-2.324585	-0.000042
H	0.828283	-2.242142	0.000086
H	5.235712	0.044871	-0.000060
H	4.395526	1.701360	-0.000092

Frequencies

42.7340	78.5156	189.3068
225.2593	258.3123	340.4389
414.3912	426.8235	429.2191
541.6262	602.7059	633.7189
638.4315	711.0051	779.2135
833.1595	860.0548	883.5984
885.7105	946.5278	958.7171
1000.3070	1017.9339	1024.3313
1031.5410	1061.5723	1117.8717
1189.9325	1206.2605	1232.1097
1305.3817	1350.3922	1363.7054
1449.4127	1500.8887	1540.0108
1654.6374	1677.8011	1718.2312
2231.8752	3149.0045	3158.7090
3184.6387	3190.4968	3200.5169
3207.0466	3222.3359	3234.2563

p15 + C₂H₂

C	-0.335532	-1.272805	0.000000
C	-1.706991	-1.050958	0.000008
C	-2.201585	0.246067	0.000007
C	-1.316111	1.320591	-0.000003
C	0.051046	1.099107	-0.000011
C	0.560621	-0.203377	-0.000008
C	2.012404	-0.467219	-0.000013
C	2.972757	0.425856	0.000024
H	0.047048	-2.288661	0.000001
H	-2.389837	-1.893076	0.000015
H	-3.271272	0.421913	0.000013
H	-1.697015	2.335801	-0.000005
H	0.741560	1.935911	-0.000020
H	2.297357	-1.525171	-0.000051
H	4.052501	0.429712	0.000029

Frequencies

70.1108	215.6764	218.6510
415.1547	453.3254	461.5542
555.4169	638.2738	644.1897
711.7005	761.6368	778.1876
847.5815	870.6971	893.4312

944.2185	1001.7396	1017.0047
1023.9478	1060.1961	1113.9564
1188.3086	1205.2318	1223.2838
1271.5988	1337.5330	1358.8956
1493.5585	1537.9963	1650.0650
1679.5613	1686.1993	3055.8186
3186.9137	3192.0816	3201.4075
3210.0778	3221.3671	3271.1238

p16 + H

C	0.990781	1.168867	-0.325973
C	2.341046	0.850983	-0.360658
C	2.765725	-0.432242	-0.037405
C	1.829272	-1.397054	0.312317
C	0.478204	-1.080560	0.344465
C	0.043430	0.210318	0.039864
C	-1.403120	0.556533	0.113794
C	-2.343785	-0.486125	-0.184421
C	-1.846043	1.770539	0.460604
C	-3.118134	-1.370042	-0.431381
H	0.666398	2.163820	-0.609330
H	3.062840	1.605107	-0.653235
H	3.820284	-0.681255	-0.068179
H	2.150834	-2.402430	0.559421
H	-0.250215	-1.837489	0.612496
H	-2.905902	1.988138	0.494565
H	-1.158188	2.562400	0.732042
H	-3.810294	-2.145591	-0.655010

Frequencies

50.8016	118.7638	163.3888
250.3658	295.9819	396.7196
419.0775	423.8267	495.0770
624.4266	637.0957	651.6085
686.5889	713.6760	716.5583
744.1369	748.9318	804.5104
871.0473	923.7524	950.4254
957.7486	1003.9789	1023.4562
1025.9888	1062.8204	1116.5011
1137.8853	1189.4142	1216.8663
1312.0014	1343.9734	1362.0650
1441.3836	1492.6675	1544.1543
1653.2984	1682.0972	1696.6267
2239.2166	3170.0420	3185.7810
3193.2370	3201.9507	3208.9580
3217.0311	3265.8153	3485.9638

p17 + H

C	-1.085539	1.429623	0.086168
C	-2.343595	0.853105	0.108329
C	-2.464396	-0.528016	0.015993
H	-0.974657	2.506022	0.139893
H	-3.224692	1.479043	0.186629
H	-3.442771	-0.994400	0.022186
C	-1.326622	-1.311507	-0.086861
C	-0.041741	-0.758756	-0.087498
C	0.070785	0.645284	-0.014186
C	1.323871	1.336613	-0.079602
C	2.334756	1.982079	-0.143526
C	2.320415	-1.539430	0.314559
C	1.093731	-1.696733	-0.174513
H	-1.426128	-2.389422	-0.160535
H	3.240628	2.535593	-0.202428
H	2.628927	-0.643472	0.837375
H	3.056629	-2.327565	0.204747
H	0.852075	-2.639371	-0.661050

Frequencies

68.4520	129.8755	161.7849
206.8289	253.7675	374.9547
392.8322	449.6923	516.4492
539.9790	572.3888	621.8733
667.3899	679.5549	708.4544
726.6332	777.2108	798.0682
840.8442	902.4853	976.9182
980.6759	1012.2925	1044.7139
1059.2127	1081.7989	1149.2742
1194.1513	1227.2756	1229.8398
1302.0825	1326.0111	1360.4865
1454.1352	1488.3887	1538.7624
1637.4821	1674.1820	1727.2576
2239.0387	3157.8327	3173.9879
3189.7359	3202.3328	3215.7180
3226.1184	3263.2457	3483.8998

p18 + C₄H₄ (1,2,3-butatriene)

C	0.000036	-1.393683	-0.000024
C	1.221183	-0.768037	-0.000003
C	1.208498	0.629507	-0.000007
C	-0.000038	1.318554	-0.000013
C	-1.208546	0.629447	-0.000006
C	-1.221124	-0.768091	0.000015

H	2.155159	-1.318490	0.000040
H	2.146618	1.174278	0.000112
H	-0.000067	2.402510	-0.000017
H	-2.146682	1.174127	0.000033
H	-2.155080	-1.318605	0.000053

Frequencies

402.8095	428.5394	603.4433
623.5234	680.7388	726.3883
828.4957	903.3153	984.3491
992.5270	1008.1169	1030.6246
1058.7046	1083.8002	1179.9680
1186.8622	1310.5168	1327.9948
1471.4512	1486.8142	1608.9858
1661.9810	3188.2868	3193.9318
3205.5201	3208.8910	3220.9839

p19 + H

C	1.138459	-1.242703	-0.000022
C	2.493462	-0.954370	-0.000039
C	2.924198	0.369725	-0.000016
C	1.997427	1.405279	0.000027
C	0.639284	1.120852	0.000041
C	0.200926	-0.205269	0.000017
C	-1.216299	-0.483531	0.000024
C	-2.557399	0.044184	-0.000007
C	-2.216157	-1.349021	0.000049
C	-3.424776	1.048767	-0.000057
H	0.794972	-2.271288	-0.000043
H	3.218528	-1.759947	-0.000074
H	3.985270	0.591923	-0.000034
H	2.334100	2.435477	0.000047
H	-0.094429	1.918567	0.000074
H	-2.538058	-2.377110	0.000089
H	-3.083950	2.076428	-0.000104
H	-4.491186	0.862472	-0.000056

Frequencies

50.6629	97.9517	113.9482
282.7412	309.3113	415.3833
415.9809	464.7122	525.0010
580.4756	636.1266	702.1530
712.5321	722.9220	762.8653
767.3418	821.2700	868.2983
873.6755	951.2883	989.4989
1004.2841	1023.4776	1025.1889

1049.9145	1059.3767	1113.3207
1129.4405	1190.4646	1205.3341
1254.1263	1331.3464	1357.3840
1454.5514	1493.3346	1534.5338
1653.1013	1673.7682	1694.4317
1899.2858	3164.6974	3193.7652
3200.5549	3209.6092	3220.7865
3226.1063	3254.2296	3284.4950

Fragments

C_2H_2

C	0.000000	0.000000	-0.598212
C	0.000000	0.000000	0.598211
H	0.000000	0.000000	-1.662213
H	0.000000	0.000000	1.662218

Frequencies

675.1654	675.1654	768.9824
768.9824	2088.1359	3423.0212
3530.5719		

C_2H_3

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

C_4H_4 (vinylacetylene)

C	1.899860	-0.173843	0.000024
C	0.734751	0.118094	-0.000054
C	-0.642291	0.494182	-0.000022
C	-1.648508	-0.378149	0.000011
H	2.929732	-0.438368	0.000098
H	-0.844898	1.561451	0.000082
H	-1.470662	-1.447350	-0.000051
H	-2.677044	-0.037433	0.000114

Frequencies

223.9483	308.2980	563.9496
676.5442	702.8308	706.3394
894.6753	963.0418	1010.7618
1117.2944	1332.3954	1445.4561
1706.1187	2243.6817	3165.3837
3181.9477	3262.9576	3487.0645

C₄H₄ (1,2,3-butatriene)

C	-0.633539	-0.000052	-0.000096
C	0.633534	0.000023	-0.000024
C	-1.943320	0.000013	0.000047
C	1.943321	0.000000	0.000036
H	-2.504304	-0.929020	0.000057
H	-2.504191	0.929115	0.000081
H	2.504268	0.929056	0.000029
H	2.504252	-0.929062	0.000054

Frequencies

221.0448	225.6155	362.6716
570.7387	782.6204	906.7813
909.7635	911.7876	1026.8500
1045.8724	1409.0971	1469.6259
1712.2877	2248.1885	3143.8532
3146.0199	3230.5441	3230.7745

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) for all intermediates, transition states, reactants, and products involved in the C₈H₅ + C₃H₆ reaction at the ωB97X-D/6-311G(d,p) level.

Reactants

C₈H₅

C	0.045775	1.219540	0.013382
C	1.426126	1.212650	-0.006714
C	2.115813	-0.000010	-0.017253
C	1.426105	-1.212662	-0.006715
C	0.045755	-1.219531	0.013384
C	-0.671544	0.000009	0.023596
C	-2.068345	0.000016	0.040729
C	-3.340546	-0.000008	-0.055969
H	-0.510694	2.148691	0.019942
H	1.973361	2.147570	-0.015716
H	3.199878	-0.000024	-0.035097
H	1.973339	-2.147581	-0.015717
H	-0.510719	-2.148680	0.019947

Frequencies

109.1212	143.9347	246.8164
390.7115	476.4153	484.9854
507.4479	629.6306	687.8436
783.4529	788.1472	862.7349
967.3232	1013.8868	1014.0002
1029.0644	1049.7885	1112.7315
1182.8967	1188.0328	1227.9584
1322.9787	1353.0819	1478.2436
1508.7173	1612.2257	1638.8824
1988.9682	3202.8066	3213.5662
3220.9948	3230.0795	3233.7590

C₃H₆

C	-1.276382	0.221005	-0.000011
C	-0.134665	-0.454315	-0.000065
C	1.230687	0.162110	0.000007
H	-2.235678	-0.284449	0.000197
H	-1.291429	1.307503	-0.000032
H	-0.168945	-1.542399	0.000050
H	1.801146	-0.152652	0.879852
H	1.175233	1.253093	-0.000755
H	1.801836	-0.153898	-0.878900

Frequencies

182.1162	433.1258	584.8547
935.9596	946.6634	949.9833
1028.6424	1072.0149	1195.7127
1328.2170	1407.9844	1453.7623
1479.9109	1496.4392	1741.6231
3037.0031	3096.8473	3127.1773
3147.8498	3161.1106	3240.4142

Intermediates

i34

C	1.000925	1.031664	-0.380732
C	2.368789	1.265085	-0.318901
C	3.235292	0.240453	0.038277
C	2.726877	-1.021946	0.331944
C	1.363045	-1.256552	0.271771
C	0.481341	-0.230847	-0.086550
C	-0.951234	-0.475032	-0.156518
C	-1.780140	-1.516814	-0.113520
C	-3.085696	-0.785976	-0.281344
C	-2.148422	0.473036	-0.321030
C	-2.365314	1.479325	0.798598
H	0.328466	1.832929	-0.668064
H	2.758786	2.249937	-0.550129
H	4.302684	0.422419	0.089790
H	3.399894	-1.824667	0.611790
H	0.962841	-2.237534	0.503653
H	-3.767187	-0.816907	0.571734
H	-3.632360	-0.990599	-1.203825
H	-2.167307	0.951248	-1.306627
H	-1.572909	2.231901	0.811900
H	-2.362162	0.974312	1.768775
H	-3.323520	1.992595	0.679037

Frequencies

57.8619	98.9766	136.0530
210.2016	249.2305	267.1636
340.4994	397.0173	416.1656
460.4796	480.7847	615.5618
637.9073	693.0859	716.2702
783.8366	791.1395	853.4209
871.1539	922.3945	944.5780
981.8952	1002.2570	1021.0096
1023.6250	1034.5861	1040.2401
1061.5721	1080.0017	1108.1485
1119.6031	1150.9845	1180.4230
1189.9150	1211.7028	1234.7351

1295.8220	1329.5314	1346.6466
1363.3778	1424.6407	1480.2775
1493.0909	1498.7184	1508.6155
1538.5071	1651.2094	1677.4747
1717.3031	3047.6699	3058.6136
3079.9292	3124.5300	3130.7349
3136.8612	3191.6308	3197.4017
3205.9317	3213.8183	3223.3144

i35

C	1.340357	1.162637	0.006442
C	2.723368	1.203709	0.130184
C	3.454553	0.023812	0.167910
C	2.796003	-1.199702	0.079774
C	1.417016	-1.242875	-0.044892
C	0.671425	-0.059322	-0.082401
C	-0.776980	-0.094645	-0.208990
C	-1.740844	-1.007032	-0.330620
C	-2.934167	-0.080505	-0.408628
C	-1.822519	1.019064	-0.261868
C	-3.968236	-0.164241	0.698763
H	0.772223	2.086605	-0.021722
H	3.229998	2.159741	0.198701
H	4.533609	0.055120	0.267108
H	3.362337	-2.123860	0.109363
H	0.901407	-2.194558	-0.113707
H	-3.410479	-0.065641	-1.392694
H	-1.738774	1.683776	-1.126715
H	-1.914880	1.597226	0.662505
H	-4.664810	0.677354	0.646267
H	-3.484337	-0.153072	1.679309
H	-4.546146	-1.088095	0.617541

Frequencies

46.9813	77.2146	121.5784
170.7255	235.6518	329.2667
333.4193	385.8735	416.6717
469.0015	514.9878	556.1814
636.2029	688.8431	716.6848
782.5693	797.4846	866.9566
880.5952	896.2555	935.3750
947.9368	1000.1255	1022.0866
1023.7668	1033.1282	1057.0663
1067.0412	1072.9184	1117.2851
1119.3302	1152.8881	1187.0521
1188.9581	1216.3059	1231.1125
1296.6354	1333.0700	1363.3635

1367.7834	1418.0048	1464.5364
1492.4426	1495.1695	1502.8357
1541.8872	1651.4433	1678.7245
1714.4034	3046.6335	3048.2621
3085.2828	3117.1975	3125.3016
3131.4917	3187.0917	3192.2390
3201.7278	3209.8959	3219.6845

i31

C	1.499277	1.035239	-0.543370
C	2.854546	1.287968	-0.390349
C	3.688716	0.323373	0.163100
C	3.160477	-0.898321	0.564409
C	1.805889	-1.156965	0.415127
C	0.959762	-0.191581	-0.141296
C	-0.439590	-0.452752	-0.296009
C	-1.615302	-0.669386	-0.428294
C	-3.051352	-0.912068	-0.573632
C	-3.910949	0.251448	-0.174126
C	-3.615889	1.061637	1.035964
H	0.845341	1.783293	-0.975670
H	3.261447	2.242141	-0.705300
H	4.747597	0.523067	0.281170
H	3.806740	-1.653948	0.996372
H	1.389908	-2.107538	0.727212
H	-3.308907	-1.799219	0.030366
H	-3.263795	-1.192292	-1.610971
H	-4.888898	0.319313	-0.637827
H	-2.561892	1.356704	1.071042
H	-3.809504	0.494364	1.960948
H	-4.231558	1.962565	1.073511

Frequencies

4.6722	47.9521	61.7764
90.8337	117.8434	147.3593
263.8775	324.7006	369.5527
381.6326	410.5264	415.2092
537.2422	555.3833	613.9493
643.2433	715.7072	735.2919
786.2041	868.8373	870.6221
886.2925	950.2608	980.7203
999.8820	1003.3142	1022.7445
1024.4117	1062.7894	1098.5052
1111.3874	1155.4144	1188.1932
1208.8406	1229.8565	1288.5254
1318.2864	1346.7635	1355.5022

1377.2049	1423.9439	1457.4012
1479.1015	1488.0072	1488.2542
1542.8321	1648.5061	1681.1614
2376.6008	2956.2596	2973.2754
3063.7102	3065.3781	3124.1634
3187.1436	3191.1970	3196.0622
3206.2386	3213.5954	3219.2794

i32

C	-1.450992	1.138832	0.369762
C	-2.819516	1.281671	0.272098
C	-3.624262	0.207404	-0.113043
C	-3.034797	-1.025035	-0.402138
C	-1.668567	-1.192524	-0.311665
C	-0.831627	-0.109335	0.078743
C	0.533010	-0.264094	0.173504
C	1.798274	-0.403678	0.239554
C	3.129965	-0.295514	-0.417579
C	3.014638	-0.721136	1.036626
C	3.678412	1.064212	-0.776670
H	-0.828385	1.973701	0.668801
H	-3.272565	2.240796	0.497696
H	-4.698337	0.329231	-0.186877
H	-3.655525	-1.862367	-0.701524
H	-1.213294	-2.149764	-0.536185
H	3.362822	-1.093597	-1.118240
H	3.195440	-1.761167	1.287353
H	3.310258	-0.004734	1.797489
H	4.770669	1.041001	-0.831539
H	3.388511	1.806315	-0.028168
H	3.293176	1.395769	-1.743968

Frequencies

36.3466	66.0763	85.7938
157.3173	194.5087	221.4221
337.4084	367.0233	382.2074
413.5533	464.6604	490.9867
547.9259	634.6799	674.7166
690.5880	757.6334	781.4015
836.4123	854.5750	869.8626
901.9234	941.2830	955.5726
989.1801	1000.5069	1002.3547
1046.4428	1051.3385	1072.1255
1110.6529	1127.8165	1136.3151
1177.9435	1179.7475	1197.5887
1305.4813	1307.0045	1349.5139

1386.5060	1423.0854	1469.1158
1471.9370	1493.1311	1502.7030
1509.7527	1595.2258	1620.3852
1990.1850	3041.3347	3115.7400
3120.5740	3122.4595	3146.6995
3185.0364	3191.1727	3205.9744
3210.7873	3213.0889	3217.9235

i33

C	1.628697	1.188702	0.115258
C	3.011774	1.208870	0.218948
C	3.738439	0.027622	0.123839
C	3.074632	-1.177074	-0.076642
C	1.691601	-1.204212	-0.181415
C	0.953053	-0.019799	-0.085951
C	-0.474752	-0.041133	-0.191312
C	-1.675191	-0.055446	-0.281406
C	-3.144436	-0.050752	-0.369020
C	-3.656960	1.328484	-0.077166
C	-3.753123	-1.102923	0.570281
H	1.058632	2.107165	0.189421
H	3.524042	2.151427	0.374993
H	4.819148	0.045964	0.206837
H	3.635798	-2.101566	-0.152079
H	1.170879	-2.141502	-0.337571
H	-3.406458	-0.311866	-1.402082
H	-3.621712	2.096473	-0.839757
H	-3.829320	1.623978	0.951868
H	-4.840012	-1.118616	0.460476
H	-3.511726	-0.868584	1.610136
H	-3.361676	-2.096907	0.345274

Frequencies

16.7567	54.5460	72.7376
163.6559	172.6515	187.7964
250.9023	294.8368	374.0759
414.2691	415.7107	457.3466
518.1501	553.2107	574.7882
609.8111	642.5141	715.2494
716.9763	787.4460	861.0120
873.9477	929.5895	951.8726
971.4223	1006.2527	1023.7951
1024.9892	1056.3304	1068.2058
1110.7940	1139.3211	1180.4512
1186.1784	1211.6585	1287.1379
1317.2344	1324.8997	1335.7367

1356.1206	1410.5010	1458.3937
1486.9704	1494.1775	1506.9274
1543.2028	1646.7520	1680.2167
2365.2987	3033.4758	3052.6092
3132.4133	3143.2657	3156.1537
3192.2361	3201.5622	3211.4837
3219.2935	3224.7042	3272.4282

i96

C	1.697874	-1.209832	-0.000006
C	3.082654	-1.203599	0.000002
C	3.781477	0.000002	0.000008
C	3.082652	1.203601	0.000006
C	1.697871	1.209831	-0.000002
C	0.980689	-0.000002	-0.000007
C	-0.431657	-0.000003	-0.000012
C	-1.659330	-0.000003	-0.000010
C	-3.023273	-0.000001	-0.000006
C	-3.798410	-1.283449	0.000009
C	-3.798402	1.283452	0.000003
H	1.151891	-2.145753	-0.000010
H	3.622034	-2.144080	0.000003
H	4.865409	0.000003	0.000014
H	3.622029	2.144083	0.000010
H	1.151886	2.145750	-0.000003
H	-4.450690	-1.339930	0.880262
H	-3.141604	-2.153368	-0.000038
H	-4.450782	-1.339898	-0.880176
H	-4.450705	1.339929	0.880239
H	-4.450751	1.339915	-0.880199
H	-3.141592	2.153367	-0.000020

Frequencies

39.0167	51.2384	51.6060
72.5408	91.5071	170.2383
219.5539	274.2307	328.6938
413.0241	429.4774	449.1673
499.8976	522.3865	603.9373
640.4490	679.8405	704.2588
772.1710	844.2504	858.1572
931.9707	964.8403	969.7461
996.2856	1010.2504	1011.8081
1022.4068	1058.5473	1061.3409
1111.3457	1184.7533	1200.7021
1227.0957	1251.6286	1313.6578
1355.1163	1401.7978	1411.1997

1433.4414	1471.8257	1474.3778
1483.6560	1490.6413	1508.0607
1554.0063	1629.7195	1656.6914
2089.4619	3015.9446	3019.4790
3068.3462	3068.4990	3145.0409
3146.4938	3194.3208	3202.1002
3213.4921	3219.8389	3226.1729

i36

C	0.957968	0.699567	-0.885701
C	2.342132	0.590207	-0.898606
C	2.979800	-0.298215	-0.040884
C	2.225037	-1.078455	0.826303
C	0.840512	-0.968838	0.838396
C	0.193310	-0.076929	-0.014814
C	-1.300818	0.034606	-0.012091
C	-1.999457	-1.102374	-0.226974
C	-2.669464	-2.186140	-0.474682
C	-1.951694	1.257895	0.205670
C	-1.293543	2.549298	0.559707
H	0.460407	1.385507	-1.562680
H	2.924145	1.197353	-1.582859
H	4.060390	-0.384979	-0.051007
H	2.715599	-1.774358	1.497595
H	0.249965	-1.577728	1.514077
H	-2.978983	-2.864191	0.319141
H	-2.948624	-2.463818	-1.490306
H	-3.035099	1.252390	0.137347
H	-1.339131	3.266264	-0.270609
H	-0.243965	2.419190	0.827232
H	-1.807399	3.020631	1.404136

Frequencies

45.3328	88.8365	100.8724
122.0751	153.6183	180.6790
227.7370	274.2369	415.8440
420.8629	441.2626	506.0003
534.4453	595.7668	607.7610
641.1544	716.3123	725.6052
728.5987	791.6020	881.1493
902.7781	947.3642	959.3584
982.5115	1009.7605	1019.3548
1024.0635	1025.8223	1060.0756
1076.3607	1113.6268	1134.3317
1185.7389	1199.2228	1210.9628
1322.9407	1353.1085	1356.2471

1412.0681	1427.3573	1451.7804
1481.8282	1489.7421	1505.4768
1543.6380	1655.0321	1681.0628
1927.6785	3019.2690	3073.2745
3097.8803	3140.4727	3168.1913
3185.9919	3189.1754	3195.3239
3203.9527	3211.7222	3220.8391

i37

C	0.787329	0.144461	1.248691
C	2.086424	-0.266413	1.220255
C	2.763733	-0.483515	0.000001
C	2.086425	-0.266414	-1.220254
C	0.787330	0.144461	-1.248691
C	0.035096	0.369745	0.000000
C	-1.466693	0.071939	0.000001
C	-1.080104	1.418488	0.000001
C	-1.319467	2.716411	-0.000002
C	-2.342978	-0.917594	0.000003
C	-1.956900	-2.363134	-0.000002
H	0.270210	0.311094	2.187105
H	2.611467	-0.428399	2.155869
H	3.796418	-0.809058	0.000001
H	2.611468	-0.428401	-2.155868
H	0.270212	0.311093	-2.187106
H	-2.334044	3.101150	-0.000001
H	-0.504065	3.430812	-0.000004
H	-3.404317	-0.676361	0.000009
H	-2.363373	-2.872154	0.879785
H	-0.871716	-2.478225	-0.000032
H	-2.363420	-2.872159	-0.879765

Frequencies

52.8046	82.4971	127.6556
139.0540	142.2953	204.4943
227.3236	375.6400	386.2374
442.0708	446.8855	525.1214
571.2721	596.9730	606.5424
648.3920	708.9963	715.1897
754.7626	787.8244	825.8154
844.6286	855.9304	929.5686
972.7272	985.5739	987.1341
1003.7832	1024.7175	1065.2928
1086.3180	1099.4702	1129.3264
1146.4593	1147.4206	1214.1540
1296.9739	1328.5489	1332.5597

1417.2632	1420.7408	1447.1713
1468.3351	1480.6130	1495.4321
1557.6841	1616.1901	1718.8660
1925.6631	3044.6651	3104.4567
3139.1389	3155.2499	3156.2572
3185.6091	3188.6259	3206.2685
3208.6286	3221.1574	3247.7962

i39

C	1.122178	0.879114	-0.650444
C	2.504228	0.761061	-0.558469
C	3.084747	-0.320144	0.095565
C	2.271944	-1.306015	0.661503
C	0.918672	-1.135696	0.535833
C	0.273650	-0.081921	-0.078749
C	-1.209055	-0.013458	-0.164446
C	-1.876773	-1.277792	-0.543927
C	-1.915939	1.098770	0.079459
C	-3.009033	-1.732627	-0.014577
C	-1.410353	2.415641	0.582837
H	0.683729	1.714796	-1.185550
H	3.135061	1.517815	-1.010526
H	4.163833	-0.405721	0.163317
H	2.700529	-2.161786	1.171032
H	-1.365893	-1.874080	-1.297088
H	-2.989098	1.039571	-0.086493
H	-3.515891	-1.199621	0.783665
H	-3.454893	-2.660359	-0.354529
H	-1.417193	3.173576	-0.208514
H	-0.397510	2.349292	0.982135
H	-2.068274	2.784920	1.375040

Frequencies

48.8074	94.6584	107.6253
166.0373	210.5672	217.2312
253.1530	317.5382	375.6441
425.7865	456.4925	493.9074
576.8512	628.9330	640.8511
713.5398	736.9319	738.8617
771.9188	879.0138	891.6234
957.1809	961.6249	971.2142
997.5143	1008.4120	1021.0479
1034.6262	1059.6879	1076.1905
1132.8562	1143.6108	1148.0443
1180.4053	1237.6550	1284.5117
1325.6258	1330.4238	1386.8240

1426.8266	1453.1137	1458.2521
1491.4082	1494.2085	1501.1562
1606.3195	1665.4309	1715.0232
1733.0073	3041.6338	3098.6975
3143.0592	3149.8666	3166.1132
3171.5922	3188.2841	3197.2949
3206.5495	3218.8033	3244.2325

i42

C	0.818353	-0.567650	1.025740
C	2.208558	-0.605968	1.013312
C	2.924586	-0.045185	-0.038322
C	2.244222	0.566750	-1.094454
C	0.875229	0.573888	-1.025136
C	0.104260	0.031131	-0.021247
C	-1.386196	0.077648	-0.024941
C	-2.038517	1.382524	0.151993
C	-2.125412	-1.030323	-0.171231
C	-1.423114	2.543651	0.366479
C	-1.631037	-2.424587	-0.390175
H	0.265540	-1.002701	1.852285
H	2.736556	-1.076268	1.834839
H	4.008739	-0.079566	-0.042282
H	2.780496	1.010933	-1.925573
H	-3.125392	1.362227	0.104028
H	-3.207310	-0.911311	-0.143474
H	-1.990546	3.458944	0.487213
H	-0.342835	2.618350	0.426945
H	-1.909119	-3.071890	0.448713
H	-0.547980	-2.466442	-0.510145
H	-2.093748	-2.853548	-1.284661

Frequencies

27.6014	85.2018	109.3899
155.3290	183.6909	199.2732
263.8467	277.7732	415.6603
425.6958	470.7574	511.6916
533.7277	607.1615	631.6376
721.7251	729.4839	740.9869
770.9168	875.7097	879.5420
943.9048	951.5416	964.8986
998.4899	1008.1499	1027.7871
1037.0889	1054.3787	1068.7552
1109.2800	1129.0603	1160.6612
1181.0603	1247.5462	1276.3624
1318.8243	1332.1069	1400.5238

1424.3476	1445.9672	1451.8251
1487.9458	1494.1274	1496.7568
1603.7610	1665.8289	1701.3580
1744.8044	3040.9753	3096.0318
3141.6257	3155.3783	3158.7796
3169.7160	3186.4440	3194.3952
3204.2027	3215.7439	3253.7255

i38

C	1.563670	0.986280	0.588232
C	2.818781	0.414858	0.754413
C	3.100891	-0.826951	0.199552
C	2.117285	-1.495392	-0.519785
C	0.863719	-0.923980	-0.685761
C	0.572120	0.325291	-0.137495
C	-0.779719	0.941004	-0.321867
C	-1.861025	0.124618	-0.315861
C	-2.894609	-0.661689	-0.295149
C	-0.912381	2.318753	-0.503894
C	-3.686183	-1.026098	0.936667
H	1.345568	1.946036	1.043418
H	3.575784	0.939878	1.326261
H	4.079941	-1.273603	0.330344
H	2.327676	-2.464564	-0.957957
H	0.098833	-1.446594	-1.249758
H	-3.231615	-1.105972	-1.234313
H	-0.040481	2.956186	-0.574456
H	-1.890555	2.767164	-0.617231
H	-4.736814	-0.747583	0.812957
H	-3.292515	-0.524575	1.821300
H	-3.651108	-2.106532	1.105126

Frequencies

46.1239	69.5714	101.9028
142.4425	176.3924	189.5510
269.6436	363.8984	401.2662
422.1960	441.7181	508.9054
552.8231	607.4746	624.9426
641.2204	724.4668	736.3973
744.6398	783.0151	801.1065
867.6030	875.5471	956.6449
1006.5603	1009.9514	1024.9677
1028.0052	1061.1210	1061.6771
1090.1087	1113.7289	1128.8737
1188.0812	1211.0232	1218.7380
1319.2142	1333.7449	1358.3203

1385.6851	1410.8316	1482.4331
1490.0475	1495.5994	1500.0066
1544.4221	1658.2547	1680.6398
1940.9442	3049.3652	3096.1793
3113.8495	3153.4858	3169.6698
3185.8605	3195.0612	3201.3583
3210.9678	3218.1166	3275.2937

i40

C	1.626496	1.170622	-0.140232
C	2.947273	0.773672	0.023614
C	3.271605	-0.565990	0.216090
C	2.259528	-1.528005	0.239326
C	0.977039	-1.075536	0.071893
C	0.580822	0.234550	-0.104198
C	-0.850947	0.599192	-0.251133
C	-1.714640	-0.440676	-0.850042
C	-2.907801	-0.844574	-0.409627
C	-1.317990	1.792943	0.127208
C	-3.644498	-0.373805	0.806571
H	1.396383	2.215671	-0.319984
H	3.734797	1.517577	-0.010252
H	4.306407	-0.865821	0.341259
H	2.485100	-2.578572	0.384324
H	-1.295253	-0.941628	-1.719457
H	-3.401970	-1.627197	-0.981191
H	-0.681598	2.530791	0.602859
H	-2.355151	2.060837	-0.033454
H	-4.486495	0.270207	0.529271
H	-3.000300	0.190798	1.482387
H	-4.063239	-1.227020	1.347420

Frequencies

39.0441	53.4512	114.4494
164.5611	177.4058	233.6770
293.7483	371.5135	401.1821
427.2772	461.4315	527.1580
584.0972	632.0988	675.9329
691.8129	746.7444	780.4085
795.9883	806.4112	882.6580
913.4308	947.0620	971.4998
975.4305	993.8242	1013.8088
1015.1466	1056.2442	1072.7174
1121.0391	1130.3252	1137.3744
1186.9493	1249.8155	1286.4144
1325.0043	1327.4778	1409.1898

1438.2261	1450.0696	1462.0060
1491.6231	1493.6641	1497.8671
1606.1948	1666.8698	1706.6061
1741.4407	3040.3169	3100.7410
3136.2218	3154.1752	3166.9636
3177.0977	3189.3901	3195.7908
3207.6489	3221.2388	3257.9285

i41

C	-1.983056	1.190527	-0.234590
C	-2.963272	0.198460	-0.253581
C	-2.656652	-1.145510	-0.019319
C	-1.352420	-1.568886	0.249966
C	-0.391842	-0.578061	0.274133
C	-0.693465	0.759133	0.032465
C	0.714050	1.174608	0.188772
C	1.101201	-0.319102	0.477705
C	2.049640	-0.945885	-0.472479
C	1.415314	2.294756	0.097194
C	3.514175	-0.949618	-0.211665
H	-2.231485	2.228574	-0.422466
H	-3.993343	0.470103	-0.456698
H	-3.457471	-1.876382	-0.047967
H	-1.128553	-2.614366	0.428208
H	1.432615	-0.451525	1.514622
H	1.692488	-1.134358	-1.480945
H	0.940459	3.240816	-0.138811
H	2.487959	2.296412	0.257107
H	4.031773	-1.700098	-0.814640
H	3.731518	-1.144729	0.843952
H	3.972003	0.023014	-0.453965

Frequencies

55.7163	82.7967	109.8732
124.4732	207.0318	231.4879
305.1870	336.1257	411.1024
450.3480	500.6441	533.8788
568.4432	625.9485	657.5035
700.9949	770.1585	780.8717
807.5694	819.4421	883.6493
917.1906	922.7775	956.1910
984.0436	1000.9608	1024.0414
1034.3451	1079.4020	1116.2562
1137.7965	1161.4185	1165.9197
1187.1744	1210.0819	1218.6484
1267.9378	1315.3757	1359.6356

1405.0835	1426.7855	1441.3519
1481.9933	1489.6513	1501.2985
1511.7424	1672.3601	1674.2306
1772.4978	2978.1553	3054.3828
3062.8153	3117.9747	3158.2921
3180.8796	3188.8660	3200.4866
3210.6671	3218.0919	3246.5503

i44

C	0.372876	-1.472671	-0.000080
C	1.721609	-1.814837	-0.000058
C	2.706719	-0.833144	0.000023
C	2.354552	0.513547	0.000072
C	1.013512	0.856135	0.000045
C	0.014505	-0.127190	-0.000011
C	-1.313063	0.542393	-0.000046
C	-1.074158	1.914678	-0.000071
C	-2.577322	-0.033021	-0.000034
C	0.388839	2.226579	0.000021
C	-2.890313	-1.494832	0.000110
H	-0.374038	-2.254585	-0.000168
H	2.006137	-2.861185	-0.000110
H	3.752818	-1.118257	0.000036
H	3.120906	1.281681	0.000122
H	-1.850286	2.669027	-0.000100
H	-3.416363	0.656532	-0.000139
H	0.689601	2.811045	-0.879197
H	0.689467	2.811048	0.879274
H	-2.477906	-2.000091	0.881628
H	-2.478401	-2.000156	-0.881607
H	-3.968474	-1.660883	0.000432

Frequencies

78.9088	161.5504	191.4840
204.9773	218.2186	263.3931
346.2475	422.8017	466.5937
492.9391	521.0784	598.7514
614.2999	670.4683	701.2818
724.3501	744.9506	755.7455
786.8187	849.7357	886.7292
931.7919	974.0554	997.5169
1005.2201	1009.1888	1017.9087
1064.9394	1099.4389	1115.2113
1148.7996	1169.9472	1188.6571
1202.1570	1230.7131	1263.1956
1331.4205	1352.4891	1395.5802

1422.2656	1426.1847	1449.3719
1474.2208	1488.0825	1506.1880
1513.8122	1529.4749	1656.7249
1689.3032	3023.0061	3025.0309
3050.9255	3075.7303	3134.9287
3179.3722	3184.6917	3197.1714
3210.2148	3232.2369	3245.7947

i43

C	-1.589361	0.892934	0.650832
C	-2.786384	0.189724	0.717718
C	-2.943613	-1.014008	0.040157
C	-1.885750	-1.526855	-0.715278
C	-0.731956	-0.788551	-0.744266
C	-0.510086	0.414647	-0.107553
C	0.760060	1.179963	-0.225831
C	2.048950	0.486176	-0.091309
C	2.237803	-0.784402	0.264849
C	0.725836	2.497559	-0.457658
C	3.579080	-1.435265	0.387544
H	-1.471392	1.821480	1.199789
H	-3.602561	0.582596	1.313025
H	-3.880549	-1.557242	0.098369
H	-1.982894	-2.464401	-1.251314
H	2.921849	1.104318	-0.295688
H	1.376175	-1.409832	0.484996
H	-0.210229	3.027097	-0.590416
H	1.641233	3.074019	-0.536446
H	3.726724	-1.839465	1.394112
H	4.388603	-0.732997	0.175767
H	3.665567	-2.277110	-0.307421

Frequencies

44.2378	87.9592	104.7258
153.4822	201.8401	218.1283
238.1207	329.5871	362.1375
427.5121	471.5146	543.6814
605.2633	610.0311	638.9647
707.3232	739.4264	754.5715
778.8995	857.8843	878.4951
932.9847	940.2315	971.3764
993.5779	1006.7318	1008.5797
1020.4901	1054.3722	1073.8275
1123.6764	1133.6237	1159.0706
1184.1692	1253.3712	1313.6825
1323.1895	1344.0413	1371.5811

1420.5269	1444.6108	1459.1815
1482.5591	1493.7090	1495.6885
1603.9152	1665.3391	1693.0615
1755.5353	3038.5904	3097.9174
3127.8752	3149.0301	3161.8850
3176.2455	3189.6936	3197.0843
3206.6215	3220.8676	3253.3281

i97

C	0.866073	-1.524841	0.000053
C	2.256499	-1.544132	-0.000203
C	2.983275	-0.356098	-0.000239
C	2.327946	0.871967	-0.000050
C	0.942751	0.891550	0.000278
C	0.211812	-0.299523	0.000390
C	-1.237956	0.018011	-0.000083
C	-1.348595	1.406653	-0.000220
C	-0.001863	2.066018	0.000180
C	-2.250443	-0.927992	-0.000146
C	-3.711798	-0.629423	-0.000633
H	0.309719	-2.456000	-0.000233
H	2.780498	-2.493403	-0.000530
H	4.067063	-0.389572	-0.000520
H	2.895280	1.797054	-0.000200
H	-2.276600	1.961899	0.000682
H	0.143051	2.707010	0.879352
H	-1.969237	-1.977185	0.004941
H	-3.919215	0.440592	-0.047673
H	-4.193054	-1.025731	0.901199
H	-4.207419	-1.105251	-0.854408
H	0.143708	2.707449	-0.878563

Frequencies

33.4340	95.6553	165.4108
182.6548	204.6719	247.5059
342.8249	424.9037	466.5629
467.5837	554.2287	591.1610
614.0746	669.5248	692.9572
693.8500	742.6240	775.9034
791.0045	850.2396	881.6855
926.3691	969.9457	984.7222
996.0425	1003.1436	1023.7155
1059.6087	1090.3775	1129.7323
1145.1205	1165.9445	1187.4551
1219.3212	1240.0147	1262.3710
1308.9657	1333.4629	1360.1631

1420.8042	1423.4219	1447.0390
1476.5602	1479.6653	1513.2031
1518.7353	1548.3586	1659.7684
1687.6833	3030.2655	3030.9398
3058.9610	3078.7679	3139.3540
3174.6751	3185.6271	3192.9628
3204.4811	3218.4919	3235.8945

i46

C	0.424015	-1.461941	0.004433
C	1.784331	-1.761665	0.002566
C	2.746715	-0.741949	-0.001811
C	2.371186	0.585263	-0.003630
C	0.996154	0.909597	-0.001488
C	0.015149	-0.132827	0.001646
C	-1.318390	0.476309	0.002000
C	-1.115437	1.988366	0.003248
C	-2.524948	-0.104954	-0.000476
C	0.370552	2.159392	-0.001157
C	-2.812802	-1.577922	-0.004535
H	-0.295927	-2.268731	0.008610
H	2.103573	-2.797532	0.004721
H	3.799237	-1.003432	-0.003372
H	3.115648	1.373608	-0.006351
H	-1.583483	2.453704	-0.873292
H	-3.388134	0.556896	0.000073
H	0.876233	3.115626	-0.002735
H	-1.577330	2.451154	0.884490
H	-2.402268	-2.071538	0.883084
H	-2.379248	-2.070871	-0.881396
H	-3.887446	-1.764895	-0.018610

Frequencies

22.7464	161.0111	175.5630
195.6472	237.2534	252.1115
354.5822	406.1184	478.4512
485.6407	527.0861	587.4638
587.8157	606.6670	697.8459
744.0278	751.2796	771.5136
823.1157	874.2208	881.2059
937.3860	960.5410	981.8070
992.0116	1010.4414	1053.1277
1053.2834	1074.9927	1119.5019
1138.5151	1161.1672	1164.3676
1199.9716	1240.1765	1273.4150
1323.4064	1328.7290	1385.4603

1399.4882	1426.0032	1461.4762
1469.8818	1491.8619	1501.9768
1519.1028	1608.6307	1629.8533
1724.1932	3029.7225	3035.1669
3057.6122	3091.5024	3133.6970
3158.5437	3186.6931	3203.0597
3214.0184	3237.0001	3253.0448

i45

C	1.388581	1.391775	0.170644
C	2.577120	0.669702	0.158917
C	2.568056	-0.708392	-0.042805
C	1.367738	-1.386684	-0.236558
C	0.183641	-0.668108	-0.226763
C	0.192433	0.713956	-0.023211
C	-1.202572	1.216257	-0.060677
C	-2.022787	0.112261	-0.288454
C	-1.235018	-1.162037	-0.403743
C	-1.598229	2.527790	0.100043
C	-1.645871	-2.228144	0.621870
H	1.402226	2.464870	0.328740
H	3.520494	1.182838	0.308119
H	3.504203	-1.255382	-0.049369
H	1.364740	-2.460510	-0.394032
H	-3.102419	0.153030	-0.366318
H	-1.357331	-1.587900	-1.410096
H	-0.879461	3.319319	0.272737
H	-2.646057	2.798791	0.055522
H	-2.691744	-2.514765	0.485223
H	-1.521368	-1.844307	1.637411
H	-1.031831	-3.126235	0.516490

Frequencies

105.1088	134.5971	163.9628
235.7655	256.4411	285.3944
395.7193	416.2907	488.2195
524.0675	535.9564	543.1151
576.1906	614.4383	673.6705
719.3531	754.0536	766.4243
781.4995	798.7419	809.1649
905.4322	932.7750	977.0549
989.9102	1015.6472	1020.1422
1057.5307	1070.7410	1106.4354
1116.8239	1163.5050	1189.0128
1219.5995	1237.9071	1259.5126
1315.6334	1330.0729	1352.8226

1401.0204	1405.3689	1421.4678
1494.6583	1502.0887	1502.2707
1517.1514	1535.7984	1661.1030
1687.1845	3013.5233	3050.4040
3129.7001	3133.9802	3163.6890
3186.4682	3193.5149	3204.7560
3217.3896	3218.3599	3261.4089

i48

C	-0.859932	-1.346416	-0.616491
C	-2.188459	-1.328424	-0.194562
C	-2.742527	-0.173788	0.351970
C	-1.982196	0.983719	0.492103
C	-0.657553	0.963833	0.074211
C	-0.105016	-0.195629	-0.484142
C	1.348530	0.057438	-0.844545
C	1.516263	1.505388	-0.413060
C	2.309937	-0.882379	-0.179884
C	0.383657	1.997274	0.101428
C	2.247262	-1.118147	1.287671
H	-0.426544	-2.247819	-1.037749
H	-2.795761	-2.221443	-0.290861
H	-3.777765	-0.178613	0.674630
H	-2.416861	1.879685	0.922086
H	1.473575	-0.007177	-1.932478
H	2.455372	2.032762	-0.518814
H	2.970206	-1.483589	-0.794054
H	0.238318	3.001207	0.480361
H	1.497925	-1.882533	1.542726
H	1.955240	-0.208256	1.822838
H	3.206502	-1.461434	1.683109

Frequencies

73.1317	87.2742	115.2759
169.7689	230.5058	258.3407
354.5015	383.3770	426.6227
468.6445	542.2085	566.5265
582.7604	659.5551	732.4337
753.7927	759.9350	795.0121
855.3711	876.2990	909.5534
929.7774	965.6843	975.4647
983.8426	1000.2102	1008.3359
1054.6858	1075.7399	1095.7734
1135.8325	1166.8167	1180.2659
1192.5495	1224.5303	1241.6597
1303.5699	1310.2767	1344.3784

1380.0753	1394.4990	1421.5979
1480.2788	1490.8954	1499.7770
1511.9874	1636.3000	1671.0546
1688.2731	2993.7865	3052.0998
3066.6489	3116.1551	3184.9743
3191.3475	3196.3160	3203.4364
3215.6574	3216.0671	3241.8810

i98

C	0.915025	-1.514259	0.000010
C	2.306201	-1.496470	0.000005
C	3.007972	-0.280344	-0.000007
C	2.339639	0.926124	-0.000011
C	0.926157	0.926360	-0.000004
C	0.220889	-0.313386	0.000004
C	-1.220859	-0.044298	0.000008
C	-1.388484	1.469927	0.000015
C	0.016976	1.990643	-0.000001
C	-2.202687	-0.950926	-0.000005
C	-3.667689	-0.647022	-0.000010
H	0.385528	-2.461098	0.000020
H	2.856064	-2.430589	0.000011
H	4.092428	-0.294628	-0.000011
H	2.884670	1.863593	-0.000020
H	-1.950915	1.812381	0.878382
H	0.275377	3.041023	-0.000009
H	-1.932726	-2.004759	-0.000029
H	-4.155872	-1.081098	-0.879130
H	-3.866485	0.426244	0.000254
H	-4.155967	-1.081544	0.878834
H	-1.950939	1.812386	-0.878333

Frequencies

76.7434	96.7692	147.7782
174.2203	232.8169	278.1069
336.5307	416.1626	464.0906
480.2361	545.3261	560.5686
595.7454	610.7131	675.6510
746.6242	756.8407	762.3383
849.2719	870.2928	879.7071
926.7459	955.2006	972.8201
987.2026	989.9353	1027.6738
1046.1402	1061.0333	1131.4506
1149.0784	1158.0421	1164.8957
1206.8651	1244.5882	1293.5765
1315.0106	1327.6866	1368.7937

1398.9176	1423.2379	1456.0655
1468.8131	1484.1686	1497.2420
1519.2170	1611.6403	1632.1210
1744.5669	3021.7784	3039.6687
3047.8516	3093.6867	3134.6096
3158.3900	3190.0439	3197.4404
3208.2042	3219.3135	3228.8253

i47

C	1.556465	1.279575	0.003018
C	2.661111	0.433096	0.003245
C	2.490188	-0.959675	-0.000423
C	1.231451	-1.525774	-0.004318
C	0.098511	-0.680799	-0.005141
C	0.283245	0.732355	-0.001042
C	-1.028744	1.388610	-0.000265
C	-2.070524	0.280545	0.000080
C	-1.271827	-0.992693	-0.008460
C	-1.279233	2.698102	-0.000611
C	-1.900004	-2.338927	0.005361
H	1.695072	2.355556	0.007030
H	3.661254	0.850525	0.007064
H	3.365185	-1.600642	0.000641
H	1.115040	-2.603844	-0.005364
H	-2.720217	0.343692	0.882956
H	-2.729808	0.349867	-0.874919
H	-0.478431	3.429290	-0.001192
H	-2.294383	3.079362	-0.000352
H	-2.633504	-2.441394	-0.803174
H	-2.441658	-2.513014	0.944237
H	-1.162380	-3.135880	-0.105592

Frequencies

78.9990	110.4088	121.0313
177.8741	246.0529	282.6489
303.5084	400.2667	472.1275
516.8569	531.4061	547.4493
561.3868	573.9299	676.4642
746.0876	753.4840	783.6865
790.1284	855.3510	894.4941
919.5817	927.6776	947.4559
956.0978	994.8053	1024.5034
1046.5033	1074.5817	1111.4200
1144.9746	1162.1219	1179.7195
1221.3061	1244.6923	1302.8059
1335.4944	1345.5036	1408.8811

1426.7870	1450.5816	1455.9640
1472.9780	1479.3628	1501.1722
1521.1562	1611.9256	1635.5445
1721.4494	3016.5201	3022.5539
3050.7652	3065.7417	3128.8773
3161.7632	3184.8698	3195.1770
3206.2369	3219.4174	3247.6752

i99

C	1.365986	1.385993	0.112518
C	2.645779	0.850146	0.214280
C	2.851079	-0.536638	0.129909
C	1.794366	-1.403918	-0.053518
C	0.487347	-0.876169	-0.157851
C	0.288644	0.532691	-0.072524
C	-1.141751	0.821719	-0.211143
C	-1.862504	-0.516810	-0.371989
C	-0.742406	-1.518039	-0.341103
C	-1.728352	2.019161	-0.198987
H	1.217169	2.458361	0.180358
H	3.495085	1.507712	0.359442
H	3.858854	-0.928775	0.212159
H	1.958279	-2.473688	-0.119430
H	-2.362141	-0.542762	-1.350044
H	-0.889272	-2.586191	-0.436831
H	-1.157058	2.932636	-0.075931
H	-2.801592	2.123914	-0.314915
C	-2.919584	-0.762053	0.714136
H	-3.703714	-0.002211	0.670944
H	-2.460162	-0.723362	1.704950
H	-3.387081	-1.742125	0.586928

Frequencies

67.1041	138.7017	207.1861
259.9935	269.3429	285.0777
361.9137	425.7713	492.1149
500.5824	537.2583	557.4668
626.2471	648.5736	687.8857
701.2552	750.0599	767.9867
792.2111	847.3784	871.7329
887.0985	916.6710	958.6915
961.2705	998.2920	1026.3380
1047.3645	1084.0507	1111.1293
1113.8809	1143.1618	1166.8876
1209.5987	1257.3383	1275.1686
1318.2428	1330.3737	1342.7826

1398.0638	1418.1550	1449.0144
1472.4784	1499.0592	1509.8143
1519.3813	1611.5305	1634.5523
1717.4401	3024.3355	3046.8012
3124.1077	3134.0117	3159.4078
3190.0252	3197.0451	3209.1808
3220.7044	3226.5681	3244.4725

i49

C	1.582045	1.246536	-0.206997
C	2.658951	0.378568	-0.029828
C	2.448440	-0.986590	0.142638
C	1.159549	-1.513878	0.144557
C	0.088098	-0.648075	-0.031932
C	0.302537	0.722994	-0.212376
C	-1.029707	1.423470	-0.378626
C	-1.998112	0.255461	-0.268181
C	-1.361091	-0.906448	-0.067707
C	-1.281215	2.478790	0.646757
C	-1.958932	-2.265018	0.096453
H	1.745741	2.311253	-0.336047
H	3.669880	0.770551	-0.024660
H	3.298401	-1.646049	0.278979
H	1.000136	-2.577970	0.283815
H	-1.100644	1.860736	-1.382736
H	-3.070998	0.386122	-0.337077
H	-1.066166	2.266491	1.687520
H	-1.817507	3.386521	0.399919
H	-3.047401	-2.230156	0.028602
H	-1.687348	-2.693457	1.066596
H	-1.587467	-2.948897	-0.673457

Frequencies

117.6735	148.6837	156.4408
163.2300	183.4249	228.4955
290.2579	379.1448	426.9702
471.4957	535.4378	541.2334
558.0121	582.1683	604.3563
683.3064	755.1134	769.9808
783.9377	807.5397	842.9335
903.7660	971.4610	985.6157
1004.8104	1007.8254	1029.9799
1056.2343	1069.8511	1094.5242
1128.3974	1139.7644	1180.2119
1195.9769	1208.9464	1253.4379
1310.8553	1329.8468	1350.2884

1384.5672	1421.5828	1460.9795
1482.8659	1496.4073	1503.0705
1517.4865	1653.3725	1685.1791
1708.3384	3043.3667	3044.7793
3103.0567	3139.9159	3154.5450
3188.0151	3193.6484	3205.0512
3218.9180	3222.9440	3268.6962

i100

C	-1.459714	1.331217	0.269304
C	-2.724971	0.765306	0.113883
C	-2.865210	-0.600402	-0.114653
C	-1.748729	-1.428855	-0.196514
C	-0.489238	-0.864607	-0.043350
C	-0.351306	0.508928	0.194798
C	1.117562	0.850663	0.323067
C	1.780993	-0.514571	0.115063
C	0.849553	-1.456537	-0.086386
C	1.583526	1.882019	-0.648108
C	3.262855	-0.679222	0.152447
H	-1.348035	2.396557	0.442316
H	-3.606842	1.393498	0.170326
H	-3.856209	-1.024339	-0.233716
H	-1.864536	-2.491793	-0.378915
H	1.335884	1.184673	1.346485
H	1.048204	-2.508877	-0.252439
H	1.248381	1.829992	-1.677412
H	2.350902	2.598776	-0.384049
H	3.670291	-0.346857	1.113332
H	3.741167	-0.073640	-0.624292
H	3.548871	-1.721618	0.001057

Frequencies

95.8906	132.0308	147.2033
148.8926	223.3837	249.2801
289.0409	334.8855	435.8290
461.3732	477.0691	520.4608
567.7256	598.8898	630.3817
659.6067	766.3297	782.6516
794.0443	856.6645	885.8712
895.9978	913.7315	977.1636
998.9054	1015.7730	1025.4806
1055.0091	1065.1611	1114.9010
1136.9635	1167.6550	1184.8612
1190.2183	1220.5291	1245.1125
1304.3822	1322.9781	1334.8755

1384.4782	1418.1122	1455.9692
1483.7877	1488.2869	1506.6038
1516.5813	1656.1054	1685.1892
1710.8669	3036.9947	3039.4390
3095.3742	3138.5768	3158.8382
3182.8633	3192.1374	3202.2955
3212.1711	3213.1837	3273.5101

i50

C	-1.254753	-1.404828	-0.392914
C	-2.503998	-0.958423	0.047830
C	-2.700910	0.381359	0.393693
C	-1.668795	1.300025	0.301603
C	-0.411025	0.868433	-0.158922
C	-0.216978	-0.501881	-0.495168
C	1.196314	-0.719530	-0.901832
C	1.856156	0.650557	-0.790044
C	2.259219	-0.487015	0.152964
C	0.796045	1.575320	-0.347521
C	1.982681	-0.492781	1.634209
H	-1.105914	-2.448736	-0.647888
H	-3.327456	-1.659110	0.125727
H	-3.677467	0.704440	0.737294
H	-1.827569	2.339306	0.567726
H	1.422080	-1.397498	-1.716469
H	2.602626	0.984885	-1.501176
H	3.217062	-0.924405	-0.114970
H	0.940690	2.632614	-0.170367
H	1.967955	-1.518975	2.012252
H	1.021902	-0.035160	1.874251
H	2.762365	0.055214	2.170236

Frequencies

108.5453	140.0414	171.5991
275.2032	295.3416	362.7154
427.1020	480.2469	494.7607
537.0227	584.5142	624.3687
670.0118	709.9700	739.5173
761.5804	782.9567	797.7035
839.7924	876.1425	880.7363
927.3083	954.4301	963.3783
993.3655	1007.1512	1047.1457
1050.7794	1066.6584	1095.9969
1131.5777	1137.0484	1172.6752
1198.0019	1220.3079	1224.5649
1273.0197	1319.1412	1353.0875

1363.4956	1392.0685	1413.4841
1440.9515	1476.3283	1497.9236
1509.9979	1516.1471	1620.4915
1641.9055	3052.7757	3116.5098
3148.4263	3163.5950	3181.5262
3188.2771	3194.0664	3196.2343
3206.9542	3217.7371	3232.4369

i52

C	-1.465396	-1.482343	-0.103559
C	-2.731056	-0.974452	0.081326
C	-2.927988	0.406490	0.214774
C	-1.839530	1.267966	0.158153
C	-0.548835	0.783931	-0.027837
C	-0.333687	-0.624405	-0.163051
C	0.959963	-1.116238	-0.346432
C	1.846320	1.209561	-0.267986
C	2.178222	-0.250459	-0.382591
C	0.603296	1.668602	-0.095757
C	3.190749	-0.667596	0.706931
H	-1.313566	-2.551786	-0.207376
H	-3.580686	-1.646894	0.123862
H	-3.926312	0.801980	0.360565
H	-1.991224	2.337974	0.260895
H	1.106167	-2.187826	-0.449290
H	2.679496	1.905257	-0.313346
H	2.685749	-0.406930	-1.349612
H	0.424461	2.735824	-0.003568
H	3.463743	-1.720350	0.596699
H	2.756418	-0.524739	1.699335
H	4.103404	-0.068843	0.638013

Frequencies

67.9964	153.6726	206.8356
245.5734	276.9158	367.6250
399.8836	431.6333	478.4746
509.7194	513.1816	600.3358
620.1621	716.1816	727.9682
759.7466	769.3849	786.4118
807.8385	871.7416	883.5785
918.2199	967.5155	980.0621
1000.7453	1011.9541	1036.5514
1058.6627	1071.7761	1138.3449
1151.2900	1168.3192	1191.5233
1212.9441	1260.3185	1300.8383
1309.8380	1346.2001	1370.0145

1404.5785	1423.1020	1449.5057
1474.3285	1495.2821	1506.2259
1522.4848	1593.1901	1634.7926
1714.6809	2959.9224	3043.2675
3123.7507	3130.4466	3171.7303
3176.1375	3183.4639	3188.0696
3194.6032	3202.0523	3216.4461

i51

C	-1.695345	-1.308915	-0.173159
C	-2.744812	-0.402883	0.009008
C	-2.485252	0.959258	0.175518
C	-1.188784	1.447597	0.149958
C	-0.124286	0.551518	-0.058696
C	-0.399650	-0.838346	-0.199805
C	0.880488	-1.580947	-0.343912
C	1.961296	-0.516207	-0.319823
C	1.268704	0.784800	-0.167534
C	1.824227	-1.498525	0.834085
C	1.977727	2.087168	-0.068158
H	-1.900147	-2.367872	-0.290219
H	-3.767766	-0.761108	0.027998
H	-3.312125	1.645278	0.323426
H	-1.001236	2.508189	0.277486
H	0.942450	-2.442624	-0.997064
H	2.850053	-0.587140	-0.937291
H	1.434813	-1.129272	1.776176
H	2.580604	-2.270723	0.912523
H	2.754779	2.171474	-0.835461
H	2.478887	2.196142	0.902930
H	1.293804	2.930548	-0.185385

Frequencies

120.1312	138.4122	160.3568
198.7626	249.3876	356.5592
416.1973	443.8176	502.6555
524.0824	553.7401	593.8761
644.6565	739.1172	755.2775
773.3019	786.7192	808.5984
875.3650	879.4318	917.2772
947.2279	962.5801	991.7864
1010.5427	1024.6049	1041.6356
1056.3296	1058.6848	1086.4408
1091.6018	1142.1997	1175.8239
1185.5206	1200.4355	1234.6809
1281.3809	1321.3531	1359.2133

1375.7260	1409.6371	1430.5653
1473.5449	1481.2248	1488.0701
1503.3210	1512.6995	1617.5900
1643.7568	3013.4462	3071.4142
3129.3681	3135.9997	3176.9391
3187.5471	3194.1319	3196.5809
3204.9693	3217.4681	3233.6915

i101

C	-1.551790	-1.379080	-0.272535
C	-2.785135	-0.725485	-0.193621
C	-2.848609	0.653913	0.022839
C	-1.694589	1.408257	0.153530
C	-0.445670	0.767509	0.056226
C	-0.393001	-0.642185	-0.145169
C	1.027243	-1.078873	-0.154074
C	1.855481	0.185523	0.011821
C	0.864971	1.283176	0.127296
C	1.791045	-0.842620	1.133356
C	3.161803	0.419301	-0.705357
H	-1.509944	-2.451686	-0.429660
H	-3.702840	-1.293111	-0.297104
H	-3.816477	1.138650	0.086858
H	-1.750043	2.479203	0.315458
H	1.351856	-1.882404	-0.805030
H	1.128741	2.323299	0.271498
H	1.226408	-0.606110	2.027850
H	2.681588	-1.441544	1.290941
H	2.989092	0.793688	-1.717874
H	3.736610	-0.507488	-0.778842
H	3.774510	1.150882	-0.169972

Frequencies

116.0427	156.6362	177.8621
256.2542	288.2805	379.3472
395.7904	438.4207	457.0534
512.4353	567.6493	601.2132
636.8948	655.2703	739.0079
762.9843	780.7674	813.9173
834.7146	880.7724	886.3943
942.4714	948.3111	960.8988
974.9111	998.6670	1026.3844
1043.4428	1055.4572	1085.3567
1110.8426	1133.4030	1168.4931
1186.3265	1200.7826	1251.3363
1270.6767	1307.3597	1347.1414

1365.4080	1415.6781	1437.2387
1467.7968	1490.6685	1491.9585
1501.4751	1518.5959	1620.5973
1640.3330	3045.3281	3117.9369
3126.2207	3137.7806	3188.5824
3189.8195	3195.3830	3206.5486
3218.6820	3226.4004	3233.3662

i102

C	-1.752388	1.265900	0.254367
C	-2.764274	0.334165	0.130291
C	-2.453600	-0.987742	-0.184361
C	-1.127188	-1.361056	-0.355377
C	-0.092485	-0.441578	-0.220166
C	-0.404448	0.903511	0.075045
C	0.642994	1.880182	0.151140
C	2.322360	0.239652	-0.412779
C	1.347298	-0.897226	-0.356487
C	1.970557	1.527756	-0.128999
C	1.731973	-1.846848	0.801792
H	-1.988321	2.300071	0.484280
H	-3.797250	0.631665	0.271080
H	-3.242301	-1.723091	-0.294712
H	-0.890981	-2.393015	-0.598270
H	0.386471	2.907901	0.381482
H	3.356879	-0.007701	-0.628963
H	1.434635	-1.476733	-1.286522
H	2.732209	2.300522	-0.127420
H	2.762896	-2.193455	0.688791
H	1.076473	-2.720717	0.825226
H	1.644490	-1.325738	1.758221

Frequencies

72.7810	149.8375	201.6342
240.1747	288.9444	377.1551
387.2706	475.6508	494.4597
508.6992	522.5121	576.5528
623.3554	697.3124	733.8571
775.0889	780.3763	798.0598
810.0426	875.7382	898.4319
944.7370	977.7286	984.8437
1001.9797	1011.0020	1064.8834
1076.7909	1096.0105	1106.5749
1154.5918	1187.8827	1190.5455
1220.2619	1240.9189	1292.0704
1301.3594	1323.2280	1366.6581

1392.8989	1411.4906	1451.1704
1482.7884	1493.4993	1502.4965
1536.0848	1576.7268	1633.7536
1665.2821	3008.8190	3047.4424
3128.2030	3134.6505	3172.6546
3178.1202	3181.9221	3193.2505
3199.6874	3209.9615	3217.5044

i53

C	1.841846	-1.251234	-0.000051
C	2.793665	-0.257946	-0.000032
C	2.403637	1.085705	0.000038
C	1.052906	1.416078	0.000068
C	0.062846	0.436819	0.000030
C	0.454450	-0.942846	-0.000008
C	-0.509215	-1.951713	-0.000009
C	-2.288457	-0.204306	-0.000014
C	-1.368196	0.769477	-0.000012
C	-1.968440	-1.665336	0.000058
C	-1.779489	2.217179	-0.000058
H	2.139536	-2.294781	-0.000100
H	3.846710	-0.516372	-0.000071
H	3.151492	1.869992	0.000060
H	0.771880	2.462591	0.000117
H	-0.188185	-2.988357	-0.000043
H	-3.341850	0.061959	-0.000063
H	-2.448537	-2.146980	-0.867781
H	-2.448435	-2.146867	0.868020
H	-2.866486	2.309722	-0.000539
H	-1.394307	2.738998	-0.881672
H	-1.395124	2.738831	0.882012

Frequencies

89.1422	166.1946	211.3560
246.3592	262.3079	285.7193
415.7639	439.0046	463.8962
486.7733	508.6565	572.2321
583.3014	687.0729	704.2518
745.1754	767.7047	777.2348
823.9861	862.3743	874.7665
938.4503	945.2739	960.3235
994.8949	1028.9130	1056.6041
1071.7985	1085.7640	1093.1618
1163.2696	1177.4738	1195.7057
1228.4925	1251.1850	1301.2205
1341.0862	1383.2039	1397.8199

1422.2861	1440.1609	1454.9058
1468.6250	1486.9502	1503.9942
1523.5322	1594.3719	1632.3189
1729.6970	2966.3884	2971.4811
3040.6152	3102.0541	3135.9496
3169.5634	3179.9885	3183.9544
3193.9404	3204.6276	3217.1217

i103

C	-1.427926	-1.507172	-0.000007
C	-2.739734	-1.050359	-0.000005
C	-2.998787	0.326851	0.000002
C	-1.959584	1.228752	0.000007
C	-0.608109	0.788800	0.000009
C	-0.355718	-0.619897	-0.000009
C	1.021580	-1.083895	0.000002
C	1.885830	1.236268	-0.000052
C	2.074372	-0.255910	0.000006
C	0.463835	1.681681	0.000026
C	3.491676	-0.742974	0.000034
H	-1.228024	-2.574311	-0.000033
H	-3.560452	-1.758067	0.000018
H	-4.022923	0.683290	0.000003
H	-2.158961	2.295548	0.000041
H	1.184749	-2.158731	-0.000024
H	2.415915	1.664172	0.867728
H	2.415744	1.664031	-0.868017
H	0.265245	2.748714	0.000102
H	3.545141	-1.833091	-0.000612
H	4.029307	-0.372734	0.880276
H	4.029642	-0.371698	-0.879568

Frequencies

94.8717	123.0779	160.3622
237.3654	262.8966	305.7824
406.3378	432.4883	441.6531
455.7633	513.2894	551.2391
622.9643	667.8240	685.5225
742.8463	763.4163	771.2442
847.5655	866.6990	883.0396
924.3713	928.1426	952.9005
987.5317	1022.1235	1047.1415
1058.8631	1067.3621	1139.3641
1166.1333	1181.4524	1206.4213
1211.5870	1269.0194	1300.8163
1338.7145	1354.7350	1409.3288

1421.9615	1441.3583	1455.0269
1471.7419	1477.9538	1496.7164
1522.4579	1593.5422	1633.8428
1733.1759	2964.0680	2969.8741
3033.2239	3088.7253	3137.0577
3172.3631	3183.6867	3186.9105
3189.2789	3203.3578	3219.9146

i104

C	-1.832664	-1.241297	-0.001097
C	-2.798430	-0.242749	-0.000158
C	-2.401363	1.097583	0.001457
C	-1.063526	1.431316	0.001408
C	-0.053255	0.432453	-0.000480
C	-0.476075	-0.935521	-0.000904
C	0.530220	-1.986026	-0.000865
C	2.365477	-0.318191	0.002264
C	1.317829	0.751480	-0.001877
C	1.837182	-1.717357	0.001007
C	1.796339	2.171925	-0.002086
H	-2.133773	-2.284460	-0.001840
H	-3.850961	-0.500548	-0.000345
H	-3.150192	1.881913	0.002927
H	-0.778548	2.476744	0.003595
H	0.182762	-3.014940	-0.001917
H	3.029562	-0.176494	0.872161
H	2.562902	-2.524279	0.001609
H	2.887150	2.218101	-0.030466
H	1.465858	2.711784	0.893332
H	1.419095	2.727745	-0.868244
H	3.035743	-0.177259	-0.862826

Frequencies

69.0962	98.1274	125.1548
186.6819	287.8054	314.7759
395.0935	428.3588	474.9312
499.1421	500.2294	546.0846
555.4407	697.2796	697.7152
756.0803	790.3104	790.6439
848.9954	863.0534	901.5534
940.2012	950.0542	992.9064
1004.7230	1009.4246	1021.3199
1058.8948	1088.5936	1144.0876
1183.3111	1189.1551	1205.4543
1213.2654	1231.1745	1299.8184
1339.8137	1377.6265	1407.5408

1418.0330	1433.6393	1448.2980
1480.4930	1484.6557	1494.0774
1519.0414	1595.1539	1637.7635
1724.4971	2961.4239	2966.8336
3023.6931	3076.9226	3125.1276
3175.7544	3178.3801	3195.1307
3202.1155	3207.1929	3219.9780

i105

C	-1.435513	-1.483532	-0.000046
C	-2.744630	-1.020977	-0.000192
C	-2.992739	0.350879	-0.000151
C	-1.936063	1.240640	0.000003
C	-0.604492	0.786389	0.000127
C	-0.359684	-0.602695	0.000134
C	1.053976	-1.133813	0.000436
C	1.821489	1.238034	-0.000048
C	2.135207	-0.094451	-0.000044
C	0.499851	1.701459	0.000147
C	3.544328	-0.594798	-0.000324
H	-1.243782	-2.552784	-0.000065
H	-3.568391	-1.725539	-0.000340
H	-4.012232	0.719956	-0.000257
H	-2.123542	2.309731	0.000004
H	1.194276	-1.793785	0.870810
H	1.194327	-1.794802	-0.869141
H	2.628272	1.965486	-0.000233
H	0.297239	2.766347	0.000160
H	3.738854	-1.221043	-0.879718
H	3.739196	-1.221079	0.878971
H	4.265408	0.224710	-0.000447

Frequencies

22.7359	100.5460	149.2590
236.5835	263.8307	297.2518
394.3068	427.5811	434.7648
482.4679	523.7738	540.1914
618.3050	694.7723	718.5193
731.4768	767.6219	784.4316
861.9445	863.4054	903.8666
921.8729	949.6607	967.1911
1000.4270	1008.9909	1046.3463
1070.8611	1125.3639	1145.2597
1183.7322	1197.2402	1220.4808
1222.7924	1241.2645	1298.8192
1320.2752	1364.0429	1368.9768

1417.0347	1443.0612	1444.9987
1481.1586	1485.0932	1493.8233
1534.6591	1585.5459	1635.2752
1665.6112	2984.5849	2999.7591
3020.7900	3070.2480	3134.5917
3178.5126	3180.6041	3187.3264
3203.3010	3207.5312	3219.1175

i106

C	1.813332	-1.211591	0.000033
C	2.775977	-0.212333	-0.000012
C	2.376983	1.121015	-0.000079
C	1.031252	1.438661	-0.000080
C	0.040363	0.438503	0.000002
C	0.455507	-0.912028	0.000035
C	-0.547950	-2.040486	0.000143
C	-2.314824	-0.273993	-0.000132
C	-1.369882	0.768550	0.000036
C	-1.971108	-1.593386	-0.000162
C	-1.817141	2.198765	0.000140
H	2.120742	-2.253517	0.000079
H	3.829047	-0.469349	0.000004
H	3.118640	1.911799	-0.000129
H	0.736858	2.481409	-0.000164
H	-0.364021	-2.688082	-0.869952
H	-0.364305	-2.687606	0.870659
H	-3.368384	-0.008690	-0.000251
H	-2.741151	-2.356767	-0.000314
H	-2.906329	2.266730	0.001004
H	-1.448784	2.736866	-0.881041
H	-1.447362	2.737134	0.880552

Frequencies

59.2824	115.0554	179.6761
207.5179	296.0926	297.6642
428.5263	434.6943	462.3842
484.0500	505.0853	571.5219
571.5960	689.1737	704.6131
741.4742	773.6861	796.2826
837.4219	871.1338	936.5166
955.7354	963.6410	969.9170
994.5669	1003.3343	1034.0078
1073.9124	1096.0912	1161.6310
1197.4572	1200.4103	1211.0007
1214.9022	1268.3108	1297.3021
1314.6697	1343.5342	1384.5674

1417.1247	1446.4872	1462.4762
1480.2101	1491.0639	1499.0358
1533.6014	1574.8368	1639.4182
1666.8554	2994.1507	3009.9014
3027.4150	3078.9336	3133.9679
3168.9331	3171.4845	3195.7277
3206.8866	3207.4288	3221.7044

Transition states

i34 – i31

C	1.164553	0.804104	-0.863004
C	2.496856	1.114946	-0.639669
C	3.275662	0.305049	0.180259
C	2.715232	-0.814967	0.784077
C	1.379242	-1.123719	0.576398
C	0.592888	-0.320765	-0.258333
C	-0.788659	-0.643106	-0.470303
C	-1.826157	-1.319983	-0.700293
C	-3.117150	-0.606428	-0.471837
C	-2.472997	0.722864	-0.073210
C	-2.514185	1.171305	1.349853
H	0.550884	1.427518	-1.502536
H	2.931842	1.989337	-1.109950
H	4.318687	0.547077	0.349391
H	3.320249	-1.446511	1.424396
H	0.930748	-1.989903	1.047829
H	-3.708877	-1.058244	0.330246
H	-3.747719	-0.556965	-1.363647
H	-2.440910	1.485326	-0.847642
H	-1.783097	1.961131	1.539217
H	-2.298293	0.339490	2.028090
H	-3.505222	1.565938	1.620982

Frequencies

-763.9086	25.4759	60.7933
100.1903	131.3946	196.1129
210.8244	312.4473	369.3373
412.9085	417.9598	486.8661
549.1431	632.5512	642.6429
703.2938	721.3442	764.6347
793.6074	855.9603	883.3473
897.6777	964.7381	1010.2184
1016.3932	1025.1116	1032.5640
1036.2361	1065.7870	1077.6377
1116.7846	1130.6142	1196.1837
1202.8603	1214.1703	1244.1036

1272.0926	1322.7999	1359.5791
1361.5937	1410.6220	1472.5577
1483.2485	1488.0095	1491.9548
1537.5985	1647.8935	1677.2666
1928.0619	2992.7544	3060.3030
3074.0737	3104.2461	3118.5029
3169.3805	3191.4687	3199.3995
3209.2350	3219.5115	3224.5557

i34 – i36

C	1.040093	1.020069	-0.439263
C	2.414249	1.157847	-0.294103
C	3.184146	0.075382	0.112361
C	2.570943	-1.145858	0.374719
C	1.197520	-1.279049	0.244831
C	0.411002	-0.196999	-0.164555
C	-1.039350	-0.350346	-0.300766
C	-1.819264	-1.458055	-0.352344
C	-3.124226	-1.180306	0.041903
C	-2.058189	0.691505	-0.268576
C	-2.018401	1.863434	0.670975
H	0.449196	1.861864	-0.783921
H	2.886184	2.110286	-0.507944
H	4.257229	0.181681	0.223451
H	3.166796	-1.994866	0.690814
H	0.713827	-2.225149	0.462924
H	-3.308917	-0.881335	1.070810
H	-3.997488	-1.580133	-0.475966
H	-2.661933	0.815176	-1.159381
H	-1.724872	2.780502	0.145292
H	-1.319496	1.699114	1.493037
H	-3.011661	2.047120	1.089794

Frequencies

-606.4163	51.7667	105.0835
135.1736	156.5193	249.3021
269.3085	289.6939	372.2929
420.0120	467.4260	499.4940
612.7411	633.0200	644.2807
679.0542	720.9039	760.6540
791.6422	802.4176	870.5561
938.7507	951.6207	967.0879
1002.9826	1020.6733	1023.3420
1025.0764	1046.7720	1062.1770
1107.7252	1114.0296	1169.1838
1188.8576	1212.3566	1229.3198

1329.5715	1338.3120	1358.6283
1399.3115	1409.6535	1481.9711
1492.3970	1498.2628	1509.7897
1538.0981	1610.4706	1654.8353
1681.7929	3029.4434	3096.5143
3105.6741	3140.7995	3186.2769
3188.3205	3192.9343	3202.5731
3207.2801	3208.9619	3218.6277

i35 – i38

C	1.518662	1.169962	0.126855
C	2.901065	1.036731	0.097672
C	3.477636	-0.223233	0.005143
C	2.663875	-1.351087	-0.062233
C	1.285038	-1.217381	-0.049476
C	0.693046	0.046461	0.045718
C	-0.763079	0.189352	0.044980
C	-1.754779	-0.723490	0.139705
C	-2.959771	-0.253110	-0.379917
C	-1.537524	1.397892	-0.202666
C	-4.292880	-0.383560	0.293530
H	1.070672	2.153206	0.227266
H	3.529081	1.918642	0.157419
H	4.556441	-0.329516	-0.011466
H	3.109841	-2.336736	-0.134983
H	0.646705	-2.091879	-0.118707
H	-2.995538	-0.088890	-1.455971
H	-1.238232	2.106961	-0.979293
H	-2.140296	1.806795	0.598207
H	-4.938989	0.456899	0.028639
H	-4.190728	-0.430975	1.378739
H	-4.796691	-1.295740	-0.045718

Frequencies

-640.9610	56.3470	83.8584
106.7857	124.5141	186.6391
255.5561	323.4994	415.6418
418.5761	445.7071	523.8553
586.9854	609.9024	635.0725
662.3156	715.1103	773.6241
799.4541	821.0802	872.4347
901.1590	923.4678	945.9422
1003.5923	1018.3793	1022.8802
1028.5311	1044.0696	1058.1708
1109.9329	1115.4890	1136.3303
1187.6029	1207.1525	1231.3165

1317.9963	1343.2122	1359.1887
1397.8268	1428.1935	1471.1828
1485.1315	1493.0064	1502.1754
1542.7394	1629.9251	1655.5452
1683.3034	3043.0490	3084.5954
3111.8775	3137.7600	3153.0816
3181.9758	3188.5098	3197.8929
3205.7880	3217.3281	3231.6966

i35 – i33

C	1.300868	1.109962	0.048921
C	2.673433	1.275841	0.164320
C	3.515868	0.170843	0.162285
C	2.978495	-1.106273	0.040764
C	1.608983	-1.282645	-0.078328
C	0.757011	-0.170869	-0.072649
C	-0.660781	-0.362083	-0.187309
C	-1.766137	-0.953333	-0.284532
C	-2.984387	-0.090845	-0.395163
C	-2.193422	1.220492	-0.357553
C	-3.999506	-0.262625	0.729180
H	0.635973	1.965365	0.050878
H	3.086741	2.273493	0.258511
H	4.587387	0.303819	0.255885
H	3.631239	-1.971793	0.037612
H	1.184635	-2.274667	-0.175287
H	-3.479626	-0.240097	-1.359740
H	-2.036658	1.757083	-1.287774
H	-2.229279	1.802795	0.559391
H	-4.796478	0.479946	0.634456
H	-3.517800	-0.128964	1.701624
H	-4.448681	-1.257777	0.704832

Frequencies

-765.9138	34.9134	69.2726
103.5200	144.2432	278.8761
308.6181	334.3521	353.1343
408.6282	414.3764	455.4972
516.2259	572.4929	635.6645
640.5901	718.2364	753.3908
774.9898	786.2583	868.9055
876.6079	942.4099	951.2508
953.9521	1008.8538	1022.0950
1027.9473	1060.0217	1099.1536
1112.0011	1124.7163	1173.5551
1189.8399	1206.0752	1243.1274

1282.6058	1318.1769	1352.6515
1355.1824	1417.6394	1430.0070
1487.2237	1503.2369	1506.8733
1531.6019	1646.7604	1676.5945
1933.5219	3046.8231	3066.4174
3123.3382	3124.9130	3136.5966
3191.1128	3198.8064	3211.2704
3216.7019	3222.7385	3246.3815

i38 – i40

C	1.704533	1.247902	0.146634
C	2.990722	0.723441	0.214624
C	3.215583	-0.646951	0.095730
C	2.148552	-1.527165	-0.092506
C	0.886909	-0.978717	-0.158963
C	0.632907	0.379787	-0.044633
C	-0.817300	0.674050	-0.159214
C	-1.505445	-0.622060	-0.203291
C	-2.729975	-1.079796	-0.006314
C	-1.366418	1.886057	-0.279932
C	-3.937374	-0.256112	0.352897
H	1.545247	2.315986	0.251875
H	3.832115	1.390353	0.365577
H	4.227577	-1.033262	0.153107
H	2.317977	-2.593885	-0.184630
H	-0.418625	-1.392717	-0.308039
H	-2.890434	-2.151714	-0.105967
H	-0.752802	2.780500	-0.265395
H	-2.430128	2.022867	-0.423234
H	-4.494069	0.034085	-0.544949
H	-3.656209	0.655381	0.884506
H	-4.616809	-0.830210	0.986956

Frequencies

-1870.0092	50.1687	119.4222
121.5254	170.7402	199.3929
272.3720	296.2021	347.3928
412.7984	458.7258	468.7698
521.0303	632.8127	650.9817
687.5277	702.5729	740.2293
795.8803	798.5723	804.3359
880.5935	887.0553	929.0653
967.7309	989.2505	1009.3602
1014.0634	1051.2373	1057.7193
1088.3165	1110.9108	1133.9114
1141.8954	1183.0346	1251.7903

1311.8054	1341.0977	1355.3905
1404.8884	1451.7602	1481.1153
1491.2701	1492.2150	1498.6390
1642.9237	1660.1801	1704.3564
1759.8078	1790.4901	3039.8766
3107.8705	3133.1638	3153.1430
3162.8665	3188.0469	3194.9311
3207.8976	3218.3984	3258.5844

i36 – i39

C	1.116183	1.219225	0.104393
C	2.496375	1.036399	0.094974
C	3.056647	-0.233374	-0.005761
C	2.235500	-1.359572	-0.094576
C	0.876639	-1.148740	-0.085951
C	0.280350	0.105015	0.006439
C	-1.198669	-0.006160	-0.005945
C	-1.518007	-1.444924	-0.014596
C	-2.125267	0.959301	-0.048183
C	-2.606391	-2.177058	0.111251
C	-1.882168	2.439274	-0.076206
H	0.714625	2.219367	0.198253
H	3.146202	1.900905	0.171531
H	4.135078	-0.349105	-0.010954
H	2.661209	-2.353967	-0.166707
H	-0.268397	-1.902941	-0.119062
H	-3.164378	0.641443	-0.073717
H	-3.586410	-1.726147	0.266281
H	-2.569086	-3.260239	0.068098
H	-2.814328	2.982689	-0.235288
H	-1.191998	2.717005	-0.879024
H	-1.449676	2.794676	0.865566

Frequencies

-1871.0166	26.9180	107.4739
167.2390	182.9554	215.7713
224.6743	300.8192	345.0933
389.3112	427.0198	449.8699
548.6533	554.3007	578.2331
665.1462	682.7712	739.0347
741.8293	793.9165	840.4740
886.7728	914.6535	966.0893
966.3637	1005.6909	1013.1326
1018.0906	1053.9833	1058.5100
1098.4846	1118.8476	1132.5113
1146.9180	1187.8779	1215.8365

1300.4828	1335.6043	1389.3384
1421.2713	1428.7464	1475.1872
1493.7385	1497.5187	1504.1273
1636.6821	1662.3578	1721.2390
1743.7256	1792.0370	3033.4859
3093.3384	3109.1023	3132.9540
3166.1070	3184.0417	3197.9695
3208.1170	3208.6798	3232.7711

i42 – i44

C	0.579914	-1.359857	0.281508
C	1.948053	-1.605105	0.206235
C	2.841234	-0.586174	-0.101904
C	2.368951	0.711591	-0.316364
C	1.011379	0.908303	-0.266436
C	0.075968	-0.079501	0.022897
C	-1.344396	0.357664	0.034181
C	-1.428593	1.815053	-0.043442
C	-2.447327	-0.412133	-0.049193
C	-0.376511	2.589477	0.349081
C	-2.530715	-1.903840	-0.161423
H	-0.082391	-2.164750	0.571900
H	2.320770	-2.603711	0.404143
H	3.904441	-0.793062	-0.163952
H	3.056334	1.524284	-0.525377
H	-2.237085	2.249288	-0.623316
H	-3.397381	0.116804	-0.059783
H	-0.318756	3.628352	0.038228
H	0.243084	2.330248	1.199370
H	-2.407105	-2.396255	0.810370
H	-1.763804	-2.301872	-0.831783
H	-3.505863	-2.202188	-0.550641

Frequencies

-580.5552	60.6278	140.0446
181.8479	191.9242	250.0553
288.4613	317.6757	402.3776
433.8286	467.5977	496.5713
565.8504	602.3930	621.3121
684.1096	731.9948	748.3551
787.8630	823.8013	853.8895
882.7642	944.0294	956.6942
964.1007	996.0730	1009.7500
1039.1427	1054.2968	1059.3351
1098.5473	1139.0931	1157.4670
1186.1756	1233.9805	1270.1441

1294.8528	1328.2430	1398.2336
1424.2285	1432.0681	1457.9086
1489.1250	1498.5407	1504.0732
1572.1082	1617.9329	1658.6757
1682.7758	3031.1909	3096.1094
3131.4990	3147.2569	3167.3979
3186.0352	3186.8048	3199.0177
3211.9722	3229.0425	3236.3545

i44 – i46

C	0.389685	-1.467508	0.030496
C	1.729737	-1.794486	0.023469
C	2.722628	-0.796944	-0.009653
C	2.378693	0.534848	-0.025379
C	1.017445	0.884180	-0.030464
C	0.006593	-0.115855	-0.011567
C	-1.304269	0.517317	-0.007661
C	-1.059862	1.931496	-0.011407
C	-2.568810	-0.044836	-0.001146
C	0.400949	2.169957	-0.033691
C	-2.876987	-1.507876	-0.025921
H	-0.351854	-2.254165	0.061483
H	2.025491	-2.837402	0.045162
H	3.767881	-1.085292	-0.017891
H	3.141407	1.305753	-0.041181
H	-1.799547	2.702435	-0.176622
H	-3.408848	0.643001	0.010803
H	0.863993	3.130160	-0.205705
H	-0.370360	2.239011	1.039258
H	-2.506765	-2.020975	0.870900
H	-2.422581	-2.007095	-0.890339
H	-3.953628	-1.677188	-0.078330

Frequencies

-1550.0917	76.2036	176.3774
180.9418	199.2442	227.9035
336.4756	350.7295	433.3019
491.7423	530.1534	559.8206
591.5713	618.6029	668.2302
709.5651	716.5496	760.3179
766.7913	790.4616	876.6890
880.3336	909.7192	972.3668
997.1023	1001.3826	1021.9740
1030.0883	1052.5244	1099.8787
1126.3354	1160.0899	1177.2862
1218.2411	1226.3617	1242.6586

1278.5508	1349.2739	1372.4750
1388.4173	1395.5488	1424.2820
1486.8052	1489.3126	1504.6064
1527.7815	1538.2781	1615.8242
1681.8742	2152.5508	3015.0261
3063.2389	3130.5460	3179.5808
3185.3535	3199.3308	3212.2273
3234.8002	3246.5097	3253.4044

i46 – i48

C	0.409828	-1.464062	0.102300
C	1.749518	-1.782189	0.048928
C	2.730709	-0.774407	-0.041915
C	2.379230	0.553324	-0.083259
C	1.013479	0.901659	-0.054025
C	0.025492	-0.115371	0.045960
C	-1.285324	0.516771	0.085935
C	-0.986811	1.982479	0.038761
C	-2.581180	-0.040693	-0.080350
C	0.385003	2.175115	-0.061103
C	-2.878619	-1.501865	-0.106571
H	-0.327890	-2.251110	0.187949
H	2.056108	-2.821459	0.083452
H	3.777565	-1.055871	-0.075629
H	3.137139	1.326646	-0.144541
H	-1.767775	2.727794	-0.028902
H	-1.237350	1.269240	1.156708
H	-3.410627	0.656797	-0.131040
H	0.885081	3.132255	-0.073544
H	-2.589385	-1.999832	0.828616
H	-2.345315	-2.013843	-0.916928
H	-3.945507	-1.675179	-0.254107

Frequencies

-1417.0540	89.3042	161.4357
180.6658	194.2753	218.0127
331.8532	352.0723	434.5183
482.0842	529.8041	545.5757
575.6780	593.9442	653.1156
712.8507	733.1046	762.5355
771.7210	799.5099	880.1681
889.0924	909.3492	972.4412
990.2321	1003.6979	1011.2798
1053.1890	1067.5277	1088.9722
1121.8873	1155.7114	1173.9106
1183.8538	1216.4498	1250.9631

1303.0774	1339.0066	1374.8522
1394.3167	1422.3867	1474.1961
1485.5093	1488.8422	1503.6965
1511.2903	1542.8528	1621.7258
1686.2072	1955.7559	3009.1448
3056.0875	3132.5979	3184.9844
3189.9142	3198.8463	3210.1677
3233.4812	3235.3505	3259.0046

i48 – i50

C	-1.121760	-1.294501	-0.677892
C	-2.394633	-1.024703	-0.177356
C	-2.674936	0.207736	0.413356
C	-1.701333	1.192677	0.512101
C	-0.428601	0.935723	-0.002066
C	-0.149427	-0.315944	-0.590301
C	1.296171	-0.354830	-0.980675
C	1.771506	1.035710	-0.667638
C	2.228288	-0.730049	0.130495
C	0.766782	1.747073	-0.045850
C	1.789940	-1.013687	1.524470
H	-0.901907	-2.257091	-1.127888
H	-3.171418	-1.777814	-0.243685
H	-3.669656	0.397671	0.801525
H	-1.927335	2.147178	0.974849
H	1.530103	-0.781817	-1.955593
H	2.734260	1.417560	-0.972887
H	3.256840	-0.924598	-0.149904
H	0.858134	2.745279	0.359921
H	1.269999	-1.979055	1.588506
H	1.085851	-0.258174	1.888710
H	2.643141	-1.040379	2.204580

Frequencies

-537.5175	102.0051	135.0308
174.1351	238.3699	277.8632
366.9880	426.8147	445.7003
521.5136	558.9298	587.3682
622.3051	638.0451	718.0750
748.6154	774.9241	803.1963
836.2088	859.0747	880.6750
900.7557	915.2614	971.7004
973.9747	1006.9093	1024.9026
1052.7553	1073.1028	1091.1082
1132.6494	1157.1135	1176.7107
1188.2398	1202.8417	1239.6004

1268.8209	1330.2410	1348.8306
1376.9332	1394.8069	1429.6849
1439.7184	1484.2889	1490.8584
1503.6743	1527.0352	1646.2453
1674.0835	3015.0760	3076.5040
3119.6176	3131.0131	3186.8731
3194.1081	3201.5409	3205.5954
3216.8446	3230.2458	3258.1347

i45 – i47

C	1.575186	1.253608	0.032191
C	2.653022	0.392651	0.028677
C	2.464299	-1.002395	-0.007962
C	1.198474	-1.543932	-0.050929
C	0.092217	-0.678658	-0.041140
C	0.278732	0.724147	0.013240
C	-1.011788	1.394786	0.010925
C	-1.992608	0.349390	-0.057462
C	-1.311836	-0.969225	-0.085517
C	-1.255822	2.747529	0.046657
C	-1.981316	-2.283865	0.151571
H	1.730617	2.326676	0.060451
H	3.660792	0.791679	0.055977
H	3.329723	-1.655747	-0.004266
H	1.058199	-2.619169	-0.084097
H	-3.060336	0.462936	0.074657
H	-1.780559	-0.327404	-1.143920
H	-0.445484	3.463002	0.106885
H	-2.267053	3.134814	0.030657
H	-3.004922	-2.282337	-0.231144
H	-2.030155	-2.497090	1.225183
H	-1.442175	-3.101570	-0.331888

Frequencies

-1556.0420	134.5269	146.0671
160.6590	208.6151	234.7788
265.2958	378.4412	419.4994
517.2022	532.4065	545.3490
549.4803	581.6470	608.5377
627.0710	715.9472	756.8198
767.1492	787.8021	798.5723
847.3459	872.1792	952.7749
964.3678	985.5660	1002.6036
1048.5327	1057.5115	1071.3264
1132.1013	1162.6738	1179.3611
1195.6706	1244.5740	1277.0132

1298.8753	1356.3389	1372.8013
1403.9940	1425.9154	1458.8247
1484.0319	1495.4473	1500.4600
1530.8276	1547.5181	1620.3945
1680.9471	2141.2856	3036.9810
3104.5900	3130.4527	3170.0551
3185.2662	3195.6238	3204.6712
3216.8292	3235.3672	3264.3802

i45 – i43

C	1.797128	0.995651	-0.124034
C	2.831695	0.068289	-0.087619
C	2.566959	-1.290652	0.060245
C	1.248781	-1.740358	0.164102
C	0.255170	-0.790524	0.153531
C	0.472696	0.569458	0.003400
C	-0.739080	1.430550	0.023673
C	-1.943462	0.605998	0.137211
C	-1.949874	-0.663661	-0.369618
C	-0.735151	2.769119	0.057998
C	-2.970655	-1.696904	0.002263
H	2.022993	2.048064	-0.261902
H	3.857002	0.407241	-0.183444
H	3.384703	-2.002983	0.090720
H	1.030978	-2.798351	0.264903
H	-2.726571	0.924334	0.819796
H	-1.402087	-0.866841	-1.285589
H	0.184795	3.341921	0.049463
H	-1.663817	3.326429	0.099818
H	-3.694566	-1.840268	-0.806569
H	-3.511203	-1.419604	0.909527
H	-2.487468	-2.661737	0.176366

Frequencies

-471.5496	75.1721	132.804
144.8604	175.1244	220.559
275.8815	356.7961	385.075
412.2010	458.3089	532.366
568.5706	583.1052	616.919
667.0326	734.9475	750.126
789.0801	801.8933	831.789
883.9550	904.0859	939.946
968.4893	994.7233	1009.359
1011.1206	1047.4807	1055.347
1124.5779	1135.5347	1154.730
1183.2437	1263.3626	1276.114

1298.4636	1328.1506	1348.530
1417.6645	1447.0418	1467.898
1487.6570	1490.1559	1494.223
1591.6255	1623.3971	1658.368
1690.3686	3044.0723	3110.212
3132.9904	3161.7088	3163.139
3178.2073	3185.0861	3191.863
3201.9877	3216.8443	3251.817

i47 – i49

C	-1.533128	1.299879	0.050883
C	-2.635333	0.470840	0.015967
C	-2.482855	-0.928946	-0.025206
C	-1.234333	-1.509187	-0.040758
C	-0.097666	-0.678539	-0.031187
C	-0.258519	0.726383	0.029398
C	1.057586	1.348415	0.053174
C	2.004277	0.189898	0.026904
C	1.293319	-1.004874	-0.032794
C	1.367032	2.709548	-0.146970
C	1.866388	-2.384386	-0.013107
H	-1.655285	2.376954	0.091555
H	-3.631689	0.897881	0.022989
H	-3.367637	-1.555899	-0.045031
H	-1.126143	-2.588197	-0.071012
H	3.076927	0.316644	-0.041612
H	1.605086	0.879445	1.134252
H	0.579321	3.449869	-0.166825
H	2.393359	3.046071	-0.214025
H	2.955162	-2.361322	-0.091448
H	1.483436	-2.981030	-0.846966
H	1.606852	-2.914613	0.910292

Frequencies

-1468.1117	95.2003	142.1092
163.6442	217.1011	226.8593
262.0332	367.8149	400.2613
448.9835	524.7304	537.3108
549.0695	573.6500	586.8317
606.3197	658.7952	762.3036
768.5111	784.0042	802.2589
868.3898	880.0476	935.1661
964.3766	997.5771	1004.6013
1048.9192	1052.8994	1066.2519
1136.9699	1140.1918	1164.3428
1187.0331	1216.8126	1249.3919

1328.4216	1345.3461	1393.9809
1410.9130	1422.9082	1481.3688
1485.2282	1492.5195	1507.0312
1530.0610	1563.6577	1626.5273
1683.9021	1954.6320	3034.3762
3092.7639	3131.1313	3179.2686
3183.0040	3194.4716	3202.9220
3217.7913	3233.2210	3283.2838

i49 – i51

C	-1.661032	-1.281276	-0.216660
C	-2.709111	-0.387685	-0.000422
C	-2.455439	0.970041	0.190237
C	-1.157454	1.465408	0.162399
C	-0.106300	0.578908	-0.071735
C	-0.368331	-0.793012	-0.252080
C	0.935938	-1.515925	-0.406013
C	1.939124	-0.402552	-0.410868
C	1.324253	0.810287	-0.162922
C	1.575234	-1.866303	0.895153
C	1.984002	2.134555	0.025859
H	-1.858828	-2.339211	-0.352992
H	-3.730082	-0.751514	0.024656
H	-3.283991	1.648488	0.361730
H	-0.968561	2.523042	0.312907
H	0.991869	-2.273966	-1.185910
H	2.982833	-0.546358	-0.651813
H	1.179156	-1.458509	1.814353
H	2.419988	-2.541358	0.927909
H	3.061258	2.065574	-0.136267
H	1.818868	2.520968	1.038505
H	1.582185	2.878168	-0.670764

Frequencies

-595.5079	141.2930	154.7183
169.4794	213.4999	230.1594
350.1614	423.1513	434.2151
493.3893	535.4619	555.0562
567.8140	597.3303	635.8009
681.4087	757.9164	769.8786
784.9071	822.4328	830.4699
897.3081	950.2063	969.1359
1004.0674	1004.8778	1034.7802
1053.6338	1058.3588	1096.7217
1105.9309	1146.9275	1179.3260
1198.4485	1206.5800	1253.0713

1282.6674	1335.1095	1351.5088
1380.2425	1417.4779	1451.5132
1472.4425	1487.5819	1498.7089
1506.9088	1545.3863	1646.6341
1676.6002	3027.9459	3081.6407
3128.1047	3133.1943	3170.8589
3187.0495	3193.7860	3204.3300
3217.1406	3245.9221	3293.2978

i45 – i99

C	1.238626	1.430811	0.202525
C	2.501690	0.881248	0.261311
C	2.710185	-0.495621	0.038439
C	1.651014	-1.330810	-0.237552
C	0.360508	-0.783049	-0.314003
C	0.146322	0.603874	-0.098718
C	-1.266400	0.911014	-0.227803
C	-1.906861	-0.342754	-0.504169
C	-0.906508	-1.401671	-0.547614
C	-1.894332	2.131944	-0.083045
H	1.092123	2.490940	0.379265
H	3.353126	1.515079	0.483726
H	3.716133	-0.896780	0.089337
H	1.810010	-2.391345	-0.402754
H	-2.904527	-0.439736	-0.908767
H	-1.061971	-2.371799	-0.996222
H	-1.331931	3.033066	0.126334
H	-2.965830	2.227543	-0.208835
C	-1.911877	-1.388428	1.056938
H	-2.938823	-1.079269	1.270187
H	-1.224829	-0.910441	1.747295
H	-1.877680	-2.476602	1.142585

Frequencies

-1035.5746	131.1573	151.4057
170.1146	212.7999	257.6541
324.6475	431.7093	451.1122
513.5794	537.0679	548.5185
567.9900	574.8112	628.9602
688.8314	722.9223	762.0614
769.5453	791.3191	841.1907
882.6771	888.2761	898.1466
962.4954	979.2606	1006.3673
1006.9742	1023.5848	1046.5191
1080.0288	1117.7308	1164.9198
1178.4256	1235.7529	1256.7476

1283.8697	1331.3969	1359.6503
1365.0577	1393.2775	1434.1070
1447.8145	1481.0029	1495.0873
1520.7530	1542.5239	1616.9542
1676.7797	3039.5330	3100.4613
3166.7981	3184.1928	3191.1535
3203.3587	3215.0300	3216.6149
3229.7796	3243.6881	3259.9615

i31 – p8

C	1.469344	1.050760	-0.473709
C	2.824346	1.307140	-0.324897
C	3.674252	0.320531	0.161858
C	3.162874	-0.926948	0.500884
C	1.808666	-1.189785	0.355767
C	0.947515	-0.202189	-0.134041
C	-0.451858	-0.465857	-0.284808
C	-1.627790	-0.680379	-0.414832
C	-3.059030	-0.917003	-0.565338
C	-3.943907	0.047927	0.181433
C	-3.522814	1.087470	0.906765
H	0.802423	1.815534	-0.853787
H	3.218535	2.281335	-0.590649
H	4.732872	0.523360	0.276765
H	3.821864	-1.699218	0.880917
H	1.405233	-2.160106	0.619769
H	-3.293661	-1.938719	-0.242959
H	-3.319323	-0.878907	-1.631040
H	-5.009590	-0.131434	0.066283
H	-2.465805	1.258526	1.081420
H	-4.227887	1.712897	1.441081
H	-3.354238	2.626736	-0.502294

Frequencies

-539.9705	10.6824	52.9703
74.9999	122.9116	144.5733
218.2261	276.8577	330.5981
338.7694	383.5643	414.8185
416.7081	544.3359	555.6532
623.2141	633.8744	643.0095
715.4572	743.8161	786.3441
870.8147	903.5829	951.4482
953.4468	985.7456	995.9548
1003.9107	1023.5830	1024.4664
1027.2712	1062.7010	1097.1691
1111.7918	1188.5085	1209.1849

1240.3358	1288.2551	1318.8417
1325.3887	1355.9067	1372.7445
1439.2512	1464.2660	1488.4068
1543.0976	1648.8404	1678.9676
1681.4793	2381.5084	3028.9157
3059.3866	3154.6558	3172.2857
3187.8779	3196.9127	3206.6684
3214.1264	3219.7534	3251.6931

i31 – p6

C	1.423944	1.127453	-0.055157
C	2.781052	1.411537	-0.056936
C	3.712166	0.380876	0.001428
C	3.279593	-0.939183	0.061198
C	1.923957	-1.231125	0.062873
C	0.980519	-0.198929	0.004626
C	-0.417800	-0.491977	0.006186
C	-1.598836	-0.731626	0.003647
C	-2.996498	-1.026969	0.025005
C	-3.960692	-0.078540	0.133014
C	-3.741976	1.391925	0.041336
H	0.694266	1.927181	-0.100330
H	3.113823	2.442128	-0.104902
H	4.772722	0.604981	-0.000210
H	4.002691	-1.745488	0.105899
H	1.581798	-2.258140	0.109135
H	-3.260718	-2.066587	0.189837
H	-3.134945	-1.499880	-1.846498
H	-4.985708	-0.421672	0.239220
H	-4.233752	1.795838	-0.851070
H	-2.680532	1.638909	-0.008298
H	-4.182216	1.902070	0.903893

Frequencies

-862.8796	20.9530	56.5136
78.3346	118.8626	147.4117
210.7440	273.5054	355.9375
367.7963	380.6709	413.4662
428.8605	532.5884	547.6495
575.3063	640.8177	656.4572
710.4773	756.3668	776.3423
780.6066	867.2536	925.1739
943.8698	998.0237	1001.0496
1013.2258	1018.3490	1023.6955
1054.8935	1062.0654	1112.0270
1125.0151	1188.8613	1207.2604

1245.6850	1301.0799	1317.2651
1355.4522	1398.6647	1436.5852
1482.8111	1485.7231	1488.0404
1541.1049	1624.2542	1646.8946
1679.9154	2355.4408	3039.1084
3096.6361	3144.1796	3179.3863
3192.7934	3196.6264	3202.8198
3211.6165	3220.0678	3225.2773

i33 – i32

C	1.494285	1.184505	-0.180942
C	2.873221	1.281638	-0.257061
C	3.673077	0.160341	-0.053671
C	3.077952	-1.066225	0.227852
C	1.700386	-1.177548	0.307529
C	0.881149	-0.050757	0.102226
C	-0.521142	-0.156707	0.185332
C	-1.746524	-0.279743	0.144864
C	-3.191868	-0.367688	0.232698
C	-2.973535	-0.650425	-1.216405
C	-3.946000	0.895884	0.609439
H	0.872301	2.057594	-0.339174
H	3.330442	2.240082	-0.476133
H	4.751950	0.242559	-0.115393
H	3.694360	-1.944010	0.386942
H	1.237179	-2.132324	0.526387
H	-3.525355	-1.237179	0.801444
H	-2.876451	-1.666457	-1.570935
H	-3.003830	0.162335	-1.929526
H	-5.013115	0.765846	0.412905
H	-3.585782	1.745494	0.024507
H	-3.807704	1.126406	1.667816

Frequencies

-669.1794	49.8010	60.5082
71.3396	171.1023	206.9278
254.3898	337.2398	349.0718
382.7083	412.9554	467.0316
512.6827	539.1626	635.7845
648.6206	678.6677	704.7682
716.7766	768.8858	854.9019
866.1651	924.4709	927.4344
950.3114	993.6049	1010.2436
1014.2267	1055.7797	1086.8571
1111.3526	1156.2971	1172.4808
1183.3027	1203.1778	1233.5691

1300.8559	1311.5864	1353.5422
1379.4868	1421.2886	1452.9674
1483.1221	1499.0944	1504.7211
1529.9129	1626.1561	1653.6431
2104.7511	3054.6027	3098.4939
3136.5920	3141.3402	3177.7909
3191.9696	3201.1085	3211.2659
3219.6001	3224.8985	3298.5651

i31 – i32

C	1.433490	1.050375	-0.552652
C	2.781127	1.265320	-0.321120
C	3.571441	0.265205	0.238994
C	2.996811	-0.959892	0.566601
C	1.650696	-1.188999	0.340057
C	0.840506	-0.184518	-0.224616
C	-0.528590	-0.411924	-0.460643
C	-1.747872	-0.567219	-0.548157
C	-3.176180	-0.190660	0.585588
C	-3.160931	-0.780297	-0.786094
C	-3.443087	1.258273	0.819400
H	0.819650	1.829737	-0.988741
H	3.221570	2.222211	-0.578511
H	4.626186	0.438669	0.417458
H	3.605711	-1.744070	1.002792
H	1.204832	-2.143483	0.593735
H	-3.171281	-0.878377	1.421769
H	-3.463596	-1.823002	-0.873722
H	-3.594675	-0.167039	-1.576546
H	-4.511964	1.443372	0.994169
H	-3.143111	1.856215	-0.046086
H	-2.897783	1.631786	1.689526

Frequencies

-665.5123	42.6133	53.4018
87.5346	132.2622	163.9038
228.5052	314.0149	372.7295
388.7364	404.1478	414.0258
511.6650	550.2211	640.4357
680.4715	707.5395	713.1569
772.0772	851.6339	878.0344
919.3045	926.7549	989.3084
990.7775	1012.5834	1013.7047
1036.2109	1058.4005	1062.2160
1113.2655	1160.2238	1187.4634
1194.7085	1203.7799	1207.7610

1311.1547	1319.0170	1355.3868
1382.7312	1425.8102	1467.2780
1484.9383	1486.0943	1498.3588
1528.5801	1626.5393	1652.4473
2115.3033	3009.8159	3082.3037
3088.0069	3122.4525	3157.4708
3192.3590	3200.9072	3211.6969
3216.6783	3219.5144	3225.2186

i33 – p22

C	-1.612423	-1.153853	0.356291
C	-2.990756	-1.138410	0.508528
C	-3.720524	-0.004612	0.169617
C	-3.064141	1.117459	-0.323426
C	-1.685920	1.109764	-0.477280
C	-0.944050	-0.027921	-0.138649
C	0.476467	-0.039732	-0.294700
C	1.674099	-0.055156	-0.427003
C	3.097097	-0.063477	-0.585768
C	3.828654	-1.207718	-0.432852
C	3.544810	1.231001	1.211611
H	-1.039819	-2.035656	0.617974
H	-3.497894	-2.016001	0.892950
H	-4.797820	0.004443	0.289154
H	-3.628702	2.003833	-0.589400
H	-1.170537	1.982210	-0.860964
H	3.507532	0.743553	-1.184573
H	4.878346	-1.229325	-0.697963
H	3.396765	-2.091919	0.019381
H	4.625090	1.311727	1.173308
H	3.130526	0.606895	1.993615
H	2.976631	2.116166	0.948307

Frequencies

-547.4312	16.5056	58.4219
68.7967	118.5171	132.1207
200.4735	227.6175	309.9898
379.5007	414.5096	420.6912
503.1306	545.5949	553.5608
566.8985	593.4098	603.2563
643.9977	714.6012	722.9802
784.9654	828.5377	869.4597
882.2987	948.1575	948.9319
980.2998	1002.7858	1022.5648
1024.2211	1061.0542	1100.9365
1112.1434	1188.6016	1209.1890

1265.7363	1298.8004	1318.6298
1355.9594	1419.8968	1424.6436
1430.6641	1488.3830	1536.9050
1556.7032	1647.5718	1680.5269
2356.0787	3093.7591	3161.9336
3172.8618	3187.8434	3196.7168
3206.8256	3214.1881	3219.8338
3258.1065	3264.6708	3267.1173

i33 – p5

C	-1.711356	1.215678	-0.002417
C	-3.097341	1.173773	-0.026756
C	-3.761115	-0.047658	-0.032469
C	-3.032156	-1.231369	-0.012656
C	-1.646114	-1.197484	0.012661
C	-0.970778	0.028250	0.017272
C	0.457668	0.065196	0.040275
C	1.661542	0.103186	0.061396
C	3.097949	0.102347	0.053749
C	3.776465	1.263514	-0.132750
C	3.757892	-1.248811	-0.132825
H	-1.189484	2.165144	0.001964
H	-3.661357	2.099387	-0.041580
H	-4.844548	-0.077389	-0.052559
H	-3.545656	-2.185968	-0.016508
H	-1.073913	-2.117439	0.029013
H	3.237414	0.043681	1.934084
H	3.267125	2.218538	-0.124062
H	4.855393	1.258416	-0.234853
H	4.836313	-1.172861	0.014092
H	3.565212	-1.607145	-1.148323
H	3.357570	-1.984095	0.565842

Frequencies

-983.7598	23.6714	59.1127
71.1850	173.0675	198.8545
239.1432	292.0287	376.3943
413.1831	416.1928	474.1270
485.6223	526.0188	541.0259
568.7910	602.6211	643.1591
678.3068	698.7077	710.7327
781.1985	866.3620	872.3053
895.5673	945.8664	977.2620
1000.8497	1018.4404	1023.4105
1035.6924	1062.1232	1068.3738
1111.8817	1187.7473	1210.6203

1232.4282	1318.4542	1346.3031
1356.8499	1413.2746	1428.8564
1487.4831	1490.6613	1500.5915
1542.9204	1602.5147	1646.2359
1679.6310	2357.6982	3056.4708
3131.5089	3153.8087	3168.7437
3194.6638	3203.4476	3212.7311
3221.3932	3226.8620	3271.5421

i33 – i96

C	1.707684	1.209163	0.045501
C	3.093870	1.189398	0.063616
C	3.780241	-0.019258	0.025501
C	3.069240	-1.212962	-0.032237
C	1.683141	-1.202618	-0.053655
C	0.982803	0.010963	-0.014256
C	-0.441456	0.024992	-0.036087
C	-1.652195	0.033889	-0.050764
C	-3.063708	0.029191	-0.110620
C	-3.818484	1.307239	0.019273
C	-3.802773	-1.259362	0.155661
H	1.171728	2.150355	0.077769
H	3.641457	2.124031	0.109337
H	4.864041	-0.031113	0.041306
H	3.597799	-2.159095	-0.062449
H	1.128070	-2.132039	-0.100749
H	-3.478819	0.637868	-1.125008
H	-3.283237	2.242020	0.101663
H	-4.884051	1.259854	0.194839
H	-4.818929	-1.212303	-0.245367
H	-3.877156	-1.434097	1.234653
H	-3.291080	-2.109293	-0.297592

Frequencies

-1909.4085	30.1295	55.3156
68.4241	168.6578	187.1035
226.1026	280.5552	356.1449
413.3308	417.2276	442.6780
491.6901	515.6431	551.8944
595.4450	642.1061	652.3157
687.5386	709.6815	776.2825
852.4522	862.3439	936.4431
959.1604	996.8316	1013.4269
1019.4054	1020.6706	1048.4423
1061.4374	1111.0933	1185.9671
1200.2258	1213.1234	1244.1662

1272.1551	1315.6449	1356.3869
1401.3699	1416.2830	1432.3435
1485.8809	1492.9832	1504.5257
1544.5612	1640.8279	1673.9859
2221.9497	2294.7400	3038.5682
3107.0930	3144.3503	3178.9465
3193.0714	3200.9789	3212.2081
3218.6367	3225.1606	3307.3078

i51 – i53

C	-1.701191	-1.280266	-0.341112
C	-2.735963	-0.377764	-0.104873
C	-2.457403	0.936867	0.259382
C	-1.141698	1.371070	0.366482
C	-0.096338	0.479204	0.129605
C	-0.383493	-0.868386	-0.199928
C	0.808107	-1.704371	-0.345346
C	2.158944	-0.314285	-0.030795
C	1.315412	0.791576	-0.015248
C	1.814446	-1.573185	0.720842
C	1.772938	2.169019	-0.375235
H	-1.923874	-2.305571	-0.617459
H	-3.765220	-0.703537	-0.205068
H	-3.270363	1.630153	0.443334
H	-0.929161	2.406465	0.612066
H	0.920935	-2.421070	-1.149694
H	3.131969	-0.255007	-0.509034
H	1.430070	-1.424858	1.731764
H	2.610183	-2.313094	0.694990
H	2.819316	2.168429	-0.687717
H	1.689477	2.845494	0.483665
H	1.164106	2.595718	-1.179496

Frequencies

-676.5430	71.2855	126.9943
154.3227	222.0233	261.6420
375.5562	408.0414	449.4991
512.3344	528.5617	549.3821
585.5447	605.6812	658.3091
743.0524	766.3543	778.8249
821.0840	853.8852	889.9668
926.6917	963.0002	999.5056
1006.1147	1032.6545	1048.7249
1056.9476	1076.5792	1138.8903
1158.9956	1172.2764	1184.9052
1221.2681	1225.6466	1266.5118

1292.3080	1328.7371	1366.6327
1408.9348	1410.3187	1460.0961
1475.0287	1493.0890	1501.0979
1506.2555	1531.6377	1633.4690
1660.4125	3028.7232	3077.5689
3084.7106	3126.4984	3171.3540
3183.5168	3184.2958	3188.4394
3202.3871	3212.6881	3217.7109

i50 – i52

C	-1.344273	-1.381367	-0.410706
C	-2.572012	-0.891986	0.032205
C	-2.704096	0.439297	0.417930
C	-1.616448	1.301428	0.348324
C	-0.383980	0.823978	-0.095095
C	-0.244352	-0.537818	-0.457484
C	1.119046	-0.908582	-0.848653
C	1.964638	0.846763	-0.630177
C	2.218248	-0.487220	0.040690
C	0.810907	1.581590	-0.389966
C	2.073910	-0.590539	1.549818
H	-1.245913	-2.421380	-0.703761
H	-3.429186	-1.554402	0.075048
H	-3.663979	0.809625	0.759788
H	-1.728458	2.346828	0.616542
H	1.312372	-1.506476	-1.731851
H	2.763962	1.263144	-1.234867
H	3.174778	-0.889574	-0.291151
H	0.757123	2.637583	-0.628303
H	2.124588	-1.637517	1.861720
H	1.123850	-0.178786	1.893652
H	2.881322	-0.042312	2.041866

Frequencies

-684.7991	115.0431	144.1635
200.3235	280.8309	300.5275
369.9991	419.3908	482.6664
501.9152	536.7530	561.9654
627.0293	653.0418	692.9554
718.6369	763.7727	796.7554
799.8517	838.0830	851.4265
884.8891	906.5849	955.9012
965.7276	999.4415	1056.7868
1067.7402	1076.8425	1117.0974
1141.1304	1181.2889	1200.8412
1224.7958	1228.2512	1243.8330

1286.5463	1328.1245	1369.9292
1388.0193	1424.2485	1427.5561
1465.1727	1500.2155	1501.6808
1506.6441	1521.1678	1635.6840
1659.3430	3051.2041	3118.6186
3122.3813	3151.6361	3185.1957
3185.8299	3194.4051	3203.9880
3204.8711	3208.7137	3215.4972

i44 – p31

C	0.398152	-1.490136	0.018199
C	1.758849	-1.794473	0.019265
C	2.715530	-0.785824	-0.014914
C	2.333372	0.553195	-0.047748
C	0.982459	0.858119	-0.049317
C	0.007995	-0.158700	-0.017948
C	-1.316729	0.497028	-0.040971
C	-1.045905	1.934010	-0.104110
C	-2.547966	-0.039308	-0.015604
C	0.292026	2.156728	-0.076105
C	-2.882901	-1.497677	0.043944
H	-0.328039	-2.291995	0.041828
H	2.073636	-2.831545	0.046511
H	3.768535	-1.044173	-0.013659
H	3.079673	1.339731	-0.067074
H	-1.820002	2.687996	-0.150314
H	-3.383460	0.656107	-0.041969
H	0.784104	3.109970	-0.212176
H	0.556602	2.626695	1.930834
H	-2.451270	-1.966910	0.933842
H	-2.487576	-2.029425	-0.827772
H	-3.961488	-1.654216	0.071808

Frequencies

-630.3154	74.4050	171.6369
186.5212	201.8108	215.4269
279.6332	301.8320	358.6005
387.8545	432.4427	493.4533
529.4867	583.5850	605.3709
649.7322	725.9460	756.6908
763.5177	772.2645	819.1738
868.5941	877.2486	900.9849
966.1169	972.4703	1004.1453
1010.6395	1056.9916	1065.3989
1087.7732	1104.1761	1125.8595
1153.1118	1189.6678	1216.9104

1231.1831	1322.1686	1346.8783
1388.4239	1406.9196	1422.9540
1493.2141	1503.0036	1505.8970
1510.8942	1565.3914	1659.4181
1688.6724	1725.1113	3044.2227
3103.1013	3144.2029	3172.9150
3188.2261	3202.6979	3214.2009
3228.2812	3243.0891	3248.4844

i44 – p33

C	-0.403315	-1.472788	0.070097
C	-1.756548	-1.794739	0.040439
C	-2.727187	-0.800727	-0.033975
C	-2.358387	0.541645	-0.062488
C	-1.013583	0.864877	-0.031903
C	-0.029453	-0.133517	0.017000
C	1.294172	0.528777	0.055766
C	1.100915	1.863298	0.065890
C	2.614469	-0.090794	0.058812
C	-0.353724	2.215831	-0.007154
C	2.923126	-1.334137	-0.332691
H	0.333550	-2.260393	0.158218
H	-2.057474	-2.835553	0.082317
H	-3.776419	-1.072600	-0.058470
H	-3.114703	1.318676	-0.100080
H	1.891784	2.602529	0.097312
H	3.420354	0.557629	0.394840
H	-0.676496	2.811793	0.854642
H	-0.582170	2.805582	-0.902891
H	2.190357	-2.009451	-0.755485
H	2.674523	-2.576518	1.530505
H	3.953790	-1.668061	-0.339666

Frequencies

-456.6783	74.9343	121.6257
166.7329	206.2750	220.7562
235.7667	281.2105	359.9108
424.8658	451.0124	497.7001
516.9643	579.0060	613.4485
694.4579	716.2260	739.9652
762.1994	789.2326	826.7831
855.3861	889.1824	947.9728
953.4389	977.7150	992.2708
1006.4566	1022.8222	1032.4193
1067.5877	1114.6116	1158.5900
1161.0701	1189.6951	1206.0949

1243.2803	1276.3358	1331.0752
1333.8100	1355.0865	1406.5894
1437.9011	1451.0782	1506.8458
1520.5986	1636.4651	1657.4414
1687.3728	1700.2871	3044.3167
3078.2827	3163.1430	3175.0630
3186.7969	3198.2184	3211.1415
3227.4886	3228.9133	3262.9494

i46 – p31

C	0.470681	-1.469130	0.079133
C	1.840841	-1.726687	0.074348
C	2.763411	-0.687509	-0.001403
C	2.336832	0.635453	-0.068434
C	0.973704	0.897756	-0.064036
C	0.033895	-0.154137	0.002052
C	-1.310704	0.453227	-0.012745
C	-1.081956	1.912751	-0.029976
C	-2.519731	-0.121386	-0.046299
C	0.249625	2.161773	-0.110850
C	-2.807397	-1.591018	-0.077265
H	-0.227612	-2.293081	0.148062
H	2.191911	-2.750689	0.133543
H	3.824364	-0.910953	-0.002768
H	3.056791	1.445003	-0.119113
H	-1.876268	2.637990	-0.142753
H	-1.358943	2.260699	1.990026
H	-3.378119	0.546199	-0.047162
H	0.714310	3.135878	-0.180399
H	-2.518953	-2.068438	0.865490
H	-2.252981	-2.088746	-0.878332
H	-3.869706	-1.780420	-0.233747

Frequencies

-620.4005	72.7478	135.2662
169.9253	195.5952	230.8187
275.5097	308.9354	359.0470
381.3504	438.5962	491.2382
529.4277	572.7351	603.8475
659.9040	723.8115	752.2926
763.2943	776.0400	825.9277
866.7676	879.2284	900.7782
959.7387	967.1849	1003.6538
1007.3461	1062.3384	1064.0577
1084.0921	1100.2962	1125.7640
1148.9048	1188.8759	1215.5413

1236.4994	1320.6367	1344.1698
1387.5093	1405.7301	1423.5595
1494.2577	1496.6350	1501.9579
1506.4612	1565.6691	1654.2850
1682.2878	1752.3128	3041.8450
3101.7137	3141.2214	3168.5367
3190.3089	3202.4413	3214.2590
3226.8377	3231.9858	3246.5155

i46 – p37

C	-0.390004	-1.495341	0.075768
C	-1.707117	-1.801906	0.042820
C	-2.729734	-0.780744	-0.048785
C	-2.415966	0.532279	-0.071640
C	-1.028586	0.922066	-0.022715
C	0.012203	-0.114352	0.020220
C	1.244043	0.483702	0.048490
C	1.030760	1.972150	0.063829
C	2.571182	-0.096692	0.082981
C	-0.448166	2.146240	-0.001518
C	2.943295	-1.294753	-0.386200
H	0.354998	-2.275387	0.168896
H	-2.020419	-2.838661	0.097449
H	-3.767637	-1.092995	-0.084112
H	-3.185789	1.294339	-0.120424
H	1.450965	2.417875	0.976155
H	1.540194	2.461125	-0.777210
H	3.341992	0.538445	0.517504
H	-0.952004	3.102625	-0.029537
H	2.255410	-1.950803	-0.906239
H	2.518088	-2.868729	1.647269
H	3.972731	-1.623729	-0.309250

Frequencies

-245.7729	81.1835	108.5853
128.5521	164.5030	189.7943
199.9445	255.9046	337.6457
388.1080	462.3537	482.2366
519.7520	529.7074	586.0555
673.9614	680.8979	702.3287
739.6679	772.6630	786.6807
862.1700	888.8596	895.0167
931.5170	972.1760	996.6846
1003.5393	1012.4713	1015.4389
1025.4436	1119.1719	1131.7558
1140.8712	1174.1457	1201.5443

1228.5025	1253.8968	1325.9848
1339.7744	1402.9088	1404.9576
1416.4090	1460.9053	1478.6980
1510.5452	1608.9144	1641.1231
1680.0795	1723.4144	3034.8448
3068.4593	3146.8032	3173.5160
3187.9518	3199.8759	3213.5072
3225.9966	3243.5575	3263.1253

i48 – p31

C	-0.460649	-1.452333	-0.145619
C	-1.824949	-1.725559	-0.064182
C	-2.751281	-0.697006	0.075684
C	-2.334328	0.630129	0.131698
C	-0.977506	0.906809	0.052362
C	-0.037031	-0.133686	-0.077646
C	1.308684	0.494154	-0.123247
C	1.057868	1.950256	-0.045544
C	2.524521	-0.067262	0.104278
C	-0.258686	2.182503	0.071142
C	2.811189	-1.528881	0.208389
H	0.241756	-2.264908	-0.279213
H	-2.168260	-2.752443	-0.118344
H	-3.808229	-0.931051	0.136172
H	-3.058463	1.431297	0.232625
H	1.308861	0.461466	-2.046218
H	1.848786	2.687828	-0.058433
H	3.371006	0.611983	0.160711
H	-0.732796	3.150496	0.163550
H	2.664231	-2.023010	-0.760047
H	2.145480	-2.017951	0.925759
H	3.840633	-1.708456	0.519545

Frequencies

-880.2638	88.5575	147.9657
178.5361	220.0060	239.3437
317.2452	348.5366	368.4896
428.7668	440.0443	490.7735
532.0875	580.0567	604.7183
639.4484	724.4477	737.7442
760.9182	774.2833	811.8361
834.2247	878.2522	898.0976
963.4861	972.8702	1003.7301
1006.0139	1045.7112	1061.3092
1086.2675	1105.0459	1123.4831
1152.6920	1187.2975	1208.7866

1232.0269	1315.9094	1343.4897
1382.0746	1404.3035	1418.7975
1487.4370	1500.0364	1507.2018
1508.7652	1623.2436	1653.8174
1665.7758	1687.5185	3029.3886
3095.5347	3143.6216	3175.3829
3189.5252	3200.0755	3214.2476
3225.8256	3230.6179	3251.6156

i48 – p35

C	-0.784674	-1.336075	-0.624573
C	-2.125752	-1.380342	-0.246611
C	-2.744654	-0.260184	0.301831
C	-2.039524	0.925726	0.483518
C	-0.702121	0.968026	0.110134
C	-0.079854	-0.160371	-0.439199
C	1.356152	0.171192	-0.762530
C	1.449794	1.623349	-0.327275
C	2.412318	-0.669490	-0.089852
C	0.284630	2.051800	0.168144
C	2.207409	-1.538582	0.905674
H	-0.303774	-2.210677	-1.049938
H	-2.691685	-2.295217	-0.380921
H	-3.788970	-0.313818	0.588642
H	-2.525822	1.797438	0.907624
H	1.513180	0.114010	-1.849330
H	2.364416	2.196662	-0.404666
H	3.430493	-0.479122	-0.421933
H	0.084617	3.041941	0.557280
H	3.033573	-2.099033	1.327383
H	1.208629	-1.796179	1.239831
H	2.273000	-0.326295	2.610465

Frequencies

-536.7309	76.7689	86.7587
147.2708	192.4754	251.8034
280.1236	333.9644	385.6038
432.9803	467.5611	524.4120
568.5134	582.4815	642.0399
695.0298	728.0318	758.8387
767.4168	797.4874	869.9315
879.8994	913.2661	964.8895
969.2207	979.0087	982.7117
1011.9703	1014.2590	1029.6647
1055.8520	1088.8483	1096.2115
1145.0829	1182.1503	1192.8417

1221.9625	1235.8761	1307.1578
1317.9413	1331.7210	1361.4391
1394.8061	1442.3751	1505.9362
1516.4702	1640.4737	1666.9712
1679.7068	1692.6293	3025.9985
3159.7037	3171.8476	3189.4887
3197.0758	3207.8157	3219.3596
3219.7892	3243.8103	3258.6507

i45 – p27

C	1.249489	1.443020	0.355529
C	2.490128	0.810123	0.307616
C	2.596249	-0.511258	-0.117692
C	1.465543	-1.231041	-0.498007
C	0.232119	-0.601562	-0.450296
C	0.125247	0.732908	-0.029142
C	-1.301733	1.121560	-0.108458
C	-2.001883	-0.050132	-0.616584
C	-1.124901	-1.091434	-0.762586
C	-1.837208	2.309233	0.209293
C	-1.386626	-2.380277	1.215262
H	1.173488	2.474657	0.682757
H	3.382125	1.351682	0.601333
H	3.570570	-0.985723	-0.152194
H	1.552799	-2.262614	-0.822211
H	-3.064327	-0.079574	-0.815828
H	-1.327938	-2.015412	-1.285757
H	-1.226236	3.128463	0.571409
H	-2.901372	2.489127	0.107355
H	-2.422848	-2.683566	1.131018
H	-1.148773	-1.593844	1.919922
H	-0.626041	-3.130037	1.032586

Frequencies

-428.6752	86.2743	92.7482
114.1195	132.8947	221.1825
266.7658	332.3411	413.4843
447.1833	480.2036	496.9114
543.1180	562.2816	574.0429
633.7885	667.9930	726.8781
766.6012	769.3846	786.4601
800.5708	822.0672	873.8584
887.8294	919.5852	926.4407
957.7967	959.8509	1002.5558
1054.9247	1078.1175	1112.9308
1153.6909	1187.7694	1220.8757

1249.1762	1333.8570	1342.8727
1392.3428	1412.5374	1419.0823
1447.1416	1472.4291	1508.3665
1526.9431	1661.8448	1681.7069
1688.4746	3102.9373	3163.2819
3187.7368	3194.9145	3204.9828
3218.1352	3229.8927	3247.9419
3254.4869	3271.1568	3282.0468

i45 – p28

C	-1.602348	1.244591	-0.021076
C	-2.670060	0.348075	-0.020917
C	-2.445275	-1.025188	-0.005076
C	-1.148414	-1.535797	0.015619
C	-0.089076	-0.643853	0.016972
C	-0.314468	0.740035	-0.005718
C	1.004376	1.410291	-0.017713
C	1.991921	0.334052	-0.026187
C	1.373462	-0.879366	0.039369
C	1.248588	2.724998	-0.022145
C	1.993106	-2.227330	-0.157404
H	-1.784918	2.313791	-0.038930
H	-3.686524	0.724707	-0.035897
H	-3.289319	-1.705720	-0.007474
H	-0.978233	-2.606900	0.033552
H	3.061563	0.494662	-0.058938
H	1.474589	-0.993147	2.037546
H	0.444039	3.451791	-0.019287
H	2.262882	3.107866	-0.029889
H	3.070139	-2.194797	0.013023
H	1.815071	-2.565304	-1.183966
H	1.559842	-2.969994	0.515918

Frequencies

-783.3857	124.5575	156.0722
176.1964	219.5582	229.9899
267.8877	328.5694	413.1623
428.3309	447.5934	529.0203
539.4857	549.0599	594.3730
619.8915	647.7165	676.2877
758.8624	774.5261	794.9824
803.6497	843.4665	889.0370
938.1121	959.2659	966.5399
1006.8222	1007.8165	1055.7143
1055.8710	1079.4508	1142.3846
1157.8182	1185.7980	1228.8401

1261.4467	1336.8695	1343.1082
1392.1155	1417.5307	1449.7027
1490.4027	1491.2410	1505.0882
1510.9243	1594.4202	1663.8242
1688.2147	1714.4678	3048.0204
3115.7978	3148.3650	3166.1179
3190.0860	3197.1707	3207.2923
3219.3514	3234.1163	3255.9264

i47 – p28

C	-1.564190	1.291794	0.018406
C	-2.665376	0.436630	0.033435
C	-2.493673	-0.945034	0.019764
C	-1.218615	-1.505186	-0.008051
C	-0.121888	-0.654859	-0.023988
C	-0.296706	0.739344	-0.013195
C	1.044729	1.358842	-0.039940
C	1.994392	0.230323	-0.018954
C	1.316779	-0.947060	-0.054007
C	1.340799	2.656921	-0.097714
C	1.883876	-2.323579	-0.073399
H	-1.706391	2.367146	0.031992
H	-3.666337	0.852159	0.057011
H	-3.363838	-1.591766	0.032356
H	-1.090229	-2.582348	-0.016358
H	3.064527	0.346817	-0.127164
H	2.436911	0.230038	2.033478
H	0.565134	3.413931	-0.128385
H	2.369560	2.998781	-0.112945
H	2.972237	-2.304894	-0.144295
H	1.489424	-2.895583	-0.919119
H	1.608246	-2.863096	0.839283

Frequencies

-525.0281	121.6235	130.8067
154.1443	182.5718	228.7505
262.9293	274.9450	287.6450
413.5154	425.5918	527.4357
537.5477	547.8409	594.7976
612.8010	661.4541	702.1573
761.7451	775.8089	797.0167
804.7289	882.6707	902.3342
949.4996	959.1067	962.1838
1003.8075	1006.4296	1056.3701
1058.0620	1081.9893	1144.7557
1155.7434	1186.7652	1225.7494

1263.0919	1335.4231	1346.7770
1389.4963	1418.3185	1453.3820
1480.7624	1488.4751	1505.3753
1509.3441	1621.2386	1663.7551
1685.0332	1746.8990	3041.3411
3101.4402	3143.9258	3164.3055
3187.3376	3195.9513	3205.0231
3218.5135	3232.6501	3253.8728

i47 – p32

C	-1.524319	1.302696	0.046401
C	-2.645372	0.486692	0.041108
C	-2.513912	-0.903300	-0.012545
C	-1.260122	-1.492342	-0.060992
C	-0.131159	-0.676228	-0.056177
C	-0.262871	0.715918	-0.002758
C	1.065382	1.352786	-0.007073
C	2.093920	0.237318	-0.081606
C	1.289574	-1.048925	-0.097068
C	1.327723	2.655691	0.043993
C	1.796895	-2.284787	-0.119852
H	-1.633047	2.380770	0.089327
H	-3.633916	0.930058	0.079426
H	-3.402150	-1.524904	-0.015968
H	-1.162617	-2.571514	-0.102612
H	2.704707	0.327139	-0.984477
H	2.771977	0.264549	0.776027
H	0.535597	3.394332	0.095242
H	2.346501	3.027015	0.036092
H	2.032524	-2.686539	2.184264
H	2.866514	-2.452827	-0.171653
H	1.159460	-3.161196	-0.146253

Frequencies

-289.1706	30.7022	101.9421
128.9227	166.1579	199.7978
275.5688	310.5389	396.5617
419.5238	482.1775	531.7703
538.5138	554.5909	592.4888
596.9583	688.5441	726.0683
750.5487	785.4841	803.2173
822.8494	890.6685	908.4290
916.1450	926.2601	956.6958
964.0816	976.1130	1011.7119
1062.4870	1100.5256	1149.3378
1161.4885	1192.3174	1194.7851

1248.6387	1277.5283	1318.5524
1344.6429	1366.1358	1448.5586
1459.0477	1461.9890	1514.8876
1518.2872	1652.4291	1682.2822
1711.9122	1749.8903	3067.4958
3107.8337	3160.5458	3161.7643
3187.7897	3198.0478	3206.9386
3218.5956	3246.9692	3248.3046

i49 – p28

C	1.532136	1.298724	-0.041958
C	2.644020	0.458949	-0.002223
C	2.488670	-0.923969	0.039457
C	1.220225	-1.500128	0.043778
C	0.112825	-0.665461	0.004324
C	0.273391	0.727311	-0.039288
C	-1.085160	1.330253	-0.055118
C	-2.014342	0.180453	-0.044131
C	-1.327612	-0.975339	0.002451
C	-1.396800	2.614205	0.238166
C	-1.868346	-2.364851	0.041080
H	1.659135	2.375290	-0.083110
H	3.639855	0.887186	-0.006224
H	3.366812	-1.559371	0.068364
H	1.105467	-2.578286	0.080011
H	-1.095864	1.403691	-1.949869
H	-3.091236	0.286244	-0.054162
H	-0.627092	3.369591	0.344776
H	-2.428888	2.931479	0.330098
H	-2.959352	-2.368073	0.040194
H	-1.521626	-2.891318	0.936006
H	-1.521251	-2.937310	-0.825316

Frequencies

-949.5196	130.6881	139.9771
158.9729	202.6355	226.2524
266.8281	334.0326	413.8920
415.8322	452.4712	525.8593
536.6886	550.7140	590.1870
605.8495	639.6966	652.9722
760.1042	772.8276	792.1115
796.5558	841.6897	889.5674
900.5918	957.9720	960.5623
1005.6451	1007.2040	1055.5274
1063.3268	1078.9793	1143.1857
1153.8743	1187.0139	1219.8577

1256.4153	1330.4539	1347.8317
1388.2580	1419.0754	1442.7925
1478.3391	1492.4137	1507.9832
1510.1010	1633.8892	1654.3770
1687.6924	1695.1098	3042.9884
3102.0136	3144.3144	3161.7601
3186.2019	3194.4365	3203.7543
3218.8381	3232.6663	3258.1401

i53 – p4

C	1.826055	-1.250139	-0.041946
C	2.776851	-0.266944	0.006788
C	2.387046	1.086342	0.054829
C	1.058022	1.426069	0.048904
C	0.048663	0.435519	-0.002336
C	0.445007	-0.930741	-0.043217
C	-0.541515	-1.942421	-0.094293
C	-2.269321	-0.240834	-0.058542
C	-1.349064	0.766325	-0.030131
C	-1.881325	-1.613357	-0.035363
C	-1.788106	2.205866	-0.033034
H	2.116884	-2.295017	-0.077185
H	3.829833	-0.524528	0.010228
H	3.143305	1.861932	0.095331
H	0.778022	2.472035	0.085350
H	-0.233259	-2.980997	-0.142890
H	-3.327274	-0.001760	-0.075682
H	-2.632916	-2.376422	-0.200783
H	-2.240979	-1.957532	1.774802
H	-2.875548	2.278431	-0.079430
H	-1.376964	2.745844	-0.891133
H	-1.454985	2.723896	0.871437

Frequencies

-893.6816	126.1121	163.8701
205.3305	240.8664	299.4558
318.4990	385.4732	428.6736
455.5643	485.4663	506.3849
522.9688	553.7236	581.5981
645.3074	720.9080	754.9427
790.7543	807.9613	839.9395
875.1226	881.8245	906.3060
979.2142	998.5966	1010.6662
1030.7469	1055.0982	1068.3807
1087.7518	1093.3002	1170.4426
1193.7845	1203.8208	1239.4722

1271.6119	1302.0693	1384.8328
1415.1594	1425.7534	1441.1657
1470.9190	1490.1668	1507.0471
1514.0811	1566.2487	1634.9253
1670.6001	1693.0604	3048.2280
3110.7982	3140.9169	3184.2411
3186.0370	3195.8034	3198.9527
3208.3729	3209.7675	3223.4720

i104 – i53

C	1.840146	-1.229474	-0.007895
C	2.791190	-0.221694	0.014034
C	2.387690	1.109180	0.022305
C	1.035879	1.425168	0.006821
C	0.050293	0.428754	-0.019317
C	0.468854	-0.940141	-0.024943
C	-0.509068	-1.990719	-0.048313
C	-2.286099	-0.288123	-0.015612
C	-1.361420	0.753596	-0.043207
C	-1.861064	-1.679116	-0.015853
C	-1.821665	2.180305	-0.014993
H	2.151318	-2.269202	-0.011447
H	3.846055	-0.471764	0.027602
H	3.126258	1.902438	0.042550
H	0.739159	2.467237	0.015433
H	-0.186458	-3.023811	-0.028861
H	-3.345962	-0.087470	-0.135893
H	-2.622139	-2.441920	-0.136410
H	-2.285867	-1.048756	1.133428
H	-2.911358	2.241749	-0.055935
H	-1.426051	2.748215	-0.864467
H	-1.493372	2.696878	0.895840

Frequencies

-1868.8082	114.9410	157.7267
213.3467	241.0352	301.0596
358.8421	442.5943	471.7549
500.0930	506.2244	514.7762
571.0740	609.2908	684.4614
710.0695	765.3908	774.2922
799.7142	811.2567	865.2205
871.1793	941.8134	980.0752
990.0884	1031.5168	1060.8859
1067.7535	1072.9908	1090.9931
1111.7979	1162.8412	1192.9068
1205.1943	1232.5021	1268.1025

1307.7049	1326.6260	1385.7408
1421.0692	1429.2736	1479.7137
1480.9549	1484.6726	1510.0778
1545.0093	1566.2435	1594.1159
1637.6000	1645.7939	3019.7315
3073.8666	3123.1952	3179.6596
3189.2555	3195.8467	3200.4707
3206.4750	3216.9593	3221.1268

i102 – p4

C	-1.880442	1.185277	-0.000707
C	-2.780850	0.154081	0.016970
C	-2.322658	-1.177709	0.024495
C	-0.978283	-1.449211	0.005760
C	-0.024211	-0.406585	-0.016082
C	-0.487060	0.935383	-0.011242
C	0.451520	2.000913	0.007092
C	2.262810	0.419774	0.054662
C	1.396479	-0.661048	-0.061606
C	1.794516	1.743534	0.059083
C	1.925640	-2.065415	0.114751
H	-2.224314	2.214585	-0.002354
H	-3.845486	0.357907	0.027588
H	-3.038685	-1.991461	0.042839
H	-0.644445	-2.479603	0.006791
H	0.082941	3.021318	0.006591
H	3.330391	0.232322	0.096836
H	1.489391	-0.711947	-1.943121
H	2.506414	2.559724	0.104591
H	3.006879	-2.084990	-0.028495
H	1.484183	-2.765996	-0.595698
H	1.707954	-2.425820	1.125387

Frequencies

-911.0310	122.9182	164.1884
218.5609	241.0660	282.4911
392.7454	424.3627	444.8392
460.5285	490.1216	513.4373
534.1505	554.4575	586.7337
643.7491	721.0954	741.9631
791.7671	805.9014	814.0667
874.9023	884.2639	912.2762
978.3155	994.5155	1000.5054
1012.1149	1054.3455	1061.9015
1084.2207	1114.6312	1172.1472
1189.6163	1198.8252	1241.0642

1264.2666	1294.2337	1373.5851
1406.6116	1417.4864	1430.7896
1473.0296	1495.2453	1502.1013
1508.7220	1564.6711	1636.5747
1652.3709	1695.8866	3052.7164
3123.9822	3147.7239	3186.8018
3190.5649	3198.6270	3200.3937
3212.3588	3217.1543	3224.0503

i52 – p3

C	1.433687	-1.510434	-0.005626
C	2.721366	-1.045474	-0.010180
C	2.978275	0.342193	-0.013117
C	1.939033	1.235778	-0.014100
C	0.598940	0.785984	-0.009369
C	0.337708	-0.610582	-0.001802
C	-1.001944	-1.061566	-0.001332
C	-1.783463	1.226838	-0.005624
C	-2.069769	-0.176983	0.069588
C	-0.504106	1.685662	-0.029341
C	-3.485389	-0.654199	-0.159518
H	1.234796	-2.577177	-0.001060
H	3.550257	-1.744220	-0.010036
H	4.002016	0.698724	-0.015948
H	2.132415	2.303634	-0.018935
H	-1.194093	-2.130221	-0.013405
H	-2.614219	1.924587	-0.015413
H	-2.249912	-0.206355	1.904095
H	-0.306634	2.752126	-0.066098
H	-3.623438	-1.673553	0.204561
H	-3.709500	-0.640274	-1.230901
H	-4.207717	-0.010575	0.345665

Frequencies

-948.2914	108.4776	125.2306
185.2217	262.4488	276.4721
380.2161	405.8197	431.8492
448.4004	484.7830	526.5966
528.5936	541.4535	635.1982
649.6706	718.5611	756.2389
780.8644	788.7425	832.5499
861.7935	897.6867	903.2083
966.7197	975.3305	997.6649
1011.9857	1033.1571	1055.0130
1062.3907	1155.5996	1171.8962
1192.2947	1199.4687	1235.2493

1285.1102	1301.7402	1388.9941
1405.6764	1419.7407	1430.4499
1472.3414	1492.3137	1501.6957
1508.8611	1555.9326	1631.2060
1669.6617	1697.4345	3051.6046
3124.7854	3150.4829	3186.5319
3187.3536	3187.8358	3192.5190
3206.1422	3207.3033	3219.6832

i52 – p38

C	-1.457828	-1.451077	-0.202144
C	-2.684385	-0.941519	0.133514
C	-2.839161	0.437993	0.380917
C	-1.759354	1.280249	0.283328
C	-0.482907	0.785658	-0.059087
C	-0.321687	-0.607418	-0.302480
C	0.953951	-1.103718	-0.651470
C	1.873934	1.144828	-0.510923
C	2.073634	-0.271209	-0.647541
C	0.650315	1.644063	-0.200956
C	2.997639	-0.687455	1.310861
H	-1.336878	-2.512810	-0.391394
H	-3.542507	-1.599901	0.209686
H	-3.814154	0.831696	0.644356
H	-1.877060	2.343608	0.466345
H	1.068044	-2.161564	-0.863720
H	2.724813	1.808202	-0.618837
H	2.990902	-0.622844	-1.105148
H	0.510931	2.711967	-0.066601
H	3.198312	-1.751913	1.251215
H	2.185034	-0.390351	1.963615
H	3.867658	-0.038464	1.306364

Frequencies

-564.3129	76.2944	121.7161
138.3768	195.6891	217.1149
370.3063	394.5560	459.7352
494.6156	509.0889	517.9771
558.4038	586.5433	620.9067
635.7958	754.0518	774.2597
779.3155	812.1581	822.9490
848.2168	888.6591	901.7275
950.6233	982.2742	992.3605
1003.8581	1011.9443	1027.0927
1055.9111	1146.4302	1168.2569
1172.3583	1188.5579	1226.6140

1273.5431	1298.9665	1393.6793
1413.2889	1421.2821	1422.6682
1430.6658	1484.7429	1496.8858
1551.2507	1614.4469	1658.7387
1683.3164	3088.1567	3184.4227
3185.8376	3188.8831	3190.9793
3202.0015	3205.1202	3214.3700
3219.9303	3245.4436	3259.4092

i52 – i102

C	-1.329030	-1.401288	-0.302834
C	-2.607824	-0.898227	-0.042941
C	-2.782105	0.443835	0.228096
C	-1.671284	1.301835	0.235721
C	-0.395093	0.825890	-0.016834
C	-0.214755	-0.561430	-0.289846
C	1.118806	-1.058937	-0.521588
C	2.024595	1.243418	-0.300833
C	2.269406	-0.148561	-0.485612
C	0.772770	1.708480	-0.040214
H	-1.194894	-2.455933	-0.521759
H	-3.459511	-1.569399	-0.053377
H	-3.770611	0.839656	0.430174
H	-1.809847	2.359885	0.434446
H	1.244052	-2.047383	-0.944710
H	2.863668	1.929334	-0.337986
H	3.195736	-0.470936	-0.943437
H	0.608054	2.765982	0.134800
C	2.111776	-1.085803	1.109936
H	1.712050	-2.083697	1.323701
H	1.636969	-0.353304	1.755285
H	3.190767	-1.129473	1.284568

Frequencies

-2559.0508	113.2564	138.8516
163.6488	255.7678	288.6503
362.4498	426.5912	492.1390
501.0479	519.0440	563.3611
579.7348	611.9909	732.5034
752.0400	764.0333	773.1543
793.6596	804.6512	845.6424
882.4284	932.6137	937.4173
946.6851	980.0777	992.5105
1009.3978	1037.9921	1068.3378
1121.6199	1135.0825	1161.5798
1182.3824	1213.1720	1230.4066

1302.2963	1322.4749	1342.0251
1351.3327	1423.3700	1443.4955
1448.9214	1486.2626	1499.9205
1514.0506	1549.8907	1619.4480
1643.6084	3005.3728	3057.6941
3180.7848	3186.0166	3188.2455
3198.6797	3199.3817	3204.9744
3208.2528	3216.8268	3219.2894

i104 – p4

C	1.867300	-1.210961	0.007917
C	2.789373	-0.197884	0.033175
C	2.359659	1.144055	0.030463
C	1.022882	1.443616	0.002846
C	0.042035	0.418870	-0.021173
C	0.481356	-0.934281	-0.019040
C	-0.479859	-1.984014	-0.057221
C	-2.256494	-0.350422	-0.013952
C	-1.355533	0.703473	-0.056031
C	-1.808752	-1.703382	-0.065716
C	-1.856346	2.119326	-0.071197
H	2.190921	-2.246831	0.009009
H	3.849315	-0.423923	0.055496
H	3.092911	1.942259	0.051515
H	0.710128	2.480896	0.003872
H	-0.129821	-3.010658	-0.083525
H	-3.310960	-0.145684	-0.164753
H	-2.542944	-2.499923	-0.090724
H	-2.945121	2.144012	-0.134226
H	-1.455170	2.677930	-0.921836
H	-1.562661	2.650273	0.840295
H	-2.730328	-0.258725	1.814445

Frequencies

-834.2682	127.8872	158.9104
176.1020	230.7502	298.8295
326.7200	361.3816	427.5506
451.5623	486.9123	502.2292
527.5422	551.8970	579.4601
655.6372	719.1551	753.1782
792.9248	808.3544	824.7924
878.0264	883.5115	972.0497
979.8417	993.4133	1011.4818
1015.9096	1054.6796	1066.1270
1090.0476	1096.9697	1172.3100
1201.3228	1202.6997	1238.9886

1269.3618	1302.5943	1380.8215
1411.7416	1424.2535	1440.7076
1469.6904	1489.1034	1507.0842
1509.0825	1569.0321	1638.9350
1666.6810	1693.9800	3044.7975
3107.6872	3141.5562	3184.5974
3189.5719	3194.3176	3199.5427
3210.8080	3220.6937	3223.4351

i104 – i102

C	-1.843995	1.216800	0.004245
C	-2.801161	0.202737	0.009172
C	-2.391503	-1.119736	0.008932
C	-1.034583	-1.433882	-0.011251
C	-0.059992	-0.430940	-0.044001
C	-0.484045	0.929191	-0.014036
C	0.509737	1.995821	0.035042
C	2.331356	0.395510	-0.025297
C	1.358224	-0.743123	-0.092062
C	1.839314	1.730522	0.060842
C	1.873263	-2.137921	0.101481
H	-2.157594	2.255740	0.025437
H	-3.856155	0.450682	0.021198
H	-3.125219	-1.917909	0.022483
H	-0.734883	-2.475079	-0.005051
H	0.153615	3.019014	0.076925
H	3.370682	0.161372	0.165371
H	1.970246	-0.147673	-1.116277
H	2.558630	2.538954	0.128421
H	2.950360	-2.183500	-0.076073
H	1.396724	-2.856075	-0.571059
H	1.693906	-2.475405	1.130216

Frequencies

-2096.6265	111.5925	151.0979
194.1526	219.7357	299.5236
366.2518	428.2400	455.1151
469.9454	499.2681	517.2682
561.1234	588.9304	698.1777
704.4637	760.8521	776.3020
794.1387	809.3793	851.1122
873.3150	938.7247	946.5527
964.7770	991.9699	1039.6472
1065.9477	1082.9762	1093.9177
1152.2987	1174.9230	1190.0493
1194.1862	1231.3418	1251.1683

1305.8566	1332.3541	1358.1464
1388.6709	1419.8894	1451.2910
1487.3973	1497.5660	1505.5284
1531.6118	1577.2646	1634.2265
1645.2134	2191.0868	3023.1282
3092.2291	3126.9118	3180.5853
3192.2131	3195.7363	3206.9173
3208.0376	3220.1551	3221.3837

i96 – p5

C	-1.676527	-1.200303	-0.000189
C	-3.062911	-1.211644	-0.023053
C	-3.772790	-0.016206	-0.029026
C	-3.089642	1.194482	-0.011469
C	-1.703273	1.214008	0.012251
C	-0.981439	0.014597	0.017809
C	0.446565	0.030151	0.041306
C	1.652394	0.056058	0.062350
C	3.079074	0.039475	0.083694
C	3.735102	-1.308819	-0.056572
C	3.778021	1.180433	0.199396
H	-1.119065	-2.129404	0.004270
H	-3.591556	-2.157864	-0.036645
H	-4.856591	-0.028261	-0.047869
H	-3.638969	2.128960	-0.016485
H	-1.166224	2.154883	0.025655
H	4.821063	-1.221257	0.002138
H	3.470576	-1.761785	-1.016285
H	3.392273	-1.987053	0.729422
H	4.860630	1.162921	0.251723
H	3.282287	2.135818	0.317506
H	4.118132	1.749644	-1.992403

Frequencies

-391.7638	31.2269	56.2275
65.6149	146.2334	157.8692
177.4630	183.8642	242.3279
296.9072	383.6951	413.3893
470.0612	499.5335	536.9077
577.5785	601.6439	642.7940
696.6494	710.6141	774.6260
781.9817	866.6135	878.2967
943.0573	946.5565	987.0704
1001.2702	1018.7642	1022.7793
1034.1115	1061.9909	1073.1891
1111.7373	1187.6796	1210.9811

1235.1206	1318.4160	1356.5768
1359.3100	1417.5302	1439.5506
1478.7457	1487.1187	1500.0275
1543.4259	1645.4317	1665.8900
1681.0765	2344.7947	3052.3380
3120.6725	3145.7773	3166.6374
3195.6187	3204.2678	3213.8826
3221.4111	3227.2234	3263.2600

i37 – i36

C	0.743469	-0.300876	1.199452
C	2.097937	-0.530735	1.194481
C	2.839530	-0.460961	0.006406
C	2.182095	-0.182246	-1.199524
C	0.827825	0.050386	-1.232603
C	0.060749	0.061943	-0.014827
C	-1.422159	0.188916	-0.041696
C	-1.014646	1.514277	0.106323
C	-1.004204	2.823901	0.161693
C	-2.474803	-0.621724	-0.040276
C	-2.371491	-2.109603	-0.126721
H	0.170613	-0.364137	2.117919
H	2.597221	-0.781710	2.124345
H	3.907127	-0.643504	0.017416
H	2.745380	-0.166475	-2.126591
H	0.319888	0.251364	-2.169093
H	-1.919959	3.406866	0.065393
H	-0.077874	3.373113	0.306390
H	-3.465116	-0.179451	0.034024
H	-2.814795	-2.581586	0.756026
H	-1.330508	-2.428219	-0.204690
H	-2.917798	-2.485922	-0.997385

Frequencies

-559.9778	38.6156	74.8862
119.9853	127.0162	160.6339
214.6628	218.2673	339.3032
411.5603	421.5048	428.5271
437.9218	539.9590	620.6138
666.6501	674.8144	721.8160
726.1446	809.4147	859.0504
871.8560	881.3157	914.2665
979.6439	989.8820	992.6758
1016.3513	1031.4368	1060.3735
1068.7945	1106.1579	1118.2351
1163.2128	1165.5774	1209.4797

1305.9051	1340.4449	1356.3650
1418.5209	1439.5534	1456.3914
1481.5453	1485.5221	1494.8320
1567.3497	1607.8568	1717.1964
1905.1227	3043.7376	3102.6835
3103.2642	3140.4886	3171.8050
3186.3400	3190.5515	3193.4559
3206.1836	3209.0012	3222.2449

i37 – i38

C	0.738544	0.226356	1.270097
C	2.019595	-0.267528	1.202552
C	2.707725	-0.330632	-0.016812
C	2.091882	0.151589	-1.180935
C	0.810793	0.647005	-1.151707
C	0.054388	0.635669	0.072359
C	-1.578283	-0.127540	-0.007597
C	-1.308814	1.232593	0.125978
C	-1.853802	2.440287	0.056249
C	-2.110807	-1.326667	0.001420
C	-1.341688	-2.588211	-0.265909
H	0.212833	0.285309	2.216266
H	2.510079	-0.596036	2.112678
H	3.716697	-0.722730	-0.055119
H	2.636943	0.144144	-2.118865
H	0.336764	1.025181	-2.050412
H	-2.926486	2.566042	-0.031258
H	-1.229044	3.325282	0.078022
H	-3.177180	-1.432744	0.215576
H	-1.432185	-3.279766	0.577620
H	-0.285499	-2.371234	-0.431509
H	-1.740116	-3.100978	-1.147168

Frequencies

-560.6243	50.8814	68.8274
107.0426	143.8680	162.5123
187.0027	258.5164	327.6514
386.7737	420.0322	474.6333
547.0463	572.0472	626.5943
669.8696	716.3454	721.6295
740.8430	802.6509	805.4316
814.9195	853.5901	927.0606
975.5023	984.7351	989.1075
1013.1250	1031.7185	1062.3852
1088.7893	1108.7601	1112.2393
1168.2002	1182.5338	1219.5970

1307.0801	1311.1227	1343.8449
1412.3538	1440.1091	1457.6942
1486.3292	1490.8321	1493.0110
1568.8410	1609.2112	1713.0881
1908.9284	3044.1324	3091.9312
3106.0038	3148.6308	3161.3409
3188.6479	3192.9953	3209.3309
3212.0980	3223.2711	3258.4896

i3l - p7

C	-1.740345	1.188671	-0.044003
C	-3.118708	1.340332	-0.038774
C	-3.945915	0.224090	0.015998
C	-3.387616	-1.048230	0.066556
C	-2.010249	-1.207912	0.061350
C	-1.170797	-0.088967	0.005982
C	0.248711	-0.250711	-0.002053
C	1.445858	-0.386663	-0.015477
C	2.861861	-0.566111	-0.011157
C	3.737548	0.466582	0.036961
C	5.215200	0.297770	0.128623
H	-1.091292	2.055239	-0.086865
H	-3.550222	2.333926	-0.079211
H	-5.023024	0.346021	0.019570
H	-4.028868	-1.921287	0.108716
H	-1.569952	-2.197092	0.099832
H	3.062608	-1.125693	-1.857565
H	3.218921	-1.574519	0.182580
H	3.349992	1.477134	-0.056945
H	5.493878	-0.751945	0.242203
H	5.621795	0.858677	0.976103
H	5.702880	0.686436	-0.772453

Frequencies

-850.7694	32.8134	52.8563
67.2349	151.4239	159.0965
167.4719	277.1008	309.7757
356.3744	393.6998	413.2516
437.0011	484.4989	534.5897
560.1329	591.2949	643.5678
710.2895	756.9197	779.7878
826.6221	867.1328	925.1795
943.6744	1001.1374	1006.5141
1017.5447	1023.9457	1045.0345
1059.1302	1068.0286	1112.1677
1136.1587	1189.1004	1207.0926

1285.4442	1306.5209	1316.8358
1330.5687	1355.6232	1417.4150
1479.4231	1488.0934	1489.1002
1540.6455	1642.9805	1646.8658
1680.4558	2357.2655	3039.1019
3097.6869	3135.4744	3166.5731
3184.0654	3191.9652	3200.8464
3211.0305	3219.8064	3224.9003

i97 – i44

C	0.558875	-1.485708	-0.236744
C	1.921056	-1.721568	-0.079197
C	2.803854	-0.667795	0.144601
C	2.340525	0.645100	0.215030
C	0.986383	0.883190	0.059362
C	0.099812	-0.176980	-0.164629
C	-1.269682	0.368852	-0.289770
C	-1.206277	1.703450	-0.143341
C	0.205985	2.169389	0.087309
H	-0.131308	-2.303915	-0.414555
H	2.302084	-2.735439	-0.132500
H	3.861920	-0.870825	0.266215
H	3.034281	1.461324	0.388816
H	-2.053704	2.375864	-0.185926
H	0.537397	2.867413	-0.690251
H	0.311195	2.690335	1.046105
C	-2.458478	-0.462038	-0.509484
C	-3.166658	-1.087299	0.643087
H	-2.716266	-0.746485	-1.524446
H	-3.499919	-0.326546	1.360323
H	-2.501466	-1.759388	1.205117
H	-4.036585	-1.663893	0.323760

Frequencies

-154.7688	79.5633	103.2467
149.7903	200.1205	217.1367
329.8434	337.5842	426.5264
481.3348	489.9067	551.6275
570.6963	641.0055	694.4469
743.7814	763.0414	790.7876
815.3922	855.0294	885.9698
952.5472	977.1980	978.5165
987.2238	997.4402	1009.4022
1053.0119	1101.1910	1115.0890
1150.0046	1162.5320	1182.0679
1203.1616	1237.0598	1267.3567

1303.7552	1327.3718	1363.6101
1384.6528	1415.7716	1451.4337
1472.2914	1491.3911	1506.0300
1510.3664	1653.2440	1683.6874
1688.5047	2996.6428	3047.1116
3050.3747	3084.8577	3126.0374
3184.0708	3185.7782	3191.9801
3203.0654	3216.4290	3226.3913

i97 – p30

C	-0.901489	-1.536146	0.037456
C	-2.294115	-1.509790	0.029790
C	-2.983343	-0.300457	-0.020395
C	-2.295740	0.909150	-0.061079
C	-0.909356	0.883073	-0.054445
C	-0.212776	-0.335296	-0.006999
C	1.235016	-0.030764	-0.024143
C	1.328773	1.427424	-0.101019
C	0.082526	1.968370	-0.087083
H	-0.375582	-2.484429	0.074677
H	-2.847724	-2.441364	0.062226
H	-4.067591	-0.302890	-0.026056
H	-2.834038	1.850071	-0.093458
H	2.253031	1.984940	-0.149735
H	-0.067944	2.514652	1.916475
H	-0.155624	3.013088	-0.234677
C	2.233425	-0.925600	0.017797
C	3.695765	-0.626408	0.001262
H	1.967138	-1.979367	0.069965
H	3.904782	0.442205	-0.052188
H	4.175119	-1.112893	-0.854589
H	4.176306	-1.025341	0.900504

Frequencies

-631.7849	90.3143	133.4715
177.5693	182.0440	234.1893
250.2292	289.0946	347.0867
379.2028	431.3305	476.7775
563.2624	581.0029	614.6464
644.7216	709.1539	753.6306
772.2246	776.0639	821.1178
870.5959	876.1519	895.4105
962.0371	973.6086	992.9041
1002.9941	1033.9464	1059.4501
1064.4684	1101.3332	1139.1855
1162.2273	1188.2845	1220.5322

1255.5173	1323.8639	1346.4774
1363.7076	1418.4845	1430.6102
1480.5339	1495.8234	1498.9046
1510.4227	1556.9126	1660.5539
1689.1656	1736.7918	3045.0266
3099.8486	3147.5599	3165.4569
3189.3593	3197.2396	3207.1623
3219.4893	3232.2661	3254.2122

i46 – i98

C	-0.639768	-1.530600	0.224078
C	-1.969780	-1.690601	0.063178
C	-2.853073	-0.559204	-0.163956
C	-2.389843	0.706545	-0.223136
C	-0.975048	0.945783	-0.058134
C	-0.081593	-0.201198	0.169217
C	1.200628	0.231216	0.295928
C	1.190133	1.734356	0.149249
C	-0.245660	2.084385	-0.071762
H	0.015806	-2.377539	0.396073
H	-2.408307	-2.681611	0.103541
H	-3.912764	-0.754198	-0.287831
H	-3.060858	1.541626	-0.392312
H	1.601853	2.219992	1.043958
H	1.825406	2.051953	-0.688815
H	-0.614948	3.090688	-0.215456
C	2.409198	-0.564368	0.503789
C	3.249822	-0.998140	-0.650341
H	2.771204	-0.727334	1.515222
H	3.760220	-0.143880	-1.121368
H	2.634391	-1.455731	-1.433687
H	4.017890	-1.713008	-0.347996

Frequencies

-236.7259	99.3180	102.5973
140.9662	182.4386	203.9766
295.2618	333.4549	412.4452
475.1522	486.0766	517.5446
553.9330	564.3011	674.1409
706.1850	734.7475	767.1226
786.4451	857.0533	880.0065
888.7157	955.1443	983.4612
986.8712	994.8726	997.9694
1015.8224	1046.9219	1093.6198
1125.7705	1145.7027	1181.1061
1199.6709	1205.7158	1240.4831

1298.4858	1366.3336	1398.8083
1399.8358	1406.8675	1421.2371
1475.5616	1477.1379	1490.3942
1596.2654	1619.8856	1651.9991
1734.0870	2987.6254	3039.2036
3057.7048	3073.4050	3126.4034
3168.2991	3187.7937	3196.0655
3209.3932	3217.8136	3237.5965

i98 – p30

C	-0.945567	-1.514897	0.038675
C	-2.337464	-1.466754	0.045544
C	-3.009720	-0.246315	0.006761
C	-2.305681	0.952202	-0.038826
C	-0.916635	0.907590	-0.047601
C	-0.238166	-0.325195	-0.011710
C	1.211516	-0.044060	-0.030995
C	1.323183	1.428350	-0.041925
C	0.079079	1.971255	-0.092025
H	-0.433740	-2.470919	0.072613
H	-2.904913	-2.389813	0.082181
H	-4.093869	-0.233185	0.014429
H	-2.830961	1.900657	-0.066322
H	1.764302	1.656357	1.984014
H	2.248861	1.971269	-0.166025
H	-0.148708	3.027404	-0.146535
C	2.197720	-0.947129	-0.048845
C	3.662214	-0.658707	-0.044368
H	1.921242	-1.999567	-0.059869
H	3.877823	0.409180	-0.004025
H	4.138835	-1.075101	-0.937774
H	4.138240	-1.134323	0.819202

Frequencies

-571.3002	87.9944	126.3679
166.5783	183.4941	232.2300
275.6501	292.6239	343.6395
357.4157	433.2452	477.8957
564.1562	570.1432	613.9503
669.8061	705.6005	746.3136
770.3710	777.0192	823.3176
871.2270	880.0965	896.4735
957.0737	964.2723	992.8018
1002.6922	1027.0419	1059.0425
1066.4114	1105.5235	1142.1165
1162.2132	1186.9886	1225.8238

1257.6003	1324.4276	1349.5431
1361.8016	1419.4165	1430.4279
1479.9842	1493.3661	1498.5609
1506.2430	1561.9168	1656.2985
1683.7023	1763.6855	3046.2772
3101.6792	3146.0023	3162.1735
3189.2189	3197.6984	3207.1851
3219.1381	3232.5223	3257.1357

i48 – p30

C	0.927862	-1.503260	0.089152
C	2.317570	-1.470508	0.003878
C	2.996215	-0.257744	-0.095194
C	2.301689	0.947920	-0.112094
C	0.916023	0.918039	-0.028590
C	0.234228	-0.305813	0.070563
C	-1.219677	-0.007695	0.126875
C	-1.309919	1.469718	0.078327
C	-0.076893	1.994103	-0.023561
H	0.408657	-2.451817	0.177042
H	2.877468	-2.398738	0.018386
H	4.078583	-0.255252	-0.159694
H	2.833105	1.890143	-0.190402
H	-1.271762	0.035117	2.035511
H	-2.236776	2.023998	0.108527
H	0.160982	3.047616	-0.089571
C	-2.210441	-0.903680	-0.111980
C	-3.667736	-0.601387	-0.181885
H	-1.931374	-1.950778	-0.202055
H	-4.103507	-1.005630	-1.100868
H	-3.876856	0.467823	-0.143109
H	-4.192048	-1.080637	0.653287

Frequencies

-895.6875	93.8844	113.8892
171.5081	186.8555	237.7588
322.3641	328.7601	354.3750
425.0007	452.8136	480.7838
563.5109	575.4557	616.0450
639.2724	709.1624	742.4312
771.8755	777.8532	808.7176
843.0886	878.2340	898.0634
960.6580	969.3393	993.1238
1006.9954	1023.7215	1051.1624
1059.2644	1106.8912	1145.4717
1161.6692	1187.6388	1223.5041

1254.5752	1320.6885	1345.6740
1361.1134	1416.3103	1426.0936
1478.2847	1491.8152	1506.0144
1510.6238	1616.0953	1660.9534
1671.9278	1689.8754	3035.2494
3091.8616	3149.0173	3173.8057
3187.8445	3195.2118	3205.6230
3217.7202	3229.3088	3256.7333

i104 – p41

C	-1.784825	-1.253073	-0.178041
C	-2.787401	-0.305054	-0.039031
C	-2.452855	1.026554	0.178719
C	-1.118860	1.403584	0.241353
C	-0.099977	0.463470	0.090849
C	-0.440442	-0.888990	-0.104986
C	0.620703	-1.893138	-0.228334
C	2.297118	-0.236636	0.526203
C	1.331058	0.836449	0.089943
C	1.888060	-1.607842	0.063746
C	1.764723	2.034430	-0.326945
H	-2.040425	-2.294943	-0.342296
H	-3.828044	-0.603738	-0.093978
H	-3.230559	1.771160	0.303868
H	-0.864385	2.440830	0.428116
H	0.334762	-2.895307	-0.531703
H	2.349780	-0.248555	1.626111
H	2.653207	-2.375057	0.012550
H	2.117530	1.623646	-2.515105
H	2.819507	2.284647	-0.304410
H	1.081092	2.814940	-0.639627
H	3.303724	0.003843	0.175612

Frequencies

-417.8972	90.2839	123.4419
158.9679	177.0600	230.6461
304.5077	367.5419	405.1756
437.6391	494.2208	514.3470
543.2539	564.9984	600.3764
698.4777	720.8475	744.2067
791.8877	795.3193	827.2007
871.6742	913.7815	928.1188
936.7634	964.5054	987.8349
1004.2008	1015.2117	1019.1463
1073.6564	1118.0042	1161.0918
1193.3340	1199.8594	1217.2939

1240.3107	1289.6769	1334.7142
1337.8866	1366.9872	1429.7056
1447.4439	1463.9369	1501.9671
1532.3538	1639.5439	1671.7766
1689.7966	1736.9462	3000.0743
3103.3341	3160.9891	3183.2795
3186.4899	3193.9065	3206.1520
3206.9545	3216.7624	3251.5486

i106 – i53

C	1.836010	-1.230724	-0.032861
C	2.789146	-0.219817	-0.022822
C	2.390610	1.106595	0.012007
C	1.030325	1.419927	0.025943
C	0.053621	0.428796	0.012015
C	0.468598	-0.934139	-0.004919
C	-0.518314	-1.983118	0.003016
C	-2.310494	-0.243057	-0.045151
C	-1.385265	0.753350	-0.008044
C	-1.964318	-1.626184	-0.017829
C	-1.805747	2.193829	-0.006570
H	2.147367	-2.269988	-0.058102
H	3.843422	-0.472963	-0.039020
H	3.127776	1.900795	0.024972
H	0.735537	2.462239	0.043180
H	-0.233395	-3.014305	-0.158753
H	-3.364871	0.011226	-0.085291
H	-2.688334	-2.397176	-0.243530
H	-1.331625	-1.937941	1.047253
H	-2.893168	2.282132	-0.031740
H	-1.402839	2.727372	-0.874650
H	-1.444900	2.715860	0.886974

Frequencies

-2094.6781	105.5054	160.8105
229.3472	252.8345	295.4000
369.5698	441.8535	455.5512
464.7899	490.2027	510.8216
572.7463	598.2546	636.3198
708.7187	757.0192	765.4225
779.1898	816.5391	856.7687
874.9945	905.4302	939.6781
960.8279	989.1401	1016.9455
1059.1988	1070.5537	1095.4831
1144.3647	1158.9979	1191.6541
1200.2952	1243.9960	1265.9024

1303.0988	1332.1110	1371.3284
1398.3315	1422.1141	1434.0157
1481.4170	1485.7402	1505.8845
1526.6992	1597.2463	1628.7776
1645.8288	2195.3499	3031.6004
3085.7970	3134.3158	3180.5355
3185.8280	3197.2851	3207.3227
3221.0158	3223.2629	3233.8656

i106 – p4

C	1.836368	-1.188438	-0.051152
C	2.760584	-0.177701	-0.038423
C	2.333425	1.164134	0.001234
C	0.996637	1.465112	0.022220
C	0.015118	0.442382	0.002235
C	0.452424	-0.906993	-0.031022
C	-0.516134	-1.959423	-0.025881
C	-2.282671	-0.312933	-0.068213
C	-1.388656	0.729587	-0.001547
C	-1.859517	-1.652009	-0.106949
C	-1.876901	2.151575	0.043337
H	2.156588	-2.225105	-0.070736
H	3.820224	-0.405560	-0.055819
H	3.068103	1.961177	0.015455
H	0.685976	2.502523	0.053303
H	-0.176650	-2.979172	-0.169866
H	-0.425694	-2.415777	1.850338
H	-3.345896	-0.097825	-0.097843
H	-2.594433	-2.446117	-0.166067
H	-2.967154	2.187046	0.032590
H	-1.512808	2.725471	-0.814443
H	-1.532310	2.661580	0.948066

Frequencies

-831.3658	125.9636	153.9968
176.0464	215.6233	292.9022
325.7467	376.9070	422.4292
448.5298	483.9987	490.5637
522.3461	568.2602	582.9238
642.2562	719.9480	765.8829
797.9266	806.1391	820.7449
877.9594	881.4053	942.3844
978.8300	996.7494	1012.5231
1018.9208	1057.0371	1062.4122
1089.2313	1103.3343	1169.6185
1198.3397	1203.1568	1234.3668

1273.8182	1303.2075	1377.4682
1410.1665	1418.9013	1435.6241
1475.7951	1484.4766	1503.8194
1509.9896	1567.5618	1637.4424
1657.0807	1698.2703	3046.4678
3107.3449	3142.8094	3185.4619
3188.7258	3198.7691	3200.2356
3211.4872	3217.8806	3224.3715

i106 – p40

C	1.808602	-1.215453	-0.001297
C	2.781122	-0.232125	0.031427
C	2.399815	1.106387	0.039943
C	1.058045	1.437740	0.005770
C	0.063134	0.453416	-0.047124
C	0.451349	-0.892869	-0.036573
C	-0.557534	-2.014329	-0.059466
C	-2.332233	-0.285456	0.089997
C	-1.376923	0.810023	-0.090085
C	-1.972902	-1.567279	0.104844
C	-1.833811	2.057634	-0.289382
H	2.098807	-2.261930	0.005320
H	3.830342	-0.503162	0.061441
H	3.149260	1.888296	0.081459
H	0.776926	2.483324	0.036182
H	-0.464496	-2.566040	-1.005240
H	-0.306625	-2.740354	0.723165
H	-3.378328	-0.013509	0.190226
H	-2.727203	-2.339624	0.218159
H	-1.826457	2.955495	2.005104
H	-2.899903	2.251759	-0.314293
H	-1.184313	2.899608	-0.489849

Frequencies

-340.2322	48.3372	98.6129
124.9072	150.3425	219.0569
314.4798	333.9838	423.7118
442.6751	471.7874	499.5059
504.1508	579.7477	612.1045
682.9334	719.1161	752.2638
784.9380	795.1360	807.2944
860.1512	884.5996	904.9277
946.3640	962.3994	983.7569
1004.2945	1010.1194	1021.4398
1079.9638	1121.5264	1165.1685
1198.6165	1214.6776	1219.9182

1232.2240	1286.1047	1337.2929
1351.4758	1390.1993	1425.1133
1462.5759	1470.0013	1509.4172
1538.9829	1647.1083	1669.9408
1688.2844	1748.4011	3022.5107
3057.4419	3173.1300	3174.5603
3175.4904	3197.3318	3199.7262
3209.3132	3223.2758	3262.4659

i102 – p38

C	1.685384	-1.265347	0.396105
C	2.716104	-0.378095	0.224978
C	2.460936	0.919681	-0.260550
C	1.176620	1.303696	-0.555398
C	0.097772	0.411648	-0.386377
C	0.352524	-0.898227	0.090278
C	-0.730387	-1.811673	0.219795
C	-2.265534	-0.161399	-0.641638
C	-1.261120	0.806631	-0.647326
C	-2.000705	-1.452025	-0.163832
C	-1.681217	1.892609	1.282044
H	1.878966	-2.267266	0.765651
H	3.732665	-0.673068	0.459503
H	3.281532	1.614627	-0.397947
H	0.975719	2.305521	-0.922204
H	-0.530352	-2.811751	0.589514
H	-3.269535	0.105799	-0.950599
H	-1.425543	1.743249	-1.168437
H	-2.805588	-2.176614	-0.108411
H	-2.707259	2.221040	1.158005
H	-0.917606	2.662165	1.257246
H	-1.515262	1.071295	1.969198

Frequencies

-538.7449	85.9506	114.1755
133.4343	185.4131	207.9188
368.0567	377.6129	479.3656
498.1428	509.8216	517.1998
550.1856	558.0286	615.8860
643.2049	731.6139	776.3065
791.3851	799.7267	811.7600
847.9310	872.6784	897.9726
951.1131	972.5354	984.3218
996.7031	1009.9641	1045.1760
1062.8055	1148.6266	1167.1158
1171.7871	1191.6008	1225.5070

1268.6228	1294.2844	1381.6695
1399.4627	1417.3889	1417.8544
1426.7939	1489.1553	1499.5888
1553.8010	1618.4904	1638.1142
1693.3442	3096.2608	3184.7182
3187.9002	3189.4218	3193.6658
3203.9639	3204.9696	3216.9375
3218.2318	3260.6925	3265.7637

i97 – p34

C	0.848774	-1.520363	0.039929
C	2.239268	-1.547213	0.000055
C	2.972928	-0.364508	-0.044217
C	2.328222	0.870668	-0.050521
C	0.945447	0.900599	-0.006300
C	0.207100	-0.288375	0.041445
C	-1.227229	0.053305	0.071624
C	-1.349696	1.394564	0.056695
C	-0.007063	2.065994	-0.005554
C	-2.300337	-0.935556	0.138200
C	-3.530738	-0.762208	-0.358811
H	0.283944	-2.446123	0.063409
H	2.758049	-2.499276	-0.000109
H	4.055822	-0.406726	-0.077102
H	2.903489	1.789940	-0.088750
H	-2.285349	1.935603	0.117562
H	0.154971	2.731631	0.850098
H	0.098911	2.680170	-0.907839
H	-2.063841	-1.870833	0.640360
H	-3.787640	0.120310	-0.935172
H	-4.594091	0.300015	1.318771
H	-4.284330	-1.536163	-0.276501

Frequencies

-379.2830	76.7024	132.0793
147.2920	198.7126	205.0320
231.7439	291.4985	348.5962
422.6071	446.9926	472.2910
557.2145	568.2992	629.2668
691.8446	722.0247	737.8921
777.1295	789.7979	819.4934
855.3262	886.2933	944.3546
962.5160	974.9777	990.0396
1005.1529	1028.8191	1050.3447
1063.2332	1094.3328	1145.9275
1153.4944	1187.6706	1206.7890

1239.7373	1280.1939	1316.0795
1335.3210	1342.5512	1376.0562
1434.9334	1464.3610	1507.3153
1517.4708	1647.7418	1678.2355
1680.9721	1690.7595	3049.9798
3084.9794	3154.6151	3170.7683
3186.0040	3193.2034	3204.4266
3218.7966	3230.4856	3249.9230

i98 – p36

C	0.872307	-1.548627	-0.020255
C	2.224127	-1.541488	0.021724
C	2.981944	-0.307232	0.055298
C	2.372691	0.897861	0.046386
C	0.932294	0.953740	0.002564
C	0.165127	-0.296694	-0.031481
C	-1.174280	-0.011047	-0.069781
C	-1.326391	1.482993	-0.059289
C	0.074495	2.002915	-0.012805
C	-2.263836	-0.954684	-0.103279
C	-3.566120	-0.641083	-0.150694
H	0.326847	-2.485221	-0.045743
H	2.769172	-2.478908	0.030712
H	4.063958	-0.370351	0.089224
H	2.945319	1.818351	0.071872
H	-1.911259	1.818741	0.806922
H	-1.860629	1.840702	-0.948769
H	0.333795	3.052649	0.005944
H	-1.988033	-2.006264	-0.081420
H	-4.327872	-1.410123	-0.181425
H	-3.906819	0.388521	-0.189653
H	-4.198641	-0.388024	2.372004

Frequencies

-277.0951	69.3570	88.4331
127.1179	169.8122	179.1914
193.3510	259.7694	341.8127
346.2664	470.5270	487.1953
519.0381	546.1514	590.1436
666.8885	677.4982	699.0798
740.8636	771.7899	782.8554
857.2451	884.6364	897.8564
919.7794	969.1911	993.0892
994.8672	1010.4984	1017.1391
1025.8899	1038.8493	1126.1589
1156.8797	1182.0656	1215.7985

1229.9414	1247.9517	1322.3794
1359.3995	1402.4442	1405.0445
1419.9078	1444.4619	1471.9263
1495.7936	1602.3331	1636.1694
1670.1577	1719.4472	3043.0934
3077.7370	3159.1058	3167.0416
3188.7114	3197.2748	3209.9531
3218.9690	3235.4017	3255.7777

i105 – p39

C	1.433822	-1.483880	0.005456
C	2.732756	-1.002055	-0.113354
C	2.965488	0.367422	-0.126667
C	1.897022	1.246943	-0.028634
C	0.590034	0.771201	0.085151
C	0.358142	-0.611740	0.108266
C	-1.048062	-1.122081	0.315547
C	-1.814931	1.259652	0.027469
C	-2.133230	-0.159312	-0.101365
C	-0.549589	1.687615	0.136069
C	-3.340139	-0.576144	-0.508104
H	1.254795	-2.554663	0.019943
H	3.560565	-1.697313	-0.194809
H	3.975711	0.749340	-0.219050
H	2.070856	2.318188	-0.048950
H	-1.182981	-2.089363	-0.174285
H	-1.175704	-1.300504	1.393574
H	-2.633256	1.971298	-0.013299
H	-0.337977	2.750226	0.203440
H	-4.397278	-0.916361	1.639342
H	-3.557849	-1.628386	-0.653234
H	-4.124758	0.131814	-0.751681

Frequencies

-348.9365	69.6573	120.9476
142.2040	164.7138	227.6597
304.5484	338.4634	409.5170
419.5070	464.8364	518.4093
524.1339	577.5204	629.1345
703.5235	734.9760	752.2465
774.6107	789.5829	836.3424
870.4547	884.3914	916.5396
931.7390	958.3624	982.6232
993.2846	1007.9033	1012.8609
1075.7205	1142.3743	1183.2125
1189.1403	1226.8031	1233.0088

1249.5070	1291.8158	1334.3583
1338.2546	1367.4623	1424.8216
1465.6874	1474.8513	1500.4814
1543.2897	1642.2760	1672.1883
1689.4867	1713.4946	3009.7614
3099.8796	3159.2362	3183.4344
3183.9997	3189.5801	3203.4149
3204.8471	3218.5380	3250.1377

i105 – p3

C	1.411059	-1.499094	-0.056288
C	2.703428	-1.043033	-0.053151
C	2.970012	0.341514	-0.010633
C	1.937460	1.240523	0.024250
C	0.593076	0.796810	0.017683
C	0.327164	-0.593616	-0.020789
C	-1.031185	-1.040042	-0.006461
C	-1.792694	1.242663	-0.017828
C	-2.082626	-0.139796	-0.060917
C	-0.503739	1.699206	0.030197
C	-3.508602	-0.610505	-0.082172
H	1.204929	-2.564196	-0.080239
H	3.527029	-1.747437	-0.080216
H	3.996221	0.690953	-0.005568
H	2.136348	2.306869	0.056727
H	-1.224058	-2.098520	-0.151336
H	-1.214275	-1.484398	1.882525
H	-2.614652	1.951531	-0.028863
H	-0.303277	2.765283	0.060740
H	-3.579692	-1.662760	-0.363307
H	-4.108459	-0.024962	-0.783450
H	-3.960231	-0.500142	0.909635

Frequencies

-761.8874	79.1122	116.0364
173.3468	253.3194	269.9695
294.8042	363.5671	414.8403
421.8114	457.1535	515.4165
527.4673	531.8947	635.6211
656.5564	718.2721	757.5048
790.0243	795.8221	834.6290
884.2900	902.7165	960.6675
975.2593	977.6678	995.7466
1012.6465	1029.0213	1056.3896
1068.9292	1157.6895	1172.1399
1192.4163	1207.1702	1240.1325

1284.8159	1300.6974	1384.3833
1406.3261	1418.6866	1425.6155
1472.6579	1490.3582	1502.6183
1516.8720	1563.2646	1635.3771
1666.9525	1704.7360	3041.5733
3108.5785	3139.9020	3185.1648
3185.5429	3187.3112	3192.4123
3204.5638	3205.9665	3219.3700

i105 – i52

C	1.451598	-1.498745	0.002659
C	2.754672	-1.015295	-0.053510
C	2.992721	0.350776	-0.068436
C	1.916869	1.237467	-0.035123
C	0.606360	0.777493	0.018209
C	0.362982	-0.622681	0.048233
C	-0.997330	-1.100824	0.122348
C	-1.812298	1.251038	0.040073
C	-2.144488	-0.140021	0.111871
C	-0.530790	1.693770	0.022574
C	-3.516955	-0.652225	-0.216958
H	1.270210	-2.568601	0.016454
H	3.583913	-1.713439	-0.081265
H	4.006988	0.730488	-0.108705
H	2.096883	2.307698	-0.056487
H	-1.217830	-2.155735	0.015813
H	-1.660631	-0.638942	1.180954
H	-2.630991	1.963388	0.008555
H	-0.324432	2.758064	-0.004375
H	-3.711511	-1.613334	0.267583
H	-3.624771	-0.804425	-1.297650
H	-4.287872	0.050321	0.107493

Frequencies

-2128.9107	98.0877	162.3039
229.2345	249.1366	259.0142
341.8316	392.8338	437.6119
453.9565	511.4811	520.8439
600.5585	616.5798	692.8003
704.5310	738.6697	768.9495
774.8671	792.4779	871.9379
874.0948	923.5717	940.2877
963.4598	992.8121	1015.8160
1055.8074	1072.5365	1128.6190
1164.3358	1172.6895	1183.6252
1230.1413	1240.9851	1259.5148

1304.3260	1325.7074	1335.0774
1398.8078	1431.7359	1462.6965
1490.6357	1493.5357	1511.0014
1527.9309	1583.8655	1633.4709
1646.6575	2187.8127	3025.2963
3091.4811	3128.2236	3184.5735
3184.7893	3189.2776	3203.1580
3205.5886	3215.9377	3219.3865

i103 – p42

C	1.453008	-1.531757	0.098029
C	2.711950	-1.056346	0.046266
C	2.968435	0.366511	-0.058142
C	1.952850	1.247466	-0.091517
C	0.568818	0.808014	-0.015353
C	0.308671	-0.643075	0.050510
C	-0.963903	-1.113916	0.007909
C	-1.879985	1.230822	0.175700
C	-2.114523	-0.239145	-0.103583
C	-0.460922	1.676509	0.008255
C	-3.331877	-0.714596	-0.409512
H	1.265579	-2.598345	0.165955
H	3.554016	-1.738470	0.076769
H	3.994941	0.711540	-0.105882
H	2.143020	2.313465	-0.162324
H	-1.136897	-2.186101	-0.012841
H	-2.552963	1.846878	-0.427796
H	-2.164055	1.426768	1.222361
H	-0.267540	2.744303	-0.030496
H	-4.182134	-0.055211	-0.544320
H	-4.428769	-0.870856	2.114832
H	-3.500339	-1.776876	-0.547634

Frequencies

-279.3014	58.7293	69.5848
96.3956	145.9861	211.6517
283.0930	287.6892	407.0225
447.2545	465.4652	484.6417
501.4797	539.0911	621.1463
691.5322	700.7182	731.7196
744.0200	755.7861	814.3797
851.2200	868.1565	890.7072
903.3849	925.4805	965.8602
995.4508	998.2317	999.5464
1011.3264	1060.0042	1166.7100
1179.0420	1198.2082	1221.3647

1228.0445	1305.0296	1332.0931
1346.8401	1407.2855	1421.4829
1448.7614	1452.6362	1476.7988
1481.9710	1621.4346	1661.6520
1690.6592	1731.3540	2981.9788
3078.9586	3152.4650	3176.0940
3180.0352	3181.0040	3185.4956
3201.1529	3212.9915	3242.5562

i103 – p3

C	-1.449015	-1.509096	0.037787
C	-2.733241	-1.030449	0.039359
C	-2.976834	0.359100	-0.001406
C	-1.930028	1.240303	-0.040172
C	-0.591322	0.774623	-0.037693
C	-0.346333	-0.624061	-0.001219
C	0.997306	-1.093786	-0.020286
C	1.805971	1.171734	-0.026659
C	2.059754	-0.238621	-0.045669
C	0.514101	1.655275	-0.081454
C	3.482544	-0.718043	-0.053937
H	-1.262263	-2.577698	0.067347
H	-3.568764	-1.720599	0.070000
H	-3.997025	0.725706	-0.000817
H	-2.111180	2.309813	-0.070935
H	1.167459	-2.166635	-0.017423
H	2.233590	1.433802	1.810706
H	2.636966	1.852194	-0.182097
H	0.336900	2.724428	-0.128792
H	3.539028	-1.807565	-0.077329
H	4.006441	-0.365900	0.840600
H	4.021436	-0.329418	-0.923165

Frequencies

-819.7271	104.3613	119.4986
166.2304	263.0882	274.3234
319.2751	373.8090	418.4724
434.5212	455.8996	486.1366
529.2647	538.0240	635.6417
662.0280	716.4752	756.1710
783.0340	790.9540	850.0581
872.0484	901.2088	907.5987
966.9044	978.2828	1011.0326
1014.8759	1027.6311	1055.2223
1067.7369	1154.5326	1170.5325
1181.2150	1205.6614	1232.5575

1284.8976	1302.7291	1392.2896
1406.0077	1416.4488	1428.8125
1468.6002	1482.9509	1502.6295
1520.3363	1557.8514	1637.3666
1674.3723	1701.0886	3044.9796
3108.2229	3140.8859	3183.6134
3187.3402	3187.9438	3193.0567
3205.7025	3206.5160	3219.3868

i103 – i52

C	1.438653	-1.502516	0.025089
C	2.741815	-1.034232	-0.001845
C	2.989668	0.337161	-0.036881
C	1.931495	1.231051	-0.043431
C	0.602605	0.785151	-0.018350
C	0.347484	-0.620825	0.017122
C	-1.005457	-1.097149	0.034374
C	-1.807230	1.219035	0.041192
C	-2.084472	-0.210839	0.064692
C	-0.504348	1.698873	-0.026511
C	-3.498608	-0.688903	-0.142948
H	1.246334	-2.570296	0.054528
H	3.567778	-1.736483	0.006101
H	4.009002	0.705884	-0.057052
H	2.122301	2.299183	-0.069246
H	-1.193069	-2.163960	0.072054
H	-2.655734	1.889389	-0.054038
H	-2.111686	0.551036	1.209368
H	-0.320613	2.765680	-0.013230
H	-3.665254	-1.646228	0.353718
H	-3.679298	-0.824823	-1.212710
H	-4.229398	0.029771	0.235489

Frequencies

-1817.5829	107.8422	163.2039
221.1519	263.5034	284.6798
360.0858	407.5716	452.4730
475.7179	524.2126	534.1996
621.0504	626.4340	697.2348
704.4429	717.2808	773.2794
773.9199	780.2790	872.3790
884.2896	915.4534	944.6289
959.2928	990.9890	1036.1941
1072.0655	1089.4747	1113.7773
1147.2631	1162.8034	1185.6110
1203.1728	1243.1236	1257.6835

1302.5699	1322.4306	1368.5662
1431.1884	1449.6047	1461.6705
1480.5469	1497.4657	1507.9013
1540.7197	1564.7848	1601.3349
1640.8691	1643.4364	3052.1363
3124.3629	3140.0012	3183.8248
3188.4140	3192.5867	3202.5322
3203.5485	3217.9774	3219.3544

i39 – i42

C	-1.014040	0.985732	0.616668
C	-2.398399	0.892460	0.521723
C	-2.998323	-0.207700	-0.079561
C	-2.202479	-1.239060	-0.586839
C	-0.847528	-1.091930	-0.459792
C	-0.182567	-0.022453	0.104575
C	1.301498	0.031814	0.195141
C	2.027783	1.114023	-0.102204
C	1.548443	2.425607	-0.647224
H	-0.562294	1.838611	1.111930
H	-3.014680	1.684892	0.930727
H	-4.078570	-0.274144	-0.150141
H	-2.645935	-2.111404	-1.053887
H	3.104213	1.027936	0.032113
H	1.563110	3.204856	0.123008
H	0.535464	2.364006	-1.047229
H	2.214166	2.761005	-1.447302
C	1.980251	-1.217331	0.651130
C	2.140258	-2.297397	-0.102409
H	2.344241	-1.221413	1.677002
H	2.626011	-3.186519	0.284293
H	1.784899	-2.330418	-1.127767

Frequencies

-131.5110	42.1000	107.7854
142.0581	176.9744	211.8044
239.2476	302.6533	362.5472
424.0266	450.9642	471.0862
570.6014	626.3914	663.0986
684.1104	723.3936	737.9818
772.0631	875.5232	886.6129
959.8352	964.9790	969.9582
996.7070	1008.6266	1019.0106
1025.2801	1058.1199	1077.8886
1113.4696	1132.6542	1151.0800
1178.5710	1241.9860	1280.3418

1318.6822	1325.0011	1390.9841
1425.9718	1446.4208	1453.4798
1489.0688	1493.4116	1499.0314
1603.2917	1665.4084	1710.7454
1753.6209	3042.4055	3101.7974
3140.9421	3146.8208	3158.6313
3160.2623	3187.9287	3196.2249
3205.3780	3219.4594	3243.5837

i99 – p29

C	1.460622	1.366090	-0.025814
C	2.732447	0.794570	-0.006902
C	2.889406	-0.588487	0.027880
C	1.781804	-1.432985	0.041713
C	0.514916	-0.865886	0.025018
C	0.358284	0.531492	-0.004249
C	-1.090253	0.820120	-0.008593
C	-1.767694	-0.504256	-0.053590
C	-0.811611	-1.471609	0.027945
C	-1.683021	2.010668	0.064134
C	-3.243856	-0.682658	0.122016
H	1.345158	2.444353	-0.057543
H	3.608322	1.433185	-0.020046
H	3.886854	-1.013300	0.041611
H	1.910023	-2.509636	0.065222
H	-1.846979	-0.528138	-2.067386
H	-1.002550	-2.536601	0.066653
H	-1.105744	2.926495	0.126393
H	-2.762938	2.107681	0.062846
H	-3.812271	-0.036100	-0.549803
H	-3.531356	-0.434609	1.149152
H	-3.534787	-1.715679	-0.074453

Frequencies

-732.9205	103.5192	140.0418
205.8510	251.5995	278.9537
287.2980	320.9682	375.2396
418.6772	429.1796	497.2813
516.4081	554.5894	577.7729
657.8496	662.2796	719.4690
753.9861	769.6695	802.0343
838.1878	853.8971	885.8504
895.9842	949.4048	959.6930
1004.3609	1012.3788	1053.7942
1058.3550	1100.1399	1133.8984
1172.6716	1185.5046	1227.2546

1250.3435	1332.5239	1356.4670
1389.8247	1417.6195	1452.6785
1491.1917	1496.9926	1506.4560
1512.3714	1600.0311	1661.1808
1685.0549	1745.4784	3046.8364
3116.2605	3145.5179	3163.6601
3186.7019	3196.4952	3204.3392
3218.3247	3228.7426	3251.1026

i99 – p27

C	1.272670	1.389185	0.262090
C	2.551917	0.861782	0.432775
C	2.796244	-0.491941	0.211643
C	1.772565	-1.349327	-0.180848
C	0.494618	-0.827954	-0.351133
C	0.252103	0.543147	-0.132826
C	-1.179104	0.795913	-0.399560
C	-1.768301	-0.537207	-0.671889
C	-0.757928	-1.459327	-0.738177
C	-1.805234	1.971310	-0.442383
C	-2.670813	-0.861439	1.486022
H	1.087490	2.443646	0.438025
H	3.363859	1.510528	0.740898
H	3.798019	-0.883039	0.350805
H	1.969136	-2.402616	-0.348471
H	-2.765466	-0.668186	-1.068107
H	-0.869683	-2.504965	-0.991173
H	-1.277700	2.901984	-0.265203
H	-2.865758	2.035994	-0.659360
H	-3.439065	-0.097714	1.475681
H	-1.762508	-0.645312	2.034529
H	-2.990740	-1.895173	1.438100

Frequencies

-448.6401	72.0111	115.8018
124.6429	140.0485	217.1484
263.1511	329.8637	420.7376
455.4257	486.7759	497.8238
544.8657	553.8371	576.4158
656.5581	700.2025	724.7242
756.1619	769.1200	791.3252
810.3226	825.7206	876.7712
908.7097	915.2686	946.9124
954.9051	978.3447	1016.3609
1055.9168	1087.5501	1114.0156
1151.1549	1183.8179	1228.1772

1256.4533	1333.2082	1345.8796
1394.4985	1412.8226	1420.9026
1436.8055	1472.4843	1504.2038
1531.3603	1653.4182	1680.0038
1746.7404	3102.7179	3161.6899
3186.9459	3193.4833	3204.7884
3217.1310	3228.9554	3247.0011
3250.1231	3273.1207	3276.3698

i41 – i43

C	2.021515	1.031402	0.113984
C	2.989175	0.033108	0.177093
C	2.647614	-1.315684	0.060780
C	1.319945	-1.714713	-0.125233
C	0.385547	-0.705546	-0.186123
C	0.698848	0.637477	-0.064985
C	-0.602479	1.299353	-0.163897
C	-1.496914	0.118375	-0.454964
C	-2.468231	-0.307803	0.416909
C	-0.969376	2.565798	-0.000142
C	-3.432082	-1.407009	0.120831
H	2.294737	2.077200	0.207194
H	4.029569	0.302800	0.320241
H	3.427915	-2.067875	0.114562
H	1.062628	-2.763910	-0.217880
H	-1.589617	-0.161480	-1.503505
H	-2.470387	0.107936	1.421712
H	-0.241126	3.336792	0.227245
H	-2.007753	2.863376	-0.090484
H	-4.460752	-1.102575	0.341234
H	-3.225369	-2.287666	0.740862
H	-3.381221	-1.713148	-0.926706

Frequencies

-585.8595	68.0889	100.2616
120.9379	128.1309	196.4802
257.5721	280.9843	357.0523
396.9452	445.0756	534.6088
565.8061	577.2057	653.7493
694.9513	720.6432	753.2787
792.3127	802.5408	877.8010
889.5243	918.0197	929.1515
967.7875	982.5490	1004.3300
1014.6474	1030.2016	1038.1646
1121.6116	1127.4445	1141.9243
1188.3834	1229.8019	1278.9950

1295.6569	1318.1964	1354.2172
1407.7074	1441.5412	1471.3490
1474.8452	1487.1611	1498.1745
1561.3543	1641.1661	1659.9714
1759.2839	3025.8528	3082.0908
3122.4396	3145.8057	3160.8043
3173.8610	3185.3326	3196.0258
3205.8589	3216.4803	3252.0563

i41 – i40

C	1.661694	1.248272	0.320306
C	2.809487	0.470992	0.442454
C	2.799143	-0.890598	0.132657
C	1.635756	-1.524335	-0.315295
C	0.516986	-0.729747	-0.429824
C	0.500763	0.619185	-0.119632
C	-0.886790	1.008415	-0.369073
C	-1.454670	-0.286674	-0.906778
C	-2.387108	-1.052420	-0.246674
C	-1.533392	2.153111	-0.176524
C	-2.736439	-0.923613	1.198293
H	1.678429	2.305449	0.563669
H	3.730958	0.927109	0.786636
H	3.713156	-1.465486	0.241196
H	1.634702	-2.581889	-0.554507
H	-1.372318	-0.415664	-1.983455
H	-2.819930	-1.892564	-0.783311
H	-1.023870	3.027212	0.214616
H	-2.589353	2.246473	-0.402956
H	-3.818717	-0.823094	1.333561
H	-2.252504	-0.060381	1.657343
H	-2.433125	-1.822695	1.747750

Frequencies

-590.1102	58.5109	105.4726
127.4262	151.9144	203.0926
263.6994	273.8946	391.9364
439.6934	456.9651	515.0840
559.3177	605.6367	673.3871
712.3731	719.5995	751.5309
794.5441	806.0257	866.1598
886.5016	911.6257	933.4670
949.9422	965.9785	1005.4431
1008.6498	1035.6139	1041.0607
1105.4929	1120.6089	1137.2800
1184.6828	1218.8968	1249.6104

1307.4428	1345.0068	1397.4129
1428.6494	1447.1457	1463.3800
1477.8321	1488.4895	1497.6504
1546.9004	1638.2101	1659.1165
1757.5091	3029.0387	3081.8572
3141.4418	3156.8526	3161.7235
3178.6280	3183.6196	3190.7044
3201.3512	3213.7110	3251.4291

i100 – i99

C	1.428511	1.374522	-0.038711
C	2.697607	0.835450	0.009500
C	2.885711	-0.560092	0.044550
C	1.814494	-1.424774	0.038870
C	0.510751	-0.893616	0.015706
C	0.330312	0.510251	-0.033328
C	-1.097807	0.794472	-0.076894
C	-1.756868	-0.550645	-0.073397
C	-0.763256	-1.526624	-0.004979
C	-1.727733	2.040907	0.111658
C	-3.235316	-0.735398	0.075952
H	1.286747	2.449439	-0.074302
H	3.562038	1.489596	0.018338
H	3.894737	-0.956459	0.077304
H	1.968988	-2.497991	0.064271
H	-1.483138	0.196434	-1.173788
H	-0.945524	-2.592143	-0.019921
H	-1.139899	2.947918	0.144135
H	-2.804288	2.124658	0.181437
H	-3.800329	-0.050218	-0.560876
H	-3.531905	-0.542923	1.111771
H	-3.525866	-1.755020	-0.181937

Frequencies

-1430.9757	128.7586	154.2859
180.5884	250.1655	265.4936
291.6476	362.4909	390.7008
460.5749	491.4262	506.6935
570.2160	578.9559	586.4179
653.6692	696.7979	735.7252
748.4257	784.3188	795.0937
826.3753	874.5939	895.8724
964.6825	1002.9217	1004.6957
1044.3499	1058.4945	1077.7679
1139.7420	1158.8517	1171.4087
1179.6915	1220.1908	1261.6423

1331.1556	1347.1624	1361.4000
1412.8064	1424.5577	1486.4077
1490.7558	1497.3656	1505.5427
1524.8402	1560.0234	1627.1847
1685.1063	1947.0660	3048.9151
3115.9209	3141.5202	3176.7094
3185.9827	3194.6496	3205.2682
3215.7475	3240.7398	3277.9384

i100 – i101

C	-1.533047	-1.344648	-0.336969
C	-2.769227	-0.719367	-0.185891
C	-2.842417	0.646173	0.090728
C	-1.692010	1.413632	0.216973
C	-0.450618	0.798233	0.048564
C	-0.384398	-0.583133	-0.226158
C	1.056242	-0.989198	-0.274126
C	1.801548	0.311024	-0.145254
C	0.892774	1.324805	0.104724
C	1.616962	-1.251397	1.084905
C	3.255101	0.486351	-0.468695
H	-1.475570	-2.409085	-0.538979
H	-3.681907	-1.296427	-0.281698
H	-3.813501	1.114321	0.208968
H	-1.758956	2.474380	0.433166
H	1.359945	-1.682347	-1.058258
H	1.150488	2.356176	0.308355
H	1.037372	-0.990328	1.958947
H	2.578333	-1.731722	1.206642
H	3.363062	0.880126	-1.484557
H	3.798652	-0.458868	-0.420831
H	3.736631	1.188920	0.215448

Frequencies

-588.6503	113.2505	128.4635
168.7579	247.4171	294.0740
353.9907	406.3028	429.9852
474.1718	514.9478	549.1252
579.3159	613.6127	646.1664
661.5365	760.4641	772.8123
793.0384	808.1604	875.6800
896.0998	901.7160	969.0304
982.6801	1009.2102	1010.8286
1048.4059	1051.0034	1102.3056
1132.7630	1138.0462	1182.0089
1187.4815	1198.5492	1250.9655

1272.5616	1321.0935	1350.0989
1376.5684	1419.4205	1449.4687
1478.1507	1493.6202	1499.9957
1508.1034	1531.4371	1646.4581
1675.8397	3046.5399	3112.6299
3125.0252	3139.0185	3169.2745
3184.1267	3193.8216	3204.2781
3216.2674	3221.8698	3290.6467

i101 – i103

C	-1.699006	-1.323427	-0.283827
C	-2.874612	-0.581696	-0.167319
C	-2.823666	0.786255	0.083719
C	-1.599162	1.434308	0.200001
C	-0.417627	0.705118	0.081527
C	-0.473400	-0.692718	-0.140401
C	0.851231	-1.320665	-0.175740
C	1.957035	0.265583	0.072860
C	0.935599	1.208429	-0.008519
C	1.754219	-0.962320	0.930053
C	3.326398	0.503921	-0.502728
H	-1.745378	-2.390502	-0.474789
H	-3.833700	-1.075675	-0.274183
H	-3.744402	1.351641	0.173191
H	-1.560253	2.506779	0.360610
H	1.129586	-2.056096	-0.920697
H	1.132773	2.215420	-0.360624
H	1.287820	-0.790822	1.901349
H	2.653152	-1.569670	1.010797
H	3.320069	1.323889	-1.223399
H	3.690235	-0.388904	-1.018401
H	4.048044	0.737220	0.288386

Frequencies

-652.1440	118.6748	143.0683
166.4489	263.2847	309.7752
373.0083	415.7993	423.4701
457.7013	486.1171	563.3354
598.0661	642.8965	674.1627
703.8071	771.5294	779.1255
800.0267	825.0885	882.5240
903.8218	970.9344	984.2957
1005.4460	1020.0898	1050.1237
1056.3986	1069.7941	1135.6399
1162.3018	1186.1603	1196.5950
1203.9258	1220.2630	1255.9010

1280.1523	1317.3365	1343.8992
1402.6605	1420.2850	1475.0519
1492.7475	1499.1490	1505.2553
1512.3703	1533.3400	1638.1629
1659.8645	3037.9635	3077.4882
3105.6791	3137.8184	3166.4719
3185.8533	3192.4741	3197.6234
3203.4382	3216.4093	3217.2207

i100 – p29

C	-1.445073	1.359697	0.062977
C	-2.720833	0.797930	0.023584
C	-2.885280	-0.582482	-0.039378
C	-1.782182	-1.434154	-0.064722
C	-0.512834	-0.877341	-0.025420
C	-0.351265	0.515752	0.037701
C	1.108084	0.792729	0.043733
C	1.769352	-0.542409	0.013007
C	0.818033	-1.491536	-0.040575
C	1.701317	1.974094	-0.237373
C	3.249912	-0.721197	0.019863
H	-1.320613	2.435906	0.120712
H	-3.592428	1.442142	0.044387
H	-3.885058	-1.001126	-0.069314
H	-1.917869	-2.508888	-0.117691
H	1.205383	0.796270	1.950987
H	0.998278	-2.558419	-0.085672
H	1.122371	2.885057	-0.334993
H	2.777837	2.055034	-0.333849
H	3.693903	-0.262505	0.908811
H	3.708463	-0.250231	-0.855803
H	3.514348	-1.779739	0.012042

Frequencies

-921.5837	115.5793	142.9627
167.9894	252.1357	275.8446
295.5799	331.8645	354.0343
422.1502	440.9796	481.8441
516.3209	558.5640	582.9363
642.7553	658.2086	684.4078
758.5798	773.0446	790.7427
836.9550	865.6375	884.2041
901.1308	911.7404	961.9589
1005.3711	1018.0123	1054.4480
1068.9773	1097.7545	1133.2028
1173.0664	1185.6954	1225.4408

1248.1954	1333.0886	1354.8493
1391.5347	1426.0008	1442.2132
1484.4761	1499.7684	1509.9298
1513.6377	1636.3333	1657.4670
1688.9824	1699.2827	3042.9081
3103.5147	3137.0183	3164.3807
3186.1744	3195.0634	3203.8193
3217.1326	3225.9495	3257.5408

Products

p22 + CH3

C	-1.090759	1.182941	0.018610
C	-2.472605	1.298989	0.012909
C	-3.270509	0.160463	-0.007568
C	-2.679933	-1.098099	-0.022595
C	-1.298927	-1.222126	-0.016316
C	-0.488769	-0.080618	0.004326
C	0.934409	-0.204802	0.012689
C	2.136120	-0.302714	0.021121
C	3.551709	-0.451036	0.037504
C	4.412494	0.563382	-0.050172
H	-0.464163	2.066764	0.034805
H	-2.929417	2.281897	0.025127
H	-4.350407	0.254598	-0.012103
H	-3.298434	-1.988253	-0.038887
H	-0.833580	-2.200446	-0.027981
H	3.923893	-1.467830	0.130110
H	5.481221	0.387012	-0.029658
H	4.071504	1.587976	-0.144469

Frequencies

37.8603	68.6306	86.0582
198.9542	234.3570	377.0909
396.1748	413.3466	511.2448
552.7850	592.4810	641.9058
700.4556	710.3587	721.8212
780.9459	866.4835	945.3717
955.9788	961.6923	1001.3475
1018.2981	1022.1640	1023.1395
1060.9032	1106.5774	1112.5288
1189.1342	1208.8206	1300.9315
1317.6602	1321.9348	1356.4636
1451.4968	1488.6456	1542.5602
1646.3072	1678.0686	1704.5522
2356.7409	3165.7967	3177.4723
3190.6170	3200.3570	3209.4294

3221.5049	3225.9779	3264.4163
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p5 + H

C	-1.670801	-1.214753	0.065242
C	-3.056960	-1.170477	0.068242
C	-3.719008	0.050155	0.002714
C	-2.987865	1.230758	-0.064972
C	-1.601648	1.194415	-0.067398
C	-0.927655	-0.030528	-0.002476
C	0.500811	-0.069765	-0.006034
C	1.705724	-0.112073	-0.010673
C	3.137029	-0.109272	-0.010111
C	3.825026	-1.249204	-0.114490
C	3.795702	1.240899	0.116914
H	-1.150468	-2.163686	0.116551
H	-3.622414	-2.093796	0.121826
H	-4.802589	0.081704	0.004707
H	-3.499712	2.184855	-0.117067
H	-1.027956	2.112078	-0.120259
H	3.324076	-2.205201	-0.204464
H	4.909459	-1.244371	-0.112629
H	4.882707	1.146529	0.100806
H	3.497857	1.724872	1.051033
H	3.486913	1.896076	-0.702242

Frequencies

24.8300	59.3319	65.7097
151.4468	174.9497	213.3614
294.5152	377.7471	413.4450
469.4386	499.4271	530.7382
569.1347	601.5227	643.1782
696.2090	710.9187	741.1538
781.8142	866.9011	878.1182
940.1797	945.7091	985.4871
1001.1144	1018.3857	1023.4713
1036.3321	1062.4233	1074.3598
1111.6857	1187.5281	1210.4418
1235.0370	1318.4256	1354.7197
1357.2346	1417.3565	1444.6273
1476.9870	1487.3563	1500.1954
1543.7899	1646.2536	1678.5162
1714.7355	2355.6684	3052.9288
3121.1490	3146.2237	3165.8034
3194.0548	3202.4040	3212.7094
3219.9562	3225.8461	3260.1567

p6 + H

C	1.374722	1.121604	-0.000792
C	2.729249	1.417870	-0.000616
C	3.669965	0.394300	0.000194
C	3.249236	-0.930960	0.000813
C	1.896204	-1.234943	0.000641
C	0.942680	-0.210152	-0.000167
C	-0.452923	-0.514494	-0.000344
C	-1.634385	-0.757867	-0.000509
C	-3.024799	-1.062970	-0.000829
C	-3.999340	-0.146767	-0.000070
C	-3.807583	1.334107	0.001243
H	0.637750	1.915875	-0.001435
H	3.052346	2.452691	-0.001121
H	4.728492	0.627872	0.000331
H	3.979593	-1.731968	0.001444
H	1.563763	-2.266220	0.001136
H	-3.283704	-2.117369	-0.001849
H	-5.025042	-0.506258	-0.000526
H	-4.279800	1.783246	-0.878412
H	-2.749847	1.601751	0.002562
H	-4.281711	1.782008	0.880481

Frequencies

13.3789	59.0167	77.3123
136.3459	149.4796	219.4138
363.6605	369.0779	385.6376
413.6148	497.7370	545.6619
561.0842	641.2578	658.3161
710.3970	745.1463	759.5801
780.5454	866.3104	931.2264
943.2479	992.5024	1000.2980
1001.7223	1017.9571	1023.7204
1062.6995	1069.6484	1112.3141
1127.8097	1188.6545	1207.8876
1258.9957	1304.9714	1317.3381
1355.7349	1403.3164	1442.2660
1485.6934	1488.3003	1491.8483
1542.4370	1646.5873	1678.2117
1723.2437	2352.4516	3043.6271
3102.8103	3139.8752	3168.1667
3188.8146	3191.3021	3202.2518
3210.2567	3221.0061	3225.5410

p7 + H

C	-1.701929	1.184397	0.010822
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C	-3.080283	1.336186	0.006421
C	-3.908070	0.219082	-0.005952
C	-3.349867	-1.054280	-0.014151
C	-1.972497	-1.213966	-0.009640
C	-1.131933	-0.094263	0.002919
C	0.287332	-0.255535	0.008668
C	1.486200	-0.386692	0.014422
C	2.896465	-0.572709	0.024370
C	3.783104	0.425396	-0.021972
C	5.265360	0.239145	-0.010094
H	-1.052535	2.051743	0.020686
H	-3.511430	2.330783	0.013117
H	-4.985183	0.341084	-0.009385
H	-3.991373	-1.928186	-0.023927
H	-1.532635	-2.204106	-0.016148
H	3.247383	-1.601285	0.074452
H	3.413124	1.446610	-0.072417
H	5.536765	-0.817739	0.037238
H	5.713939	0.748323	0.849055
H	5.718657	0.672206	-0.907546

Frequencies

16.0976	54.2526	64.2902
157.6758	165.9411	197.6054
311.3012	316.4827	403.3336
413.4543	457.9635	533.3826
559.5941	592.9607	643.5710
710.3477	757.8738	779.9005
821.3627	866.3493	931.3685
943.1995	991.5854	1000.7698
1017.0997	1023.9961	1047.8534
1069.2215	1073.6320	1111.9369
1135.9572	1188.8489	1206.8942
1290.0967	1316.2369	1329.0344
1335.7765	1355.4051	1422.3438
1481.3289	1488.3410	1496.4685
1541.0633	1646.4914	1678.1189
1736.0671	2354.5849	3040.6229
3101.0750	3129.0735	3159.4301
3175.9082	3190.6371	3200.3848
3210.0046	3220.6828	3225.4162

$p8 + H$

C	1.499181	1.048489	-0.545050
C	2.859417	1.245431	-0.358649
C	3.640801	0.244192	0.206592

C	3.055050	-0.958069	0.586046
C	1.695255	-1.161159	0.403139
C	0.902252	-0.158490	-0.165162
C	-0.502682	-0.362213	-0.353274
C	-1.682680	-0.531395	-0.511844
C	-3.117446	-0.722498	-0.693898
C	-3.991028	0.147705	0.178721
C	-3.563651	1.029923	1.069045
H	0.885627	1.825649	-0.985188
H	3.311832	2.184604	-0.656009
H	4.703499	0.400828	0.351872
H	3.660243	-1.741895	1.027150
H	1.233804	-2.096000	0.698296
H	-3.364733	-1.774678	-0.508567
H	-3.372074	-0.540772	-1.745209
H	-5.058331	0.002935	0.029273
H	-2.504137	1.193076	1.238634
H	-4.262546	1.614758	1.655750

Frequencies

23.6224	61.9992	89.5464
146.4634	177.5749	293.1133
330.9072	382.4401	414.2712
416.3487	546.2607	553.5081
594.0463	626.9746	643.6583
715.3122	744.3548	786.6776
864.2298	904.2609	950.8057
962.9435	990.9330	997.8075
998.4519	1024.2541	1024.4574
1052.6695	1062.3926	1099.1715
1112.9245	1191.9914	1207.7412
1249.1173	1288.4630	1317.4516
1338.3959	1356.1341	1377.2011
1446.7643	1475.4476	1490.3471
1541.9188	1649.3786	1679.9188
1741.7443	2382.8611	3037.9888
3067.0880	3154.6118	3172.1719
3194.4238	3204.6130	3213.4582
3222.1320	3227.1669	3249.8376

p27 + CH3

C	-0.283258	0.916700	0.000000
C	-1.638560	1.206877	0.000001
C	-2.546009	0.149096	0.000001
C	-2.103668	-1.170580	0.000000
C	-0.740371	-1.463695	-0.000002

C	0.163069	-0.416549	-0.000001
C	0.898299	1.790337	-0.000001
C	2.010334	1.035938	-0.000002
C	1.642422	-0.390664	-0.000001
C	2.477235	-1.430707	0.000003
H	-1.989376	2.233230	0.000005
H	-3.610533	0.355163	0.000003
H	-2.827279	-1.977693	0.000001
H	-0.402384	-2.494749	-0.000005
H	0.857665	2.871771	0.000003
H	3.031848	1.391509	0.000000
H	2.110951	-2.451567	0.000002
H	3.552149	-1.288179	0.000006

Frequencies

126.3582	196.3357	255.8370
313.8011	412.8448	458.3690
542.6148	554.4088	574.9900
658.3506	666.3424	725.7150
767.1655	773.9117	794.1780
817.7328	873.0931	895.0496
943.1760	948.9898	958.1894
966.3736	1004.5593	1051.1091
1088.7123	1111.2229	1153.0305
1186.7821	1220.3516	1252.6485
1330.5703	1344.3044	1400.8573
1453.2807	1500.9889	1510.8398
1619.4568	1667.6097	1688.2438
1745.1369	3161.5054	3187.7651
3193.1102	3205.8447	3220.0934
3225.5656	3248.2399	3251.5142

$p28 + H$

C	1.551949	1.273287	-0.000027
C	2.642006	0.402778	-0.000008
C	2.450089	-0.975158	0.000018
C	1.165289	-1.517375	0.000021
C	0.082461	-0.652435	-0.000001
C	0.277257	0.738199	-0.000018
C	-1.059320	1.372975	-0.000021
C	-2.019102	0.259062	-0.000026
C	-1.369208	-0.920037	-0.000009
C	-1.337285	2.677402	0.000044
C	-1.951037	-2.293067	0.000003
H	1.709229	2.346759	-0.000054
H	3.649012	0.804298	-0.000015

H	3.310500	-1.635074	0.000034
H	1.022084	-2.592823	0.000042
H	-3.093271	0.393567	-0.000032
H	-0.551732	3.424933	0.000073
H	-2.361204	3.034386	0.000065
H	-3.041692	-2.263074	-0.000009
H	-1.620769	-2.853371	0.880783
H	-1.620750	-2.853394	-0.880755

Frequencies

121.5205	134.5283	149.2009
208.1938	226.7606	271.8448
405.8236	412.4674	526.1516
537.4549	546.9907	593.4777
612.8245	655.2922	685.8467
760.1962	774.2661	795.8717
805.0824	853.2049	888.4833
946.1275	956.8758	964.7880
1004.9928	1007.9692	1055.9956
1062.0863	1080.6245	1143.4048
1157.2544	1185.8860	1227.6910
1264.9977	1336.3700	1346.3197
1392.5187	1420.2871	1454.7203
1477.9189	1491.3117	1507.5697
1510.9404	1652.8582	1687.1664
1694.2547	1745.4813	3040.0416
3098.3810	3142.6711	3164.0059
3187.0821	3194.9374	3204.4225
3218.0572	3228.4253	3252.8008

p29 + H

C	1.432119	1.365687	0.000001
C	2.707931	0.800067	-0.000003
C	2.869772	-0.581207	-0.000004
C	1.763668	-1.431405	0.000000
C	0.497006	-0.870346	0.000004
C	0.334866	0.525536	0.000003
C	-1.118456	0.802162	0.000003
C	-1.784034	-0.522064	0.000004
C	-0.838584	-1.480020	0.000006
C	-1.718366	1.992505	0.000000
C	-3.265973	-0.700373	-0.000007
H	1.311532	2.444050	0.000003
H	3.580698	1.443118	-0.000005
H	3.868695	-1.003041	-0.000009
H	1.897443	-2.507778	-0.000003

H	-1.023099	-2.547321	0.000005
H	-1.147610	2.914701	-0.000003
H	-2.799274	2.082071	0.000000
H	-3.718192	-0.235192	-0.881667
H	-3.718220	-0.235100	0.881590
H	-3.531671	-1.758755	0.000043

Frequencies

106.6854	136.1469	162.4407
255.6493	286.3439	292.7937
333.3137	415.8243	482.1895
515.8159	557.4890	579.7438
658.8068	663.8281	721.3165
756.0437	771.9024	803.0559
840.7576	860.7374	884.3235
897.6539	948.9560	956.1171
1002.2275	1018.3355	1054.0203
1069.6374	1100.9942	1133.5754
1173.9041	1185.8864	1228.2828
1247.2248	1332.8963	1361.4027
1396.4762	1427.0311	1454.6306
1484.3776	1501.0598	1508.9302
1514.0387	1655.3218	1687.1313
1695.3703	1745.7802	3043.2924
3103.3945	3135.4066	3160.3444
3185.4704	3194.9360	3203.1023
3217.2554	3223.6426	3247.3543

p30 + H

C	-0.905507	-1.504890	0.000012
C	-2.298666	-1.474463	-0.000021
C	-2.983953	-0.262159	-0.000020
C	-2.292586	0.946547	0.000005
C	-0.905377	0.918200	0.000027
C	-0.213240	-0.305963	0.000035
C	1.234398	-0.002134	0.000043
C	1.324261	1.466874	0.000017
C	0.087555	1.996571	0.000004
C	2.230462	-0.895912	0.000004
C	3.693571	-0.596939	-0.000024
H	-0.382266	-2.455509	0.000006
H	-2.855014	-2.405016	-0.000054
H	-4.068307	-0.261093	-0.000044
H	-2.829587	1.888996	0.000006
H	2.250014	2.024766	-0.000071
H	-0.153614	3.051561	-0.000202

H	1.964312	-1.951223	-0.000030
H	3.902060	0.473184	0.000138
H	4.173396	-1.039879	-0.878824
H	4.173493	-1.040165	0.878576

Frequencies

89.0842	125.8736	181.0283
182.5426	258.7555	323.6586
344.6195	428.7803	476.3211
563.9240	572.8404	614.4216
653.1372	707.4640	736.7012
771.6050	776.0033	813.4992
871.9033	877.7239	896.4388
956.1081	964.4678	992.4640
1001.3195	1029.8060	1058.8568
1066.2942	1103.3197	1142.3511
1161.4208	1187.8097	1222.5064
1257.6289	1323.0301	1347.9275
1365.1287	1419.8164	1432.5068
1479.5845	1497.2089	1506.3974
1508.5605	1616.4245	1664.7079
1688.7554	1762.8733	3045.9194
3100.9721	3144.4775	3160.7674
3188.4763	3196.1468	3206.1969
3218.5498	3223.2993	3250.0692

p31 + H

C	-0.422300	-1.453130	0.000048
C	-1.787224	-1.740865	0.000025
C	-2.730727	-0.719673	-0.000021
C	-2.331692	0.615356	-0.000037
C	-0.976601	0.905685	-0.000015
C	-0.015224	-0.126903	0.000015
C	1.315731	0.514926	0.000028
C	1.053090	1.963638	0.000031
C	2.538716	-0.032955	0.000003
C	-0.270967	2.190821	-0.000005
C	2.859987	-1.496536	-0.000054
H	0.293756	-2.264564	0.000101
H	-2.115141	-2.774256	0.000048
H	-3.787046	-0.964543	-0.000039
H	-3.069497	1.410404	-0.000063
H	1.836281	2.710167	0.000043
H	3.381827	0.653997	0.000022
H	-0.758187	3.156808	-0.000023
H	2.441740	-1.993023	-0.881537

H	2.442164	-1.992995	0.881649
H	3.937358	-1.664181	-0.000305

Frequencies

82.3303	178.1382	196.8338
207.9617	252.2322	358.5765
364.8824	430.8201	490.8106
529.0420	575.6608	605.8604
655.8834	725.3488	733.0667
763.8279	772.0102	819.7641
868.4924	878.1846	902.0718
962.3611	969.0567	1001.8940
1010.3765	1060.0926	1060.7645
1086.2264	1105.5238	1124.5123
1153.4166	1187.1315	1216.4788
1229.9281	1317.4815	1346.7516
1387.6987	1409.9201	1424.2853
1496.4761	1501.9071	1508.2611
1512.1823	1625.0999	1664.6197
1687.3560	1751.2899	3045.9469
3105.3673	3143.4287	3170.5453
3187.4181	3201.1905	3212.8044
3229.0644	3232.8125	3251.7230

p32 + H

C	-1.371718	-1.404028	-0.000064
C	-2.565127	-0.698538	-0.000006
C	-2.565126	0.698542	-0.000009
C	-1.371716	1.404031	-0.000068
C	-0.170762	0.699368	-0.000115
C	-0.170764	-0.699367	-0.000113
C	1.211584	-1.208735	-0.000081
C	2.132134	-0.000002	-0.001008
C	1.211587	1.208733	-0.000081
C	1.594610	-2.482607	0.000729
C	1.594616	2.482604	0.000732
H	-1.377549	-2.488480	-0.000098
H	-3.508144	-1.233419	0.000015
H	-3.508142	1.233424	0.000011
H	-1.377547	2.488483	-0.000106
H	2.780852	-0.000003	0.879317
H	2.778598	-0.000003	-0.883019
H	0.873983	-3.292825	0.001396
H	2.644024	-2.755627	0.000793
H	2.644031	2.755621	0.000800
H	0.873993	3.292825	0.001401

Frequencies

33.4972	102.4526	182.1181
250.9359	286.4052	394.7673
414.5271	476.6356	525.9396
537.0011	552.7167	588.6218
596.0686	680.4278	708.8557
748.0650	781.7528	802.9343
819.0324	888.6662	906.2938
914.5608	917.0221	950.0978
964.1723	976.4388	1008.0590
1056.8850	1097.1796	1148.3378
1152.3292	1196.4693	1198.0536
1236.3497	1280.7352	1316.0225
1336.8723	1364.8612	1441.1435
1449.7293	1455.8637	1512.1020
1516.4468	1653.1596	1681.4726
1739.1701	1752.1362	3064.2613
3104.5175	3158.2098	3158.5154
3193.3414	3201.4637	3211.3923
3222.0331	3244.9714	3244.9783

p33 + H

C	0.450178	-1.479838	-0.134096
C	1.817761	-1.731414	-0.089122
C	2.732565	-0.690218	0.033600
C	2.291718	0.629182	0.097390
C	0.932346	0.882299	0.052075
C	0.004228	-0.164855	-0.046382
C	-1.352622	0.425353	-0.089903
C	-1.232883	1.766082	-0.054126
C	-2.637220	-0.275133	-0.142087
C	0.199332	2.195089	0.058989
C	-2.885479	-1.519868	0.259922
H	-0.244213	-2.300821	-0.257903
H	2.175448	-2.752793	-0.157038
H	3.794314	-0.906588	0.069466
H	3.005521	1.442977	0.173007
H	-2.061831	2.462787	-0.077878
H	-3.465429	0.322390	-0.516953
H	0.505105	2.837721	-0.774915
H	0.378850	2.763691	0.979146
H	-2.120913	-2.158206	0.685468
H	-3.886395	-1.931236	0.200045

Frequencies

71.9253	135.8578	187.6531
209.9425	247.7474	356.2326
421.7867	441.7232	495.5413
515.7344	570.6126	610.7520
691.4492	706.6942	740.5310
760.5925	790.7951	828.5469
853.9885	888.5576	949.5899
956.9855	977.4523	990.1417
1006.8136	1024.1785	1038.6836
1062.0848	1111.7113	1158.2932
1162.3649	1185.2224	1202.1576
1240.8736	1270.0001	1328.6465
1335.9425	1352.5323	1402.3400
1440.1215	1454.8284	1506.4799
1513.3126	1644.8371	1664.8863
1686.8270	1739.8903	3048.7027
3082.5763	3160.7315	3175.7054
3187.2687	3197.7632	3213.3957
3225.0123	3229.5220	3260.1078

p34 + H

C	0.765382	-1.521114	-0.046334
C	2.153909	-1.567200	0.029778
C	2.902305	-0.394616	0.093614
C	2.274682	0.849472	0.083992
C	0.894116	0.898615	0.003920
C	0.141064	-0.280339	-0.063782
C	-1.287037	0.079943	-0.131548
C	-1.392295	1.421152	-0.118528
C	-0.043068	2.076212	-0.019030
C	-2.371719	-0.901853	-0.219924
C	-3.578633	-0.751616	0.318722
H	0.187624	-2.438363	-0.084730
H	2.659578	-2.526221	0.043342
H	3.983253	-0.451910	0.155188
H	2.861570	1.760606	0.138049
H	-2.319654	1.973774	-0.198998
H	0.047286	2.685743	0.888082
H	0.151231	2.742014	-0.867804
H	-2.145065	-1.817676	-0.762006
H	-3.831725	0.127620	0.902777
H	-4.346340	-1.507516	0.200829

Frequencies

78.9352	131.2554	193.2994
204.5443	242.6065	343.3383

420.2157	438.7037	472.6973
556.3944	561.3974	628.9595
691.5750	709.9733	738.9596
776.1993	791.5335	820.9280
855.8999	886.8877	946.6300
964.3182	975.5859	988.5872
1005.7411	1037.6161	1049.9976
1061.1241	1093.9128	1144.5322
1154.1031	1187.0496	1206.4389
1238.6138	1278.4000	1315.5165
1333.8843	1346.0101	1378.8752
1437.0073	1464.4172	1508.8177
1516.8768	1650.6704	1685.5614
1693.2972	1725.4545	3048.6827
3083.5697	3147.6166	3162.7086
3184.7604	3192.0187	3202.8541
3217.8192	3230.3353	3241.2321

p35 + H

C	-0.728536	-1.346576	-0.585096
C	-2.081527	-1.394779	-0.252891
C	-2.726247	-0.271814	0.258904
C	-2.035343	0.921234	0.448045
C	-0.686117	0.967535	0.120216
C	-0.037047	-0.164255	-0.390758
C	1.405528	0.175190	-0.673744
C	1.473793	1.632239	-0.256554
C	2.453103	-0.654391	0.031869
C	0.289879	2.060143	0.193444
C	2.233955	-1.580298	0.955111
H	-0.228108	-2.222910	-0.983188
H	-2.636775	-2.315072	-0.394864
H	-3.779692	-0.328658	0.509554
H	-2.541759	1.795794	0.841832
H	1.591262	0.107115	-1.755663
H	2.385612	2.212655	-0.314152
H	3.478150	-0.424906	-0.253366
H	0.069161	3.055203	0.558355
H	3.061273	-2.103085	1.421662
H	1.232219	-1.841501	1.278551

Frequencies

83.0982	114.8897	158.1446
250.9297	268.4208	384.7384
431.8263	460.8400	523.0577
568.4421	576.8375	629.6190

677.3639	726.0448	758.5366
766.1064	797.8660	868.7849
878.7822	910.8313	965.9003
967.7384	974.9852	981.8447
1013.1414	1022.4819	1048.0264
1055.7702	1090.2961	1095.2888
1145.0202	1182.5282	1194.6983
1226.5498	1235.1479	1307.2883
1319.6031	1336.1537	1364.0152
1394.1861	1449.0105	1506.7864
1515.3531	1640.3098	1673.2586
1692.1887	1732.7811	3023.7521
3147.6439	3165.0214	3190.0008
3198.8515	3208.5499	3217.8616
3219.5729	3241.8439	3249.3585

p36 + H

C	-0.826462	-1.549228	-0.000002
C	-2.177046	-1.533133	-0.000003
C	-2.929224	-0.292355	0.000000
C	-2.314255	0.908348	0.000001
C	-0.871404	0.957029	0.000000
C	-0.109460	-0.299845	0.000001
C	1.228333	-0.023116	0.000002
C	1.389423	1.469782	0.000001
C	-0.008557	1.999447	0.000000
C	2.316689	-0.976794	0.000007
C	3.617766	-0.673823	-0.000006
H	-0.286271	-2.489233	-0.000004
H	-2.728636	-2.466809	-0.000006
H	-4.012136	-0.349856	0.000001
H	-2.882433	1.831987	0.000002
H	1.951213	1.812912	-0.878238
H	1.951210	1.812913	0.878240
H	-0.260990	3.051023	-0.000001
H	2.030974	-2.026084	0.000027
H	4.374688	-1.448528	0.000002
H	3.967557	0.353802	-0.000027

Frequencies

81.2239	150.8086	176.6469
184.5300	252.4158	336.8752
344.2629	470.4824	487.3051
516.9435	548.0225	590.1471
668.2377	669.3391	699.9799
741.0909	772.5121	784.1407

856.7709	888.6616	898.4431
927.8787	971.0752	993.7270
995.4294	1011.7005	1022.7389
1027.0510	1040.2384	1126.3269
1156.5216	1190.6408	1216.4553
1228.3952	1257.3770	1338.6852
1358.2715	1403.9157	1405.2785
1421.6392	1452.1893	1489.1168
1585.1900	1612.2760	1644.9637
1707.7777	1732.9650	3043.9348
3078.4371	3157.0685	3165.6425
3188.7122	3197.1132	3210.5956
3219.1145	3235.2319	3253.2870

p37 + H

C	0.442654	-1.506134	-0.162315
C	1.771753	-1.740834	-0.107969
C	2.734570	-0.667668	0.049741
C	2.349291	0.623548	0.116748
C	0.942748	0.940605	0.049703
C	-0.037722	-0.150826	-0.059775
C	-1.297523	0.375683	-0.091289
C	-1.171574	1.872594	-0.039587
C	-2.587251	-0.291010	-0.176715
C	0.294152	2.128356	0.065273
C	-2.895012	-1.492153	0.318144
H	-0.259210	-2.318631	-0.305501
H	2.145960	-2.754819	-0.196828
H	3.787198	-0.923900	0.098550
H	3.075860	1.422606	0.214604
H	-1.600469	2.332973	-0.940472
H	-1.724238	2.293721	0.810707
H	-3.374364	0.275086	-0.673304
H	0.741073	3.109778	0.144802
H	-2.180688	-2.081033	0.882460
H	-3.887637	-1.908743	0.193223

Frequencies

97.3375	148.5910	185.2643
190.2935	251.8674	332.8876
391.0427	458.3443	482.1572
519.8509	531.6938	585.5940
674.2811	683.9745	709.4121
739.8290	773.7499	791.1490
862.8536	889.8869	896.9519
954.6863	973.2466	995.3882

1002.5806	1011.4852	1018.7265
1038.3561	1114.1826	1131.6367
1139.9714	1174.5211	1200.0691
1222.4767	1256.8535	1321.9912
1341.2494	1402.2440	1406.7278
1414.7632	1462.2245	1481.8258
1584.8169	1618.1307	1649.3342
1706.0523	1732.2804	3038.0795
3071.9927	3139.7675	3164.9150
3187.2384	3198.5055	3211.7610
3226.2512	3237.5211	3252.8495

p38 + CH3

C	0.000000	-0.710183	0.000000
C	0.000000	0.710183	0.000000
C	1.240907	1.396272	0.000000
C	2.421887	0.706735	0.000000
C	2.421887	-0.706735	0.000000
C	1.240908	-1.396272	0.000000
C	-1.240907	-1.396272	0.000000
C	-2.421887	-0.706734	0.000000
C	-2.421886	0.706734	0.000000
C	-1.240907	1.396272	0.000000
H	1.237769	2.481481	0.000000
H	3.364789	1.241538	0.000000
H	3.364790	-1.241538	0.000000
H	1.237770	-2.481481	0.000000
H	-1.237770	-2.481481	0.000000
H	-3.364794	-1.241538	0.000000
H	-3.364800	1.241541	0.000000
H	-1.237769	2.481481	0.000000

Frequencies

171.5891	183.9252	367.4296
394.8906	481.3061	485.9152
521.6916	523.1722	637.8144
641.6353	727.5514	785.3336
791.1627	804.1738	811.8000
850.9893	902.7167	954.8211
972.0033	989.1822	1008.7409
1014.3510	1042.9674	1056.7628
1162.3137	1162.7224	1182.5444
1197.4560	1240.5369	1271.7387
1292.4368	1400.4451	1424.5318
1430.5037	1499.3545	1507.2749
1569.3899	1653.8108	1674.8670

1714.8066	3188.8241	3189.5136
3193.0047	3195.1937	3207.7492
3208.4595	3220.8476	3221.7931

p3 + H

C	-1.404538	-1.509654	0.000002
C	-2.691889	-1.045462	0.000008
C	-2.949915	0.343258	0.000004
C	-1.912687	1.235712	0.000001
C	-0.569478	0.784598	0.000004
C	-0.309067	-0.610015	-0.000003
C	1.036661	-1.060626	-0.000023
C	1.813991	1.209031	-0.000006
C	2.089149	-0.184385	-0.000021
C	0.532167	1.678569	0.000002
C	3.518423	-0.655749	0.000023
H	-1.205739	-2.576591	0.000002
H	-3.520704	-1.744437	0.000015
H	-3.974117	0.698773	0.000003
H	-2.105285	2.303829	-0.000002
H	1.222728	-2.130972	-0.000048
H	2.644735	1.908098	-0.000021
H	0.340188	2.746819	-0.000005
H	3.580328	-1.745463	-0.000770
H	4.050242	-0.286500	0.881936
H	4.050719	-0.285207	-0.881053

Frequencies

73.2695	115.7947	181.9132
264.9901	281.4546	402.6285
416.2783	456.4724	485.8276
519.9192	531.2685	637.4324
649.3701	717.8813	754.3360
788.3549	793.1639	835.2625
866.4121	904.0400	908.2899
974.0452	976.2160	995.2258
1012.2165	1026.9152	1054.1666
1067.8975	1159.0486	1172.7059
1193.1987	1208.2723	1238.3418
1287.4364	1302.4088	1396.9977
1413.8415	1418.3968	1433.6409
1476.8416	1484.6902	1506.0069
1522.8716	1567.5205	1652.2029
1683.3706	1721.2031	3048.6893
3112.0664	3139.2399	3181.5918
3182.1302	3185.7006	3190.5646

3201.9201	3204.7811	3218.3837
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p4 + H

C	-1.847395	-1.196224	-0.000023
C	-2.756016	-0.174174	-0.000032
C	-2.309838	1.164270	0.000010
C	-0.970500	1.448043	0.000041
C	-0.000500	0.412188	0.000022
C	-0.454316	-0.935190	0.000011
C	0.493260	-1.990433	0.000025
C	2.280079	-0.376108	-0.000023
C	1.404813	0.679440	-0.000017
C	1.829765	-1.714954	0.000018
C	1.913979	2.096070	-0.000018
H	-2.182277	-2.228606	-0.000049
H	-3.819018	-0.387045	-0.000072
H	-3.034436	1.970742	0.000013
H	-0.646311	2.481890	0.000084
H	0.136617	-3.015228	0.000033
H	3.347730	-0.180975	-0.000069
H	2.555599	-2.520270	0.000025
H	3.004840	2.114141	-0.000993
H	1.569422	2.643609	0.882508
H	1.567839	2.644176	-0.881564

Frequencies

127.4312	150.5757	176.6390
245.9094	288.6763	418.7345
445.7635	480.9815	488.4051
523.1424	547.1521	581.4000
644.2405	721.0279	745.5692
794.4175	807.6769	815.7169
877.6185	880.9331	917.3952
979.2128	996.4349	1004.5161
1012.3358	1053.9502	1065.1122
1086.8323	1108.1260	1173.4135
1199.9980	1203.0492	1241.7189
1276.9526	1301.0518	1387.2733
1413.1669	1426.6647	1441.4108
1475.3628	1484.2044	1508.8061
1513.2069	1572.7917	1662.4634
1677.0095	1709.5024	3045.7479
3106.7352	3141.8477	3184.2791
3186.4721	3192.9463	3198.7168
3210.0701	3216.5640	3222.6925

p39 + H

C	1.402288	-1.469895	0.022994
C	2.688376	-0.966917	-0.140632
C	2.894562	0.405954	-0.185710
C	1.812520	1.267479	-0.074044
C	0.518534	0.770456	0.085153
C	0.313566	-0.615876	0.139897
C	-1.077202	-1.147099	0.396312
C	-1.894824	1.214679	0.079289
C	-2.189705	-0.215292	-0.024742
C	-0.636829	1.667545	0.151556
C	-3.382538	-0.658560	-0.427263
H	1.243454	-2.543258	0.062646
H	3.526621	-1.648338	-0.232182
H	3.894464	0.804739	-0.312795
H	1.966010	2.341068	-0.119629
H	-1.204680	-2.129178	-0.065231
H	-1.173188	-1.297935	1.481378
H	-2.727312	1.910372	0.047600
H	-0.442675	2.734609	0.198895
H	-3.589279	-1.717984	-0.533693
H	-4.185907	0.031061	-0.663847

Frequencies

75.5000	145.5932	223.0846
303.6816	334.1376	409.3632
419.0582	464.1474	516.7245
522.4715	573.1917	629.3623
691.9247	733.9759	751.1156
774.6537	785.2910	831.9716
869.1790	887.0486	917.3690
930.9355	960.3791	984.5927
991.7112	1007.7535	1014.3822
1076.1922	1142.2043	1182.2187
1188.4469	1226.4241	1232.2401
1249.8823	1291.6713	1333.8429
1336.3722	1367.9186	1424.3537
1465.4352	1474.6527	1500.5274
1544.1734	1644.1926	1679.1747
1699.1812	1737.5787	3011.4025
3097.2644	3156.1813	3181.9988
3183.1354	3188.3103	3202.0934
3203.6220	3217.3248	3245.0206

p40 + H

C	-1.722820	-1.265296	0.043545
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C	-2.745332	-0.335112	-0.005895
C	-2.433162	1.019771	-0.066128
C	-1.109756	1.419911	-0.067265
C	-0.064061	0.490771	-0.000644
C	-0.383248	-0.872616	0.043823
C	0.680448	-1.942040	0.091792
C	2.366864	-0.133236	-0.125142
C	1.358495	0.923803	0.005787
C	2.072244	-1.430118	-0.086817
C	1.752361	2.196832	0.135750
H	-1.957872	-2.324911	0.080855
H	-3.779395	-0.660741	-0.006337
H	-3.221748	1.761621	-0.118404
H	-0.885086	2.477360	-0.134321
H	0.614709	-2.475316	1.050157
H	0.465571	-2.697683	-0.673667
H	3.398583	0.185999	-0.235955
H	2.864021	-2.168271	-0.168549
H	2.807298	2.446539	0.124144
H	1.061725	3.019381	0.269232

Frequencies

50.1875	126.4525	215.7600
313.8890	330.0758	423.4863
442.8765	470.1894	499.0219
502.1866	579.2752	608.2983
672.3616	717.8255	750.7953
783.6811	794.0409	806.5789
860.0879	885.5160	910.0740
946.1492	964.2331	986.0267
1003.9621	1009.1157	1023.3899
1080.1371	1120.1533	1165.1914
1198.9126	1211.0047	1217.7877
1230.6738	1290.9928	1337.8849
1351.5533	1388.4595	1424.3622
1462.1281	1473.7538	1508.3101
1542.4370	1648.7547	1685.6907
1695.5854	1761.0360	3022.1291
3052.3424	3168.6438	3176.8974
3178.1652	3196.7977	3199.8497
3209.8049	3223.4774	3257.9432

p41 + H

C	-1.722988	-1.286816	-0.142103
C	-2.750488	-0.365553	-0.002349
C	-2.451148	0.979949	0.175370

C	-1.127524	1.398159	0.196330
C	-0.085834	0.485537	0.042299
C	-0.389124	-0.880590	-0.110208
C	0.701495	-1.854564	-0.227066
C	2.331920	-0.130070	0.473185
C	1.337309	0.899815	-0.005521
C	1.962989	-1.524046	0.043599
C	1.725117	2.084751	-0.475356
H	-1.950634	-2.339796	-0.273957
H	-3.782486	-0.696954	-0.023675
H	-3.247702	1.704144	0.302516
H	-0.898236	2.446400	0.352362
H	0.443367	-2.872003	-0.503621
H	2.371006	-0.110179	1.573337
H	3.335095	0.129233	0.126488
H	2.750137	-2.269307	-0.000364
H	2.775425	2.351474	-0.523274
H	1.013691	2.817559	-0.838901

Frequencies

102.7000	131.9421	190.6557
297.3980	359.2403	402.1489
432.3681	494.4096	516.2755
541.7656	561.8544	599.6573
692.5190	719.0426	725.0237
787.5255	791.6843	822.6638
870.3770	912.0320	930.4466
935.9319	967.5245	986.0905
1005.1206	1013.3579	1018.3895
1073.4504	1115.3894	1160.2827
1190.7897	1200.5695	1215.5771
1241.2875	1289.4851	1333.5524
1336.7448	1365.5651	1430.2439
1450.4924	1466.0226	1500.5432
1533.6008	1640.5951	1679.0259
1727.8295	1737.9697	3002.2451
3104.4456	3154.6453	3179.4066
3186.1418	3194.8941	3204.9371
3206.1061	3217.0962	3241.4061

p42 + H

C	-1.428207	-1.515668	0.130038
C	-2.672416	-1.017596	0.019198
C	-2.896556	0.408042	-0.139339
C	-1.864793	1.268066	-0.160525
C	-0.491681	0.805714	-0.017269

C	-0.261971	-0.650213	0.094046
C	0.998013	-1.145345	0.096493
C	1.952084	1.183140	0.267802
C	2.169846	-0.289720	-0.008795
C	0.550830	1.654565	0.028939
C	3.376170	-0.785412	-0.309500
H	-1.264847	-2.582862	0.238364
H	-3.529064	-1.681860	0.040451
H	-3.913598	0.770220	-0.237625
H	-2.030967	2.334608	-0.271726
H	1.152174	-2.220615	0.104264
H	2.181601	1.367292	1.329952
H	2.667009	1.788450	-0.296404
H	0.380655	2.724555	-0.043548
H	3.528068	-1.851274	-0.440522
H	4.241051	-0.141951	-0.429738

Frequencies

71.4025	145.4369	210.7495
283.0831	288.1003	405.2593
448.7377	465.0683	483.3582
500.4622	541.8139	620.4739
688.4497	701.4752	739.3369
748.3194	757.1544	816.7215
855.3484	869.7824	889.8718
912.1515	925.6196	971.5271
994.0798	1003.4182	1007.0140
1018.1068	1062.9082	1167.7335
1188.9184	1226.5011	1229.8415
1236.3824	1313.0016	1344.9641
1365.8709	1411.3836	1432.2985
1451.1191	1464.2727	1479.6313
1627.7899	1637.9838	1681.4082
1712.4397	1748.4506	2984.7390
3090.4776	3157.3316	3182.7227
3185.5202	3187.1347	3190.9377
3205.7057	3217.3935	3245.9296

Fragments

CH_3

Cartesian coordinates

C	-0.000147	0.000018	0.0
H	0.598306	-0.900124	-0.0
H	0.481424	0.967479	-0.0
H	-1.078846	-0.067462	-0.0

Frequencies

470.9451	1399.8856	1409.5749
3117.6199	3301.0861	3304.8947

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