

Electronic Supporting Information

From the Laboratory to Space: Unveiling Isomeric Diversity of C₅H₂ in the Reaction of Tricarbon (C₃, X¹Σ_g⁺) with the Vinyl Radical (C₂H₃, X²A')

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Methods

Experimental

The gas-phase reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 ; X^2A') was carried out under single-collision conditions using the crossed molecular beams machine.^{1,2} The experimental setup, data acquisition, and data processing are described elsewhere in detail.³⁻⁵ Compared to ‘classic’ crossed-molecular beam experiments where active species are generated only in the primary beam, our setup was altered *ad hoc* to introduce a second laser beam to generate radicals in the secondary source (Figure 1); this restricted the lowest detector position angle to 24° and changed the timing scheme of the experiment (Figure S1). Briefly, a supersonic molecular beam of tricarbon was prepared *in situ* in the primary source chamber by laser ablation (3mJ, 266nm, 30 Hz; Quanta-Ray) from a rotating carbon rod.^{6,7} The ablated species were seeded in neat carrier gas (Helium, 99.9999%, Airgas) released by a Proch-Trickl pulsed valve operating at 60 Hz and a backing pressure of 4 atm. A four-slot chopper wheel located between the skimmer of the primary source and the cold shield allowed to select the segment of the pulsed tricarbon beam with a peak velocity of $v_p = 1761 \pm 15 \text{ m s}^{-1}$ and speed ratio $S = 5.7 \pm 0.3$. The secondary pulsed supersonic beam of the vinyl radicals was generated via photodissociation of vinylbromide (CH_2CHBr ; Aldrich, 99%) seeded at a level of 1% in helium (He, 99.9999 %, Airgas) at a backing pressure of 1 atm using the 193 nm output of the excimer laser (Coherent, CompEx110; 40 mJ pulse⁻¹; 30 Hz) focused ($2 \times 5 \text{ mm}^2$) at the exit of the primary pulsed valve 2 mm downstream.^{8,9} This yielded a vinyl radical beam with a v_p of $1607 \pm 30 \text{ ms}^{-1}$ and S of 8.5 ± 0.3 . Two molecular beams intersected at an angle of 90° in the scattering chamber at a mean collision energy of $E_C = 44 \pm 1 \text{ kJ mol}^{-1}$. The reaction products scattered from a collisional region were monitored using a triply differentially pumped (10^{-12} Torr) quadrupole mass spectrometric detector (QMS; Extrel, QC 150; 1.2 MHz) operated in the time-of-flight (TOF) mode with electron ionization (80eV, 2mA).¹⁰ This, also called ‘universal’, detector can be rotated within the plane defined by the primary and the secondary reactant beams to record angular resolved TOF spectra. Integration of the TOF spectra at distinct laboratory angles allows us to derive the laboratory angular distribution (LAD) – the signal intensity of an ion with a specific mass-to-charge ratio (m/z) versus the laboratory angle.

To gain information on the reaction dynamics, TOF spectra and the laboratory angular distribution (LAD) were transformed from the laboratory to the center-of-mass (CM) frame by a forward-convolution routine.^{9,11,12} This approach uses initially a trial angular flux $T(\theta)$ and translational energy $P(E_T)$ distributions of products in the CM frame to simulate the laboratory data (TOFs and LAD). CM functions were iteratively varied until the best fit of the TOF spectra and LAD was achieved. Together, the CM functions constitute the reactive differential cross sections $I(\theta, u) \sim P(u) \times T(\theta)$, where u is the CM velocity, θ is the angle in the CM system. The reactive differential cross sections can be represented as a flux contour map that depicts the probability of the products to scatter at a specific angle (θ) with the specific kinetic energy (u).

Computational

Geometry optimizations of various stationary points on the doublet C_5H_3 potential energy surface (PES), including reactants, products, intermediates, and transition states and vibrational frequency calculations for the optimized structures were performed using the long-range corrected hybrid ω B97X-D density functional¹³ in conjunction with Pople’s 6-311G(d,p) basis set,¹⁴ as implemented in the Gaussian 09 software package.¹⁵ The ω B97X-D method includes Grimme’s dispersion correction, which accounts for London dispersion interactions that are not always well described by standard density functionals. The optimized reactants, intermediates, and products exhibited only real, positive vibrational frequencies. In contrast, transition states were characterized by a single imaginary frequency, with all remaining frequencies being real and positive. The zero-point energy (ZPE) correction is calculated as one-half the sum of all vibrational frequencies, excluding any imaginary frequencies associated with transition states.

Specifically, the ω B97X-D method provides reasonably accurate structural geometries; bond lengths are typically determined to within 0.01-0.02 Å, bond angles to within 1-2°, and vibrational frequencies to within 30-40 cm⁻¹. The nature of each transition state was further confirmed through intrinsic reaction coordinate (IRC) calculations¹⁶ at the ω B97X-D/6-311G(d,p) level of theory.

To improve upon a typical 12-20 kJ mol⁻¹ error associated with DFT relative energies, single-point energy calculations were performed using explicitly correlated coupled-cluster CCSD(T)-F12b^{17,18} theory with the cc-pVTZ-f12 basis set¹⁹ in Molpro 2015.²⁰ However, these single-determinant CCSD(T)-F12b calculations revealed the need for a multireference treatment for certain species. Specifically, the T1 diagnostic values for suspected structures exceeded established thresholds (0.02/0.025 for singlet/triplet products and 0.03 for doublet intermediates/transition states), indicating significant multireference character. For structures deemed unreliable by CCSD(T)-F12b, multireference CASPT2 calculations^{21,22} were then employed, utilizing both cc-pVTZ and cc-pVQZ basis sets¹⁹ to allow for extrapolation to the complete basis set (CBS) limit. The CBS extrapolation was performed using a two-point scheme:²³ $E(\text{CBS})=E(\text{VQZ})+0.69377\times[E(\text{VQZ})-E(\text{VTZ})]$.

The CASPT2 calculations utilized initial orbitals obtained from full-valence, multireference CASSCF calculations^{24,25} employing the same basis sets.¹⁹ The active space, selected to balance the computational efficiency with sufficiently accurate wavefunction description, comprised all π orbitals. This balance resulted in an active space of 13 electrons in 13 orbitals for doublet intermediates and transition states, and 12 electrons in 12 orbitals for singlet and triplet products. To combine CCSD(T)-F12b and CASPT2 energies on the PES, relative CASPT2 energies were computed. For suspected intermediates and transition states, these energies were referenced to the energy of the nearest intermediate **ix** on the PES, chosen because its T1 diagnostic was below 0.03, indicating the reliability of the single-determinant CCSD(T)-F12b method for that species. For suspected singlet products, two approaches were used. Either the composite triplet-singlet gap method^{26,27} was employed if the corresponding triplet state at the singlet geometry possessed a T1 value below 0.025 in CCSD(T) calculations. Or in the other case, relative CASPT2 energies were computed with respect to the energy of a singlet product **p5** with a very low T1 value. For suspected triplet products, relative CASPT2 energies were referenced to the energy of the triplet product **p2**, also chosen for its low T1 diagnostic (T1 < 0.025). This approach, referencing to nearby single-reference species on the PES rather than bimolecular reactants, circumvents the issue of size consistency in the CASPT2 method. The final relative energy for each considered case was then calculated using the following expressions:

$$E(\text{rel})_{\text{final}}(i/ts) = E(\text{rel})_{\text{CCSD(T)-F12/cc-pVTZ-f12}}(i_x) + \Delta E_{\text{CASPT2(13,13)/CBS(VQZ,VTZ)}} + \text{ZPE}[\omega\text{B97X-D/6-311G(d,p)}] \quad (1)$$

where

$$\Delta E_{\text{CASPT2(13,13)/CBS(VQZ,VTZ)}} = E_{\text{CASPT2(13,13)/CBS(VQZ,VTZ)}}(i/ts) - E_{\text{CASPT2(13,13)/CBS(VQZ,VTZ)}}(i_x) \quad (2)$$

$$E(\text{rel})_{\text{final}}(\text{singlet } p_x) = E(\text{rel})_{\text{CCSD(T)-F12/cc-pVTZ-f12}}(\text{triplet state of } p_x) + \Delta E_{\text{CASPT2(12,12)/CBS(VQZ,VTZ)}} + \text{ZPE}[\omega\text{B97X-D/6-311G(d,p)}] \quad (3)$$

where

$$\Delta E_{\text{CASPT2(12,12)/CBS(VQZ,VTZ)}} = E_{\text{CASPT2(12,12)/CBS(VQZ,VTZ)}}(\text{singlet } p_x) - E_{\text{CASPT2(12,12)/CBS(VQZ,VTZ)}}(\text{triplet state of } p_x) \quad (4)$$

$$E(\text{rel})_{\text{final}}(\text{singlet/triplet } p_y) = E(\text{rel})_{\text{CCSD(T)-F12/cc-pVTZ-f12}}(\text{singlet } p_5 / \text{triplet } p_2) + \Delta E_{\text{CASPT2}(12,12)/\text{CBS}(\text{VQZ,VTZ})} + \text{ZPE}[\omega\text{B97X-D/6-311G(d,p)}] \quad (5)$$

where

$$\Delta E_{\text{CASPT2}(12,12)/\text{CBS}(\text{VQZ,VTZ})} = E_{\text{CASPT2}(12,12)/\text{CBS}(\text{VQZ,VTZ})}(\text{singlet/triplet } p_y) - E_{\text{CASPT2}(12,12)/\text{CBS}(\text{VQZ,VTZ})}(\text{singlet } p_5 / \text{triplet } p_2) \quad (6)$$

The combined CCSD(T)-F12b/cc-pVTZ-f12// ω B97X-D/6-311G(d,p)+ZPE[ω B97X-D/6-311G(d,p)] theoretical scheme, incorporating multireference $E_{\text{CASPT2}(13,13 \text{ or } 12,12)/\text{CBS}(\text{cc-pVQZ,cc-pVTZ})}$ corrections where necessary, is anticipated to yield relative energies with an accuracy of 4 kJ mol⁻¹ or better.²⁸

Microcanonical rate constants for the unimolecular steps following bimolecular reactions on the doublet C₅H₃ PES were calculated using RRKM statistical theory.^{29–31} In RRKM statistical calculations, vibrational frequencies are essential for determining the density of states of intermediates and the sum of states of the activated complex. Within the harmonic approximation, these rate constants, which depend on the internal energy of the intermediate or transition state, were calculated for all unimolecular reaction steps following the formation of a collision complex from the initial recombination of reactants in a single collision event. The internal energy of each structure on the PES was determined as the sum of the collision energy and the chemical activation energy (defined as the negative of the relative energy with respect to the separated reactants). To mimic the single-collision conditions in crossed molecular beams experiments relevant to deep space environments, the statistical calculations were performed in the zero-pressure limit. The Unimol code³² was employed for these rate constant calculations. Product branching ratios were then determined by solving first-order kinetic equations using the steady-state approximation.^{32,33}

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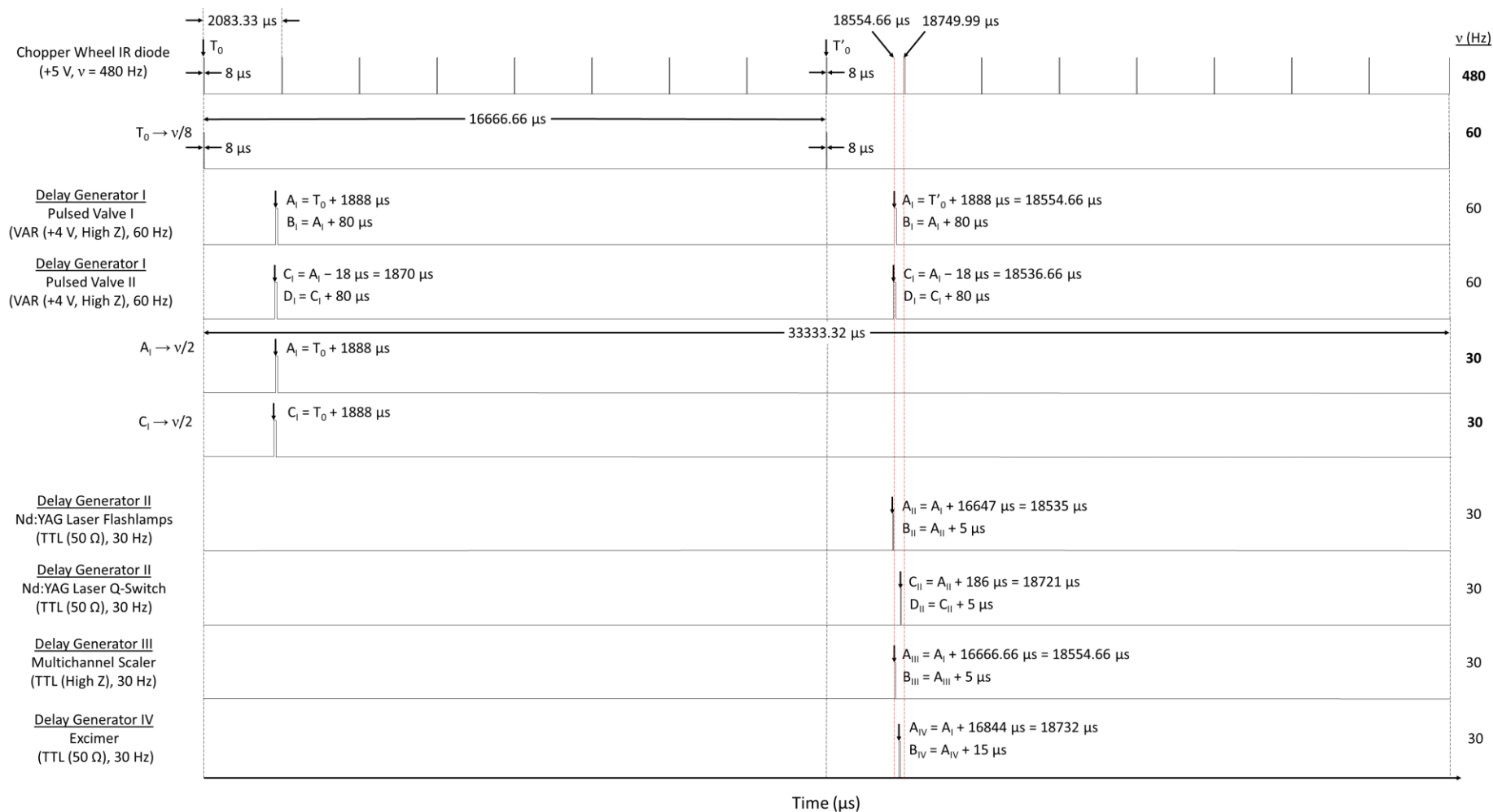


Figure S1. Timing chart for the crossed molecular beam experiment for the reaction of the tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A')

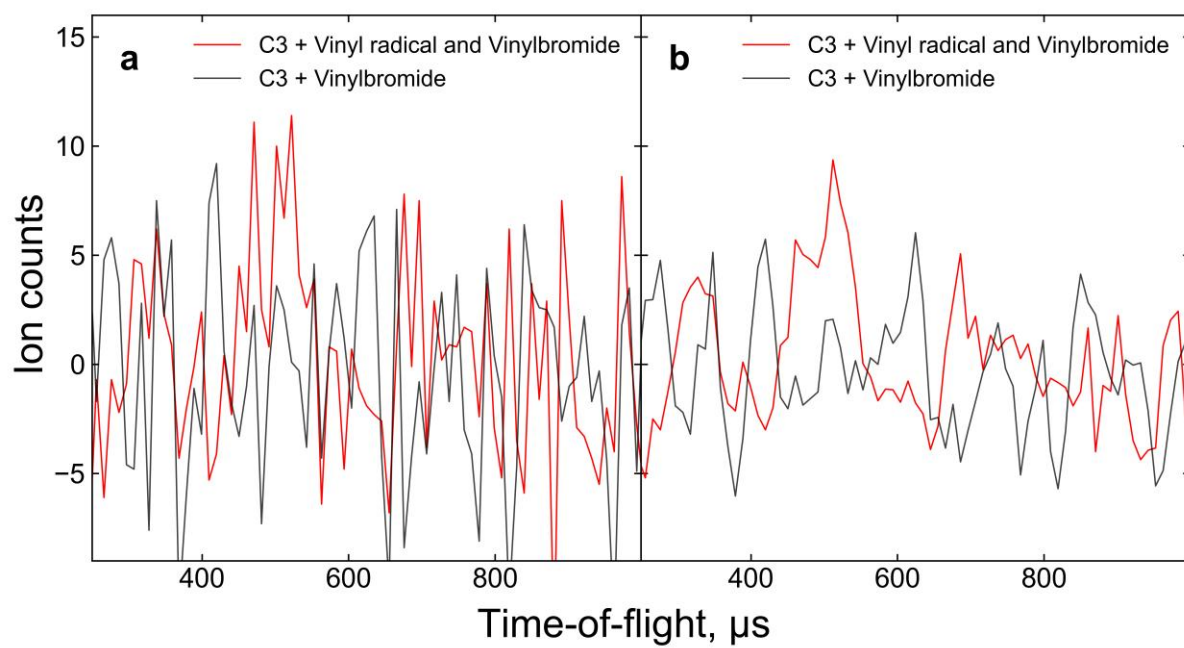


Figure S2. The TOFs for $m/z = 62$ recorded for the same amount of time at CM angle 34.25° with photodissociation in secondary beam (red) and without (black). (a) Raw data, (b) smoothed.

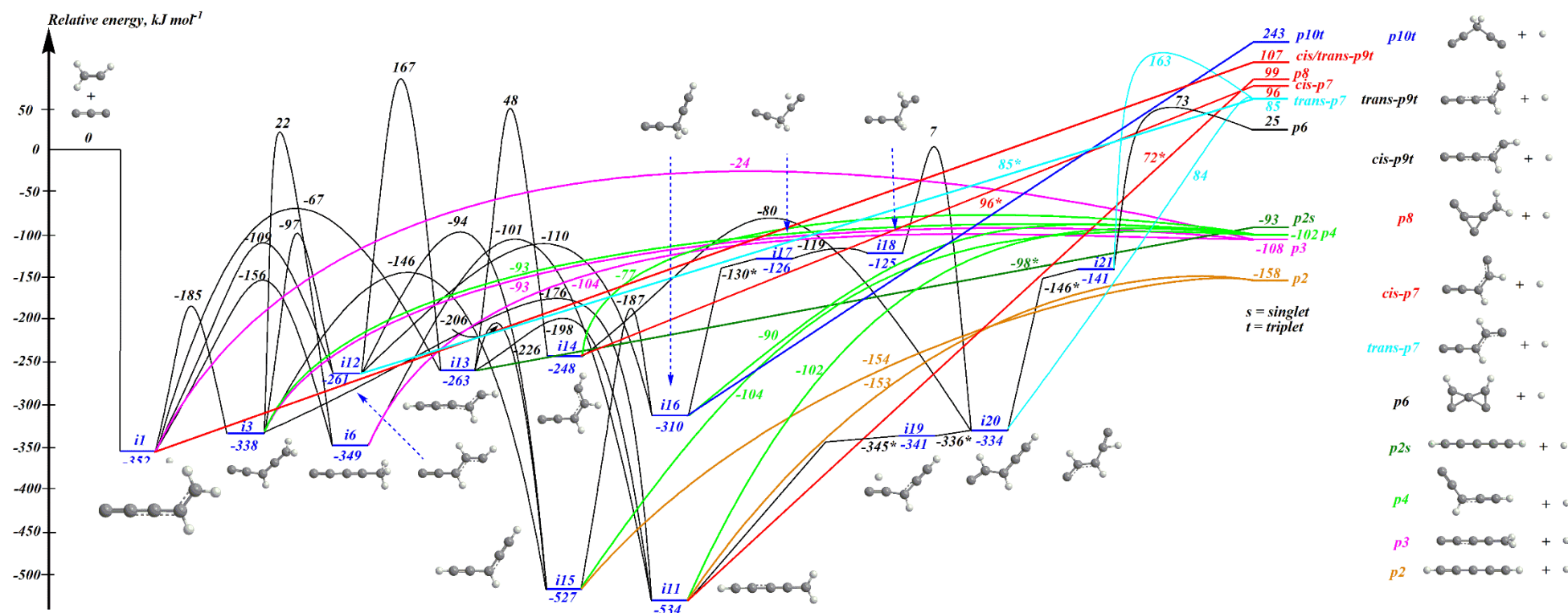


Figure S3. Potential energy surface for the bimolecular reaction of the tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') leading to C_5H_2 isomers plus the atomic hydrogen calculated at the CCSD(T)-F12/cc-pVTZ-f12// ω B97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1} . Part I.

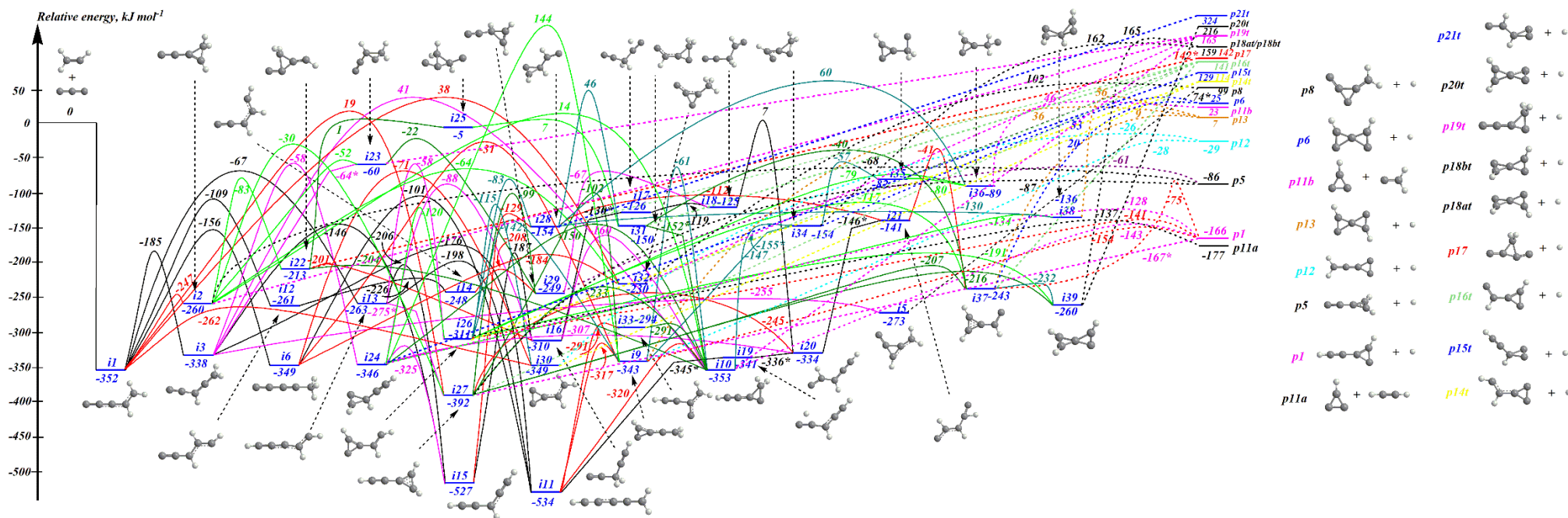


Figure S4. Potential energy surface for the bimolecular reaction of the tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') leading to C_5H_2 isomers plus the atomic hydrogen calculated at the CCSD(T)-F12/cc-pVTZ-f12// ω B97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1} . Part II.

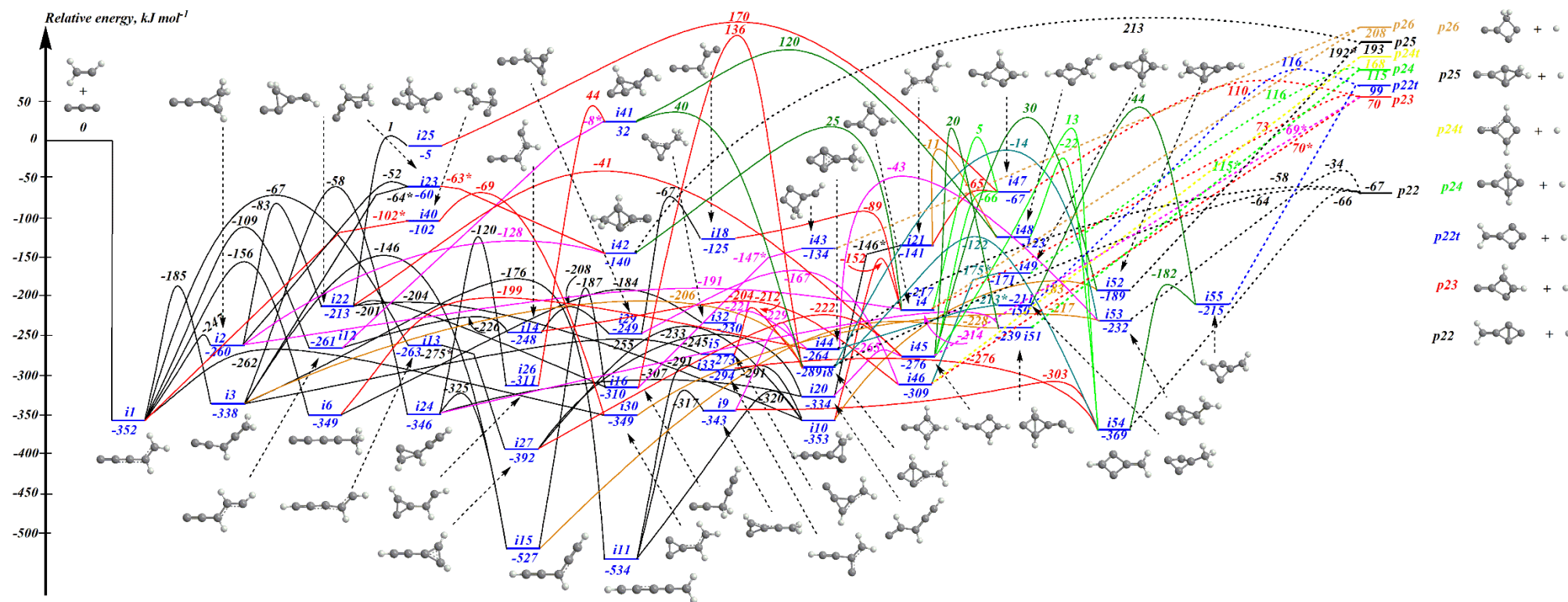


Figure S5. Potential energy surface for the bimolecular reaction of the tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') leading to C_5H_2 isomers plus the atomic hydrogen calculated at the CCSD(T)-F12/cc-pVTZ-f12// ω B97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1} . Part III.

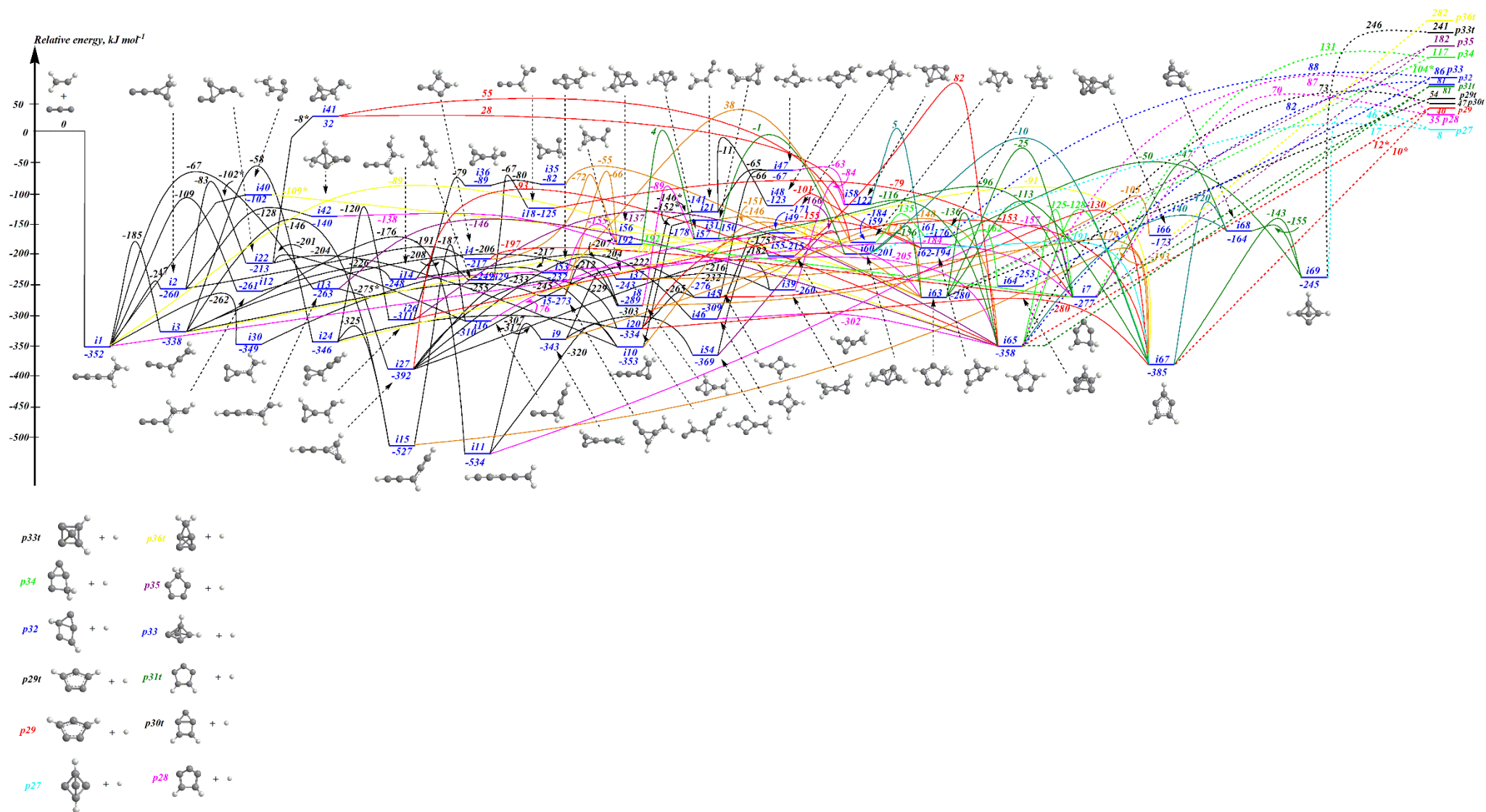


Figure S6. Potential energy surface for the bimolecular reaction of the tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') leading to C_5H_2 isomers plus the atomic hydrogen calculated at the CCSD(T)-F12/cc-pVTZ-f12// ω B97X-D/6-311G(d,p) level of theory. Relative energies are given in kJ mol^{-1} . Part IV.

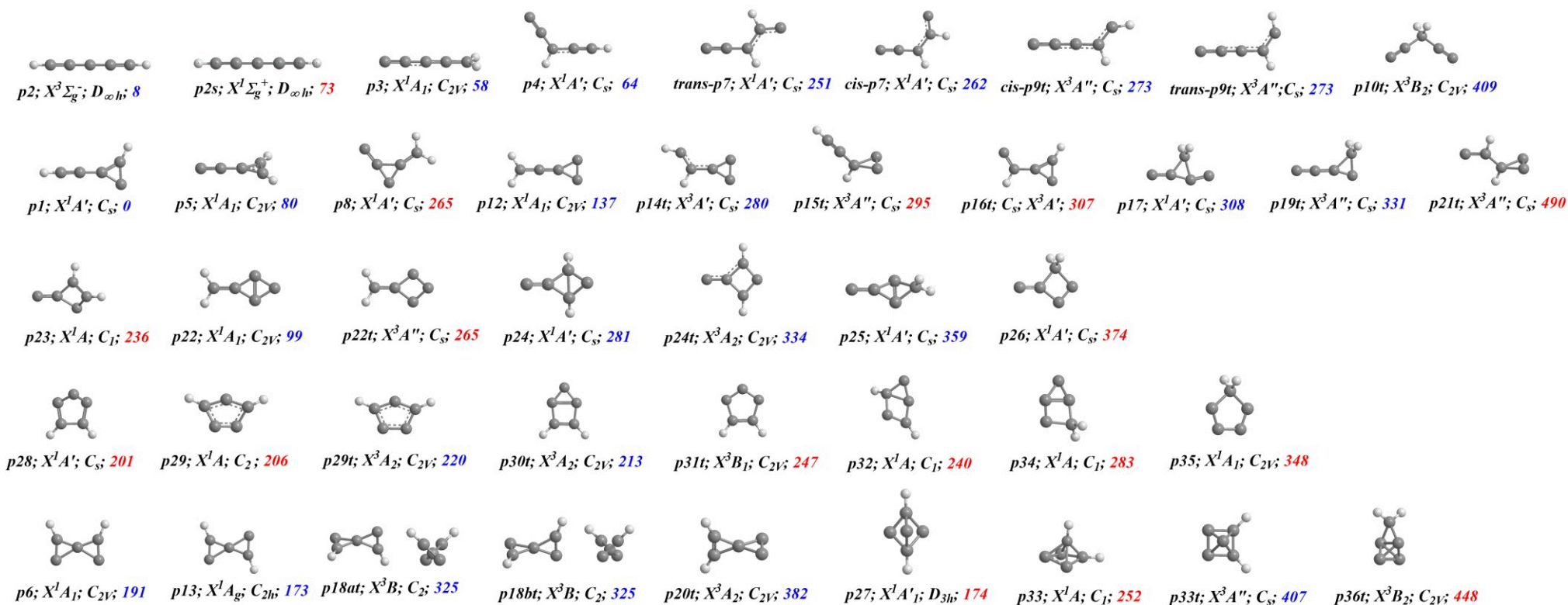


Figure S7. C_5H_2 isomers considered in this work. Relative energy in kJ mol^{-1} were calculated at different levels of energy: CCSD(T)-F12/cc-pVTZ-f12 (blue values) and CASPT2(12,12)/CBS(cc-pVQZ,cc-pVTZ) (red values).

Table S1. RRKM calculated statistical product branching ratios (%) for the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') at different collision energies.

Products	E_{col} , kJ mol ⁻¹					
	0	10	20	30	44	50
$p1+H$	10.7	10.1	9.5	9.0	8.2	7.9
$p2+H$	79.8	77.8	75.5	72.9	69.0	67.3
$p2s+H$ *	0.0	0.0	0.0	0.1	0.1	0.1
$p3+H$	7.4	9.4	11.4	13.4	16.3	17.5
$p4+H$	1.6	2.3	3.2	4.2	5.8	6.6
$p5+H$	0.0	0.1	0.1	0.1	0.2	0.3
$p11a+C_2H_2$	0.3	0.3	0.3	0.3	0.3	0.3

* s – singlet

Table S2. RRKM calculated rate constants ($k(E)$, s⁻¹) of the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') as functions of the internal energy (E , kJ mol⁻¹) of the intermediates for unimolecular reaction steps corresponding to different collision energies (E_{col} , kJ mol⁻¹)

E_{col} , kJ mol ⁻¹	0	10	20	30	44	50
$i44 - p22+H$	9.35E+06	2.07E+07	4.19E+07	7.85E+07	1.71E+08	2.32E+08
$i1 - i2$	8.96E+10	1.00E+11	1.11E+11	1.23E+11	1.40E+11	1.48E+11
$i2 - i1$	3.59E+12	3.66E+12	3.72E+12	3.78E+12	3.86E+12	3.90E+12
$i2 - p5+H$	1.48E+08	2.96E+08	5.48E+08	9.55E+08	1.91E+09	2.50E+09
$i1 - i3$	1.80E+10	2.27E+10	2.82E+10	3.46E+10	4.53E+10	5.05E+10
$i3 - i1$	3.20E+10	3.99E+10	4.92E+10	5.98E+10	7.73E+10	8.58E+10
$i1 - i12$	1.11E+08	1.75E+08	2.66E+08	3.92E+08	6.47E+08	7.90E+08
$i12 - i1$	3.59E+09	5.15E+09	7.19E+09	9.78E+09	1.45E+10	1.70E+10
$i1 - i6$	3.07E+09	4.13E+09	5.44E+09	7.06E+09	9.90E+09	1.14E+10
$i6 - i1$	8.50E+09	1.14E+10	1.51E+10	1.97E+10	2.77E+10	3.17E+10
$i1 - i65$	4.62E+06	8.41E+06	1.45E+07	2.39E+07	4.52E+07	5.82E+07
$i65 - i1$	3.20E+08	5.88E+08	1.02E+09	1.70E+09	3.26E+09	4.21E+09
$i13 - i27$	1.26E+13	1.25E+13	1.23E+13	1.22E+13	1.20E+13	1.19E+13
$i27 - i13$	7.30E+12	8.21E+12	9.18E+12	1.02E+13	1.18E+13	1.25E+13
$i1 - i13$	2.93E+05	6.05E+05	1.17E+06	2.12E+06	4.50E+06	6.07E+06
$i13 - i1$	4.82E+05	8.98E+05	1.57E+06	2.61E+06	4.91E+06	6.30E+06
$i2 - i4$	5.21E+10	5.79E+10	6.39E+10	7.01E+10	7.91E+10	8.31E+10
$i4 - i2$	3.70E+12	3.90E+12	4.10E+12	4.29E+12	4.56E+12	4.67E+12
$i2 - i22$	2.05E+08	3.51E+08	5.68E+08	8.80E+08	1.52E+09	1.89E+09
$i22 - i2$	7.25E+09	1.16E+10	1.77E+10	2.58E+10	4.14E+10	4.98E+10
$i44 - i53$	9.10E+05	2.15E+06	4.58E+06	9.00E+06	2.07E+07	2.86E+07
$i53 - i44$	9.54E+06	2.16E+07	4.42E+07	8.36E+07	1.83E+08	2.49E+08
$i3 - i63$	2.24E+09	2.76E+09	3.38E+09	4.08E+09	5.21E+09	5.76E+09
$i63 - i3$	3.74E+11	4.40E+11	5.12E+11	5.90E+11	7.11E+11	7.66E+11
$i1 - i27$	2.75E-02	4.70E-01	7.00E+00	6.62E+01	7.43E+02	1.75E+03
$i27 - i1$	1.31E-02	2.30E-01	3.52E+00	3.42E+01	3.97E+02	9.48E+02
$i3 - i15$	4.45E+08	6.06E+08	8.09E+08	1.06E+09	1.51E+09	1.74E+09
$i15 - i3$	1.28E+06	1.95E+06	2.88E+06	4.18E+06	6.79E+06	8.27E+06
$i3 - i12$	8.32E+07	1.41E+08	2.28E+08	3.55E+08	6.26E+08	7.84E+08
$i12 - i3$	7.54E+08	1.18E+09	1.77E+09	2.57E+09	4.11E+09	4.96E+09
$i3 - i11$	3.11E+10	3.97E+10	5.00E+10	6.20E+10	8.23E+10	9.23E+10
$i11 - i3$	3.31E+07	4.72E+07	6.61E+07	9.09E+07	1.38E+08	1.64E+08
$i3 - i8$	7.17E+09	8.43E+09	9.82E+09	1.13E+10	1.37E+10	1.48E+10
$i8 - i3$	6.66E+11	7.49E+11	8.37E+11	9.30E+11	1.07E+12	1.13E+12
$i3 - p4+H$	6.79E+08	1.25E+09	2.18E+09	3.62E+09	6.92E+09	8.94E+09
$i12 - i14$	2.12E+12	2.24E+12	2.35E+12	2.47E+12	2.62E+12	2.69E+12
$i14 - i12$	5.03E+12	5.22E+12	5.40E+12	5.58E+12	5.82E+12	5.92E+12
$i65 - i14$	2.57E+11	3.09E+11	3.68E+11	4.33E+11	5.38E+11	5.88E+11
$i14 - i65$	2.83E+11	3.03E+11	3.23E+11	3.44E+11	3.72E+11	3.84E+11
$i12 - i15$	1.87E+08	2.93E+08	4.42E+08	6.46E+08	1.04E+09	1.26E+09

<i>i15 – i12</i>	5.95E+04	1.13E+05	2.03E+05	3.52E+05	7.15E+05	9.51E+05
<i>i3 – i15</i>	3.22E+08	5.01E+08	7.53E+08	1.10E+09	1.79E+09	2.18E+09
<i>i15 – i3</i>	9.30E+05	1.61E+06	2.69E+06	4.33E+06	8.06E+06	1.04E+07
<i>i14 – i29</i>	4.13E+12	4.45E+12	4.76E+12	5.07E+12	5.51E+12	5.70E+12
<i>i29 – i14</i>	1.69E+13	1.83E+13	1.96E+13	2.09E+13	2.28E+13	2.36E+13
<i>i14 – i46</i>	5.82E+11	6.26E+11	6.69E+11	7.13E+11	7.74E+11	8.01E+11
<i>i46 – i14</i>	2.29E+11	2.64E+11	3.01E+11	3.42E+11	4.03E+11	4.31E+11
<i>i65 – i7</i>	3.24E+08	4.71E+08	6.67E+08	9.23E+08	1.41E+09	1.67E+09
<i>i7 – i65</i>	3.36E+09	4.53E+09	5.99E+09	7.75E+09	1.08E+10	1.24E+10
<i>i65 – i67</i>	8.55E+08	1.24E+09	1.76E+09	2.44E+09	3.73E+09	4.43E+09
<i>i67 – i65</i>	1.52E+08	2.25E+08	3.25E+08	4.58E+08	7.14E+08	8.54E+08
<i>i1 – i7</i>	8.33E+08	1.03E+09	1.26E+09	1.53E+09	1.96E+09	2.17E+09
<i>i7 – i1</i>	2.99E+11	3.48E+11	4.00E+11	4.57E+11	5.43E+11	5.82E+11
<i>i4 – i7</i>	3.64E+12	3.69E+12	3.74E+12	3.79E+12	3.86E+12	3.88E+12
<i>i7 – i4</i>	4.59E+11	5.05E+11	5.52E+11	6.01E+11	6.71E+11	7.01E+11
<i>i65 – i7</i>	7.55E+07	1.17E+08	1.76E+08	2.58E+08	4.20E+08	5.11E+08
<i>i7 – i65</i>	7.84E+08	1.13E+09	1.58E+09	2.16E+09	3.23E+09	3.79E+09
<i>i4 – i7</i>	2.18E+12	2.25E+12	2.33E+12	2.41E+12	2.50E+12	2.55E+12
<i>i7 – i4</i>	2.75E+11	3.08E+11	3.44E+11	3.81E+11	4.36E+11	4.60E+11
<i>i67 – i26</i>	9.84E+08	1.35E+09	1.82E+09	2.40E+09	3.46E+09	4.01E+09
<i>i26 – i67</i>	7.11E+08	9.17E+08	1.16E+09	1.45E+09	1.94E+09	2.18E+09
<i>i22 – i45</i>	1.07E+07	2.56E+07	5.43E+07	1.05E+08	2.34E+08	3.19E+08
<i>i45 – i22</i>	1.39E+06	3.64E+06	8.41E+06	1.76E+07	4.34E+07	6.16E+07
<i>i15 – i24</i>	4.35E+10	4.92E+10	5.55E+10	6.22E+10	7.25E+10	7.73E+10
<i>i24 – i15</i>	1.62E+13	1.66E+13	1.69E+13	1.73E+13	1.78E+13	1.80E+13
<i>i9 – i10</i>	2.40E+05	5.03E+05	9.81E+05	1.80E+06	3.87E+06	5.23E+06
<i>i10 – i9</i>	3.87E+05	8.21E+05	1.62E+06	3.01E+06	6.56E+06	8.92E+06
<i>i63 – i7</i>	1.86E-01	9.31E+00	3.04E+02	2.67E+03	2.14E+04	4.43E+04
<i>i7 – i63</i>	2.26E-01	1.12E+01	3.64E+02	3.20E+03	2.55E+04	5.25E+04
<i>i3 – p3+H</i>	2.89E+08	5.32E+08	9.28E+08	1.54E+09	2.95E+09	3.81E+09
<i>i3 – i63</i>	1.15E+09	1.45E+09	1.81E+09	2.22E+09	2.91E+09	3.25E+09
<i>i63 – i3</i>	1.92E+11	2.30E+11	2.74E+11	3.22E+11	3.97E+11	4.32E+11
<i>i13 – p2s+H</i>	2.02E+09	3.47E+09	5.66E+09	8.84E+09	1.55E+10	1.93E+10
<i>i6 – p3+H</i>	1.95E+09	3.41E+09	5.69E+09	9.12E+09	1.67E+10	2.12E+10
<i>i22 – i10</i>	7.71E+12	7.89E+12	8.05E+12	8.21E+12	8.43E+12	8.51E+12
<i>i10 – i22</i>	1.79E+10	2.15E+10	2.56E+10	3.02E+10	3.74E+10	4.08E+10
<i>i63 – i67</i>	2.20E+09	3.16E+09	4.41E+09	6.00E+09	8.91E+09	1.04E+10
<i>i67 – i63</i>	4.57E+07	7.15E+07	1.08E+08	1.60E+08	2.64E+08	3.23E+08
<i>i15 – p2+H</i>	8.40E+08	1.34E+09	2.08E+09	3.14E+09	5.38E+09	6.70E+09
<i>i13 – i14</i>	1.96E-09	1.49E-07	1.06E-05	6.93E-04	2.11E-01	1.94E+00
<i>i14 – i13</i>	9.12E-08	6.90E-06	4.86E-04	3.18E-02	9.61E+00	8.83E+01
<i>i63 – i16</i>	1.82E+11	2.16E+11	2.53E+11	2.94E+11	3.57E+11	3.86E+11
<i>i16 – i63</i>	4.12E+09	5.02E+09	6.04E+09	7.19E+09	9.03E+09	9.90E+09
<i>i27 – i45</i>	2.95E+10	3.54E+10	4.22E+10	4.98E+10	6.19E+10	6.77E+10
<i>i45 – i27</i>	5.71E+12	6.22E+12	6.75E+12	7.29E+12	8.05E+12	8.39E+12
<i>i11 – p2+H</i>	7.18E+08	1.15E+09	1.80E+09	2.74E+09	4.74E+09	5.93E+09
<i>i11 – i7</i>	2.39E+06	3.55E+06	5.15E+06	7.34E+06	1.17E+07	1.41E+07
<i>i7 – i11</i>	4.52E+11	5.70E+11	7.08E+11	8.66E+11	1.12E+12	1.25E+12
<i>i11 – i10</i>	1.52E+10	1.74E+10	1.97E+10	2.23E+10	2.63E+10	2.81E+10
<i>i10 – i11</i>	2.63E+13	2.73E+13	2.83E+13	2.92E+13	3.05E+13	3.10E+13
<i>i13 – i15</i>	5.27E+11	5.80E+11	6.36E+11	6.93E+11	7.75E+11	8.11E+11
<i>i15 – i13</i>	3.29E+09	4.42E+09	5.86E+09	7.67E+09	1.09E+10	1.26E+10
<i>i8 – i9</i>	3.28E+12	3.58E+12	3.88E+12	4.19E+12	4.64E+12	4.83E+12
<i>i9 – i8</i>	4.05E+10	4.62E+10	5.23E+10	5.89E+10	6.88E+10	7.32E+10
<i>i12 – i16</i>	2.40E+09	3.53E+09	5.02E+09	6.95E+09	1.05E+10	1.24E+10
<i>i16 – i12</i>	1.00E+09	1.56E+09	2.34E+09	3.41E+09	5.52E+09	6.69E+09
<i>i15 – i16</i>	1.51E+08	2.09E+08	2.84E+08	3.80E+08	5.57E+08	6.52E+08
<i>i16 – i15</i>	1.98E+11	2.40E+11	2.88E+11	3.42E+11	4.27E+11	4.67E+11
<i>i11 – i9</i>	9.24E+09	1.06E+10	1.21E+10	1.37E+10	1.61E+10	1.73E+10
<i>i9 – i11</i>	9.94E+12	1.02E+13	1.05E+13	1.07E+13	1.11E+13	1.12E+13
<i>i27 – i29</i>	4.66E+06	8.04E+06	1.33E+07	2.12E+07	3.84E+07	4.88E+07
<i>i29 – i27</i>	1.53E+09	2.32E+09	3.38E+09	4.77E+09	7.40E+09	8.81E+09
<i>i65 – i63</i>	9.08E+08	1.28E+09	1.76E+09	2.37E+09	3.50E+09	4.10E+09

<i>i63 – i65</i>	7.79E+09	1.02E+10	1.32E+10	1.67E+10	2.27E+10	2.56E+10
<i>i13 – i26</i>	3.69E+02	2.32E+03	9.55E+03	3.04E+04	1.15E+05	1.88E+05
<i>i26 – i13</i>	2.00E+03	1.35E+04	5.89E+04	1.99E+05	8.14E+05	1.38E+06
<i>i65 – i46</i>	1.44E+13	1.52E+13	1.60E+13	1.69E+13	1.80E+13	1.85E+13
<i>i46 – i65</i>	6.26E+12	6.31E+12	6.36E+12	6.41E+12	6.47E+12	6.50E+12
<i>i13 – i15</i>	3.81E+10	4.44E+10	5.11E+10	5.84E+10	6.93E+10	7.42E+10
<i>i15 – i13</i>	2.38E+08	3.38E+08	4.72E+08	6.46E+08	9.76E+08	1.16E+09
<i>i13 – i11</i>	2.02E+11	2.26E+11	2.51E+11	2.77E+11	3.14E+11	3.31E+11
<i>i11 – i13</i>	4.66E+08	6.38E+08	8.59E+08	1.14E+09	1.65E+09	1.93E+09
<i>i14 – p4+H</i>	3.63E+09	6.78E+09	1.19E+10	1.97E+10	3.70E+10	4.73E+10
<i>i29 – p5+H</i>	8.36E+07	1.76E+08	3.42E+08	6.17E+08	1.28E+09	1.71E+09
<i>i16 – p4+H</i>	7.18E+08	1.31E+09	2.25E+09	3.69E+09	6.93E+09	8.89E+09
<i>i65 – i45</i>	1.01E+09	1.52E+09	2.23E+09	3.19E+09	5.06E+09	6.08E+09
<i>i45 – i65</i>	2.68E+09	3.74E+09	5.09E+09	6.77E+09	9.76E+09	1.13E+10
<i>i26 – p11a+C₂H₂</i>	9.81E+10	1.37E+11	1.87E+11	2.50E+11	3.62E+11	4.21E+11
<i>i9 – i26</i>	9.65E+08	1.34E+09	1.82E+09	2.43E+09	3.53E+09	4.10E+09
<i>i26 – i9</i>	2.11E+09	2.86E+09	3.79E+09	4.93E+09	6.93E+09	7.95E+09
<i>i8 – i26</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.15E+01
<i>i26 – i8</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.81E+00
<i>i3 – i5</i>	2.11E+11	2.31E+11	2.52E+11	2.74E+11	3.05E+11	3.19E+11
<i>i5 – i3</i>	1.68E+12	1.72E+12	1.75E+12	1.79E+12	1.84E+12	1.86E+12
<i>i27 – i10</i>	4.81E+10	5.69E+10	6.66E+10	7.75E+10	9.45E+10	1.02E+11
<i>i10 – i27</i>	3.32E+11	3.83E+11	4.38E+11	4.98E+11	5.89E+11	6.31E+11
<i>i26 – p1+H</i>	2.92E+10	4.09E+10	5.60E+10	7.51E+10	1.10E+11	1.28E+11
<i>i65 – i26</i>	2.48E+09	3.51E+09	4.87E+09	6.60E+09	9.80E+09	1.15E+10
<i>i26 – i65</i>	3.18E+08	4.32E+08	5.74E+08	7.47E+08	1.05E+09	1.21E+09
<i>i9 – p12+H</i>	2.14E+05	1.12E+06	4.37E+06	1.39E+07	5.45E+07	9.15E+07
<i>i9 – p1+H</i>	7.84E+10	1.09E+11	1.48E+11	1.97E+11	2.85E+11	3.31E+11
<i>i10 – p1+H</i>	9.52E+09	1.38E+10	1.94E+10	2.67E+10	4.05E+10	4.79E+10
<i>i63 – i60</i>	1.39E+10	1.72E+10	2.11E+10	2.55E+10	3.25E+10	3.59E+10
<i>i60 – i63</i>	7.83E+11	8.71E+11	9.60E+11	1.05E+12	1.18E+12	1.24E+12
<i>i13 – i11</i>	8.69E+04	2.42E+05	5.93E+05	1.31E+06	3.42E+06	4.96E+06
<i>i11 – i13</i>	2.00E+02	6.84E+02	2.03E+03	5.37E+03	1.80E+04	2.89E+04
<i>i2 – i27</i>	7.54E+04	2.17E+05	5.40E+05	1.20E+06	3.18E+06	4.63E+06
<i>i27 – i2</i>	4.48E+02	1.45E+03	4.06E+03	1.01E+04	3.08E+04	4.74E+04
<i>i67 – i45</i>	4.02E+08	5.97E+08	8.64E+08	1.22E+09	1.91E+09	2.29E+09
<i>i45 – i67</i>	6.00E+09	8.11E+09	1.07E+10	1.38E+10	1.93E+10	2.20E+10
<i>i30 – i53</i>	2.84E+10	3.31E+10	3.83E+10	4.40E+10	5.27E+10	5.68E+10
<i>i53 – i30</i>	5.74E+12	5.89E+12	6.03E+12	6.17E+12	6.35E+12	6.43E+12
<i>i26 – i39</i>	2.76E+10	3.29E+10	3.88E+10	4.53E+10	5.55E+10	6.03E+10
<i>i39 – i26</i>	1.58E+12	1.79E+12	2.00E+12	2.22E+12	2.55E+12	2.70E+12
<i>i6 – i11</i>	3.55E+07	5.85E+07	9.27E+07	1.42E+08	2.45E+08	3.05E+08
<i>i11 – i6</i>	2.43E+04	4.42E+04	7.70E+04	1.29E+05	2.52E+05	3.30E+05
<i>i3 – i6</i>	1.58E-01	1.39E+00	1.15E+01	7.72E+01	6.89E+02	1.53E+03
<i>i6 – i3</i>	2.45E-01	2.20E+00	1.83E+01	1.24E+02	1.13E+03	2.52E+03
<i>i53 – p22+H</i>	1.46E+06	4.37E+06	1.11E+07	2.51E+07	6.69E+07	9.73E+07
<i>i65 – i13</i>	8.27E+09	1.15E+10	1.57E+10	2.10E+10	3.06E+10	3.56E+10
<i>i13 – i65</i>	1.96E+08	2.44E+08	3.00E+08	3.63E+08	4.63E+08	5.10E+08
<i>i38 – i24</i>	1.13E+13	1.14E+13	1.15E+13	1.16E+13	1.17E+13	1.17E+13
<i>i24 – i38</i>	4.67E+08	6.69E+08	9.35E+08	1.28E+09	1.92E+09	2.25E+09
<i>i65 – i58</i>	1.53E+08	2.34E+08	3.47E+08	5.01E+08	8.03E+08	9.71E+08
<i>i58 – i65</i>	6.97E+12	7.23E+12	7.46E+12	7.69E+12	7.97E+12	8.09E+12
<i>i4 – i10</i>	3.36E+10	5.02E+10	7.21E+10	1.00E+11	1.52E+11	1.79E+11
<i>i10 – i4</i>	3.87E+07	6.71E+07	1.11E+08	1.76E+08	3.18E+08	4.03E+08
<i>i15 – i67</i>	1.93E+07	2.62E+07	3.49E+07	4.59E+07	6.60E+07	7.65E+07
<i>i67 – i15</i>	2.32E+10	2.93E+10	3.65E+10	4.50E+10	5.91E+10	6.61E+10
<i>i7 – i18</i>	1.80E+08	3.07E+08	4.96E+08	7.69E+08	1.34E+09	1.66E+09
<i>i18 – i7</i>	1.29E+10	1.60E+10	1.93E+10	2.29E+10	2.81E+10	3.05E+10
<i>i8 – i5</i>	1.08E+12	1.21E+12	1.34E+12	1.49E+12	1.69E+12	1.79E+12
<i>i5 – i8</i>	9.24E+10	1.01E+11	1.10E+11	1.19E+11	1.31E+11	1.37E+11
<i>i16 – i24</i>	1.21E+08	2.11E+08	3.50E+08	5.57E+08	1.00E+09	1.27E+09
<i>i24 – i16</i>	3.44E+07	6.18E+07	1.05E+08	1.72E+08	3.21E+08	4.12E+08
<i>i45 – i20</i>	1.83E+13	1.87E+13	1.90E+13	1.94E+13	1.98E+13	2.00E+13

<i>i20 – i45</i>	6.53E+10	7.00E+10	7.48E+10	7.97E+10	8.66E+10	8.96E+10
<i>i10 – i24</i>	3.69E+09	5.09E+09	6.89E+09	9.15E+09	1.32E+10	1.54E+10
<i>i24 – i10</i>	2.15E+09	2.95E+09	3.96E+09	5.22E+09	7.49E+09	8.67E+09
<i>i26 – i30</i>	1.12E+08	1.67E+08	2.42E+08	3.41E+08	5.29E+08	6.31E+08
<i>i30 – i26</i>	2.71E+07	4.18E+07	6.24E+07	9.06E+07	1.47E+08	1.78E+08
<i>i26 – i24</i>	8.25E+08	1.24E+09	1.80E+09	2.54E+09	3.97E+09	4.75E+09
<i>i24 – i26</i>	3.54E+08	5.48E+08	8.21E+08	1.20E+09	1.94E+09	2.35E+09
<i>i6 – i30</i>	2.08E+06	4.13E+06	7.68E+06	1.35E+07	2.76E+07	3.67E+07
<i>i30 – i6</i>	1.61E+06	3.20E+06	5.92E+06	1.04E+07	2.12E+07	2.81E+07
<i>i6 – i44</i>	2.68E+10	3.24E+10	3.88E+10	4.60E+10	5.75E+10	6.30E+10
<i>i44 – i6</i>	8.01E+11	8.87E+11	9.77E+11	1.07E+12	1.20E+12	1.26E+12
<i>i1 – i30</i>	2.54E+11	2.79E+11	3.04E+11	3.30E+11	3.69E+11	3.86E+11
<i>i30 – i1</i>	5.45E+11	5.97E+11	6.52E+11	7.08E+11	7.90E+11	8.27E+11
<i>i1 – i30</i>	2.15E+11	2.36E+11	2.58E+11	2.81E+11	3.14E+11	3.28E+11
<i>i30 – i1</i>	4.62E+11	5.07E+11	5.53E+11	6.02E+11	6.72E+11	7.03E+11
<i>i22 – i16</i>	4.54E+12	4.66E+12	4.77E+12	4.88E+12	5.02E+12	5.08E+12
<i>i16 – i22</i>	2.16E+10	2.51E+10	2.89E+10	3.31E+10	3.94E+10	4.23E+10
<i>i56 – i42</i>	7.94E+11	9.16E+11	1.04E+12	1.18E+12	1.37E+12	1.46E+12
<i>i42 – i56</i>	1.41E+12	1.42E+12	1.43E+12	1.44E+12	1.45E+12	1.45E+12
<i>i67 – i20</i>	5.85E+11	6.44E+11	7.06E+11	7.71E+11	8.66E+11	9.08E+11
<i>i20 – i67</i>	6.25E+10	6.57E+10	6.88E+10	7.20E+10	7.64E+10	7.82E+10
<i>i8 – i54</i>	7.57E+09	1.09E+10	1.52E+10	2.08E+10	3.11E+10	3.65E+10
<i>i54 – i8</i>	1.08E+09	1.67E+09	2.50E+09	3.64E+09	5.92E+09	7.20E+09
<i>i8 – i53</i>	1.40E+04	6.59E+04	2.38E+05	7.11E+05	2.61E+06	4.26E+06
<i>i53 – i8</i>	7.36E+04	3.21E+05	1.08E+06	3.02E+06	1.01E+07	1.60E+07
<i>i4 – i47</i>	4.85E+02	1.73E+04	1.44E+05	6.67E+05	3.52E+06	6.41E+06
<i>i47 – i4</i>	7.73E+06	1.59E+08	8.06E+08	2.40E+09	7.30E+09	1.07E+10
<i>i24 – i20</i>	4.93E+12	5.13E+12	5.33E+12	5.53E+12	5.80E+12	5.92E+12
<i>i20 – i24</i>	8.49E+11	8.70E+11	8.89E+11	9.08E+11	9.35E+11	9.45E+11
<i>i27 – i10</i>	2.08E+09	2.91E+09	3.99E+09	5.36E+09	7.88E+09	9.22E+09
<i>i10 – i27</i>	1.44E+10	1.96E+10	2.62E+10	3.44E+10	4.92E+10	5.68E+10
<i>i3 – i23</i>	4.82E+05	1.01E+06	1.97E+06	3.60E+06	7.63E+06	1.03E+07
<i>i23 – i3</i>	9.07E+12	8.84E+12	8.65E+12	8.50E+12	8.33E+12	8.27E+12
<i>i20 – i19</i>	5.75E+12	5.75E+12	5.75E+12	5.75E+12	5.75E+12	5.75E+12
<i>i19 – i20</i>	3.83E+12	3.85E+12	3.86E+12	3.87E+12	3.89E+12	3.90E+12
<i>i67 – i45</i>	2.14E+05	4.64E+05	9.33E+05	1.75E+06	3.89E+06	5.33E+06
<i>i45 – i67</i>	6.40E+06	1.26E+07	2.31E+07	3.98E+07	7.85E+07	1.03E+08
<i>i47 – i21</i>	8.66E+12	8.99E+12	9.27E+12	9.51E+12	9.81E+12	9.93E+12
<i>i21 – i47</i>	5.39E+08	7.90E+08	1.10E+09	1.47E+09	2.09E+09	2.39E+09
<i>i38 – i28</i>	9.07E+12	9.25E+12	9.42E+12	9.58E+12	9.77E+12	9.85E+12
<i>i28 – i38</i>	1.05E+12	1.14E+12	1.23E+12	1.31E+12	1.43E+12	1.48E+12
<i>i22 – i25</i>	1.48E+01	9.05E+03	7.33E+04	3.30E+05	1.67E+06	2.98E+06
<i>i25 – i22</i>	1.27E+10	1.02E+12	1.89E+12	2.65E+12	3.60E+12	3.98E+12
<i>i3 – i10</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.42E-01	1.03E+01
<i>i10 – i3</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.45E+00	2.03E+01
<i>i29 – i23</i>	1.40E+05	5.48E+05	1.67E+06	4.29E+06	1.31E+07	1.99E+07
<i>i23 – i29</i>	3.00E+10	5.97E+10	1.00E+11	1.51E+11	2.37E+11	2.78E+11
<i>i27 – i20</i>	1.22E+11	1.42E+11	1.64E+11	1.87E+11	2.23E+11	2.40E+11
<i>i20 – i27</i>	8.47E+10	9.36E+10	1.03E+11	1.13E+11	1.27E+11	1.33E+11
<i>i7 – i56</i>	9.52E+10	1.08E+11	1.22E+11	1.36E+11	1.57E+11	1.66E+11
<i>i56 – i7</i>	7.97E+12	8.00E+12	8.03E+12	8.05E+12	8.08E+12	8.09E+12
<i>i39 – i58</i>	1.02E+08	1.68E+08	2.64E+08	3.99E+08	6.71E+08	8.23E+08
<i>i58 – i39</i>	6.28E+11	7.76E+11	9.34E+11	1.10E+12	1.35E+12	1.46E+12
<i>i24 – i51</i>	3.85E+10	4.53E+10	5.27E+10	6.09E+10	7.37E+10	7.96E+10
<i>i51 – i24</i>	2.25E+13	2.36E+13	2.47E+13	2.58E+13	2.73E+13	2.80E+13
<i>i58 – i41</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.07E+06	5.16E+06
<i>i41 – i58</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.32E+12	8.34E+12
<i>i23 – i42</i>	3.54E+12	3.46E+12	3.40E+12	3.34E+12	3.28E+12	3.26E+12
<i>i42 – i23</i>	5.67E+09	8.75E+09	1.27E+10	1.77E+10	2.64E+10	3.08E+10
<i>i29 – i46</i>	1.42E+11	1.66E+11	1.91E+11	2.19E+11	2.60E+11	2.78E+11
<i>i46 – i29</i>	1.37E+10	1.70E+10	2.09E+10	2.54E+10	3.27E+10	3.62E+10
<i>i68 – i69</i>	8.22E+10	1.11E+11	1.45E+11	1.85E+11	2.51E+11	2.82E+11
<i>i69 – i68</i>	8.43E+08	1.32E+09	1.99E+09	2.88E+09	4.60E+09	5.54E+09

<i>i65 – i45</i>	1.21E+10	1.68E+10	2.27E+10	3.02E+10	4.38E+10	5.08E+10
<i>i45 – i65</i>	3.22E+10	4.12E+10	5.18E+10	6.42E+10	8.45E+10	9.43E+10
<i>i4 – i56</i>	2.23E+08	3.71E+08	5.84E+08	8.80E+08	1.47E+09	1.79E+09
<i>i56 – i4</i>	2.36E+09	3.76E+09	5.69E+09	8.27E+09	1.31E+10	1.57E+10
<i>i14 – i20</i>	1.04E+08	1.75E+08	2.82E+08	4.33E+08	7.43E+08	9.19E+08
<i>i20 – i14</i>	8.95E+05	1.65E+06	2.87E+06	4.77E+06	9.08E+06	1.17E+07
<i>i58 – i47</i>	3.70E+10	5.20E+10	6.97E+10	9.01E+10	1.23E+11	1.39E+11
<i>i47 – i58</i>	2.13E+12	2.17E+12	2.21E+12	2.24E+12	2.27E+12	2.28E+12
<i>i67 – i69</i>	1.77E+08	2.49E+08	3.41E+08	4.59E+08	6.76E+08	7.90E+08
<i>i69 – i67</i>	3.44E+10	4.23E+10	5.12E+10	6.12E+10	7.69E+10	8.43E+10
<i>i48 – i21</i>	1.32E+07	6.41E+07	2.00E+08	4.93E+08	1.35E+09	1.95E+09
<i>i21 – i48</i>	5.44E+04	2.74E+05	8.79E+05	2.23E+06	6.31E+06	9.23E+06
<i>i56 – i53</i>	2.27E+12	2.49E+12	2.73E+12	2.96E+12	3.28E+12	3.42E+12
<i>i53 – i56</i>	6.53E+10	7.62E+10	8.79E+10	1.00E+11	1.19E+11	1.27E+11
<i>i67 – i68</i>	3.31E+07	5.01E+07	7.35E+07	1.05E+08	1.68E+08	2.02E+08
<i>i68 – i67</i>	3.14E+11	3.58E+11	4.04E+11	4.52E+11	5.19E+11	5.48E+11
<i>i69 – p27+H</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.21E+02
<i>i15 – i19</i>	4.61E+11	5.16E+11	5.76E+11	6.40E+11	7.37E+11	7.81E+11
<i>i19 – i15</i>	1.97E+13	1.97E+13	1.97E+13	1.97E+13	1.97E+13	1.97E+13
<i>i69 – i61</i>	2.40E+07	5.09E+07	9.88E+07	1.79E+08	3.72E+08	4.94E+08
<i>i61 – i69</i>	1.48E+09	2.78E+09	4.84E+09	7.88E+09	1.43E+10	1.80E+10
<i>i45 – i52</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.66E+02	3.37E+03
<i>i52 – i45</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.27E+04	7.43E+04
<i>i54 – i33</i>	4.71E+12	5.17E+12	5.64E+12	6.14E+12	6.86E+12	7.19E+12
<i>i33 – i54</i>	7.50E+11	7.64E+11	7.78E+11	7.92E+11	8.10E+11	8.18E+11
<i>i11 – p3+H</i>	1.67E+07	3.16E+07	5.72E+07	9.93E+07	2.02E+08	2.68E+08
<i>i25 – i31</i>	2.34E+07	1.39E+11	5.07E+11	8.62E+11	1.34E+12	1.54E+12
<i>i31 – i25</i>	3.46E-01	1.38E+04	1.93E+05	9.34E+05	4.64E+06	8.09E+06
<i>i10 – i52</i>	6.30E+09	7.90E+09	9.78E+09	1.20E+10	1.56E+10	1.73E+10
<i>i52 – i10</i>	7.14E+12	7.26E+12	7.37E+12	7.48E+12	7.62E+12	7.67E+12
<i>i10 – i33</i>	2.10E+12	2.23E+12	2.37E+12	2.51E+12	2.71E+12	2.80E+12
<i>i33 – i10</i>	2.40E+12	2.40E+12	2.41E+12	2.42E+12	2.43E+12	2.43E+12
<i>i10 – i34</i>	2.89E+09	3.98E+09	5.37E+09	7.11E+09	1.02E+10	1.19E+10
<i>i34 – i10</i>	1.22E+13	1.25E+13	1.28E+13	1.31E+13	1.35E+13	1.36E+13
<i>i10 – i60</i>	2.41E+08	3.26E+08	4.32E+08	5.61E+08	7.91E+08	9.08E+08
<i>i60 – i10</i>	1.24E+12	1.40E+12	1.57E+12	1.75E+12	2.00E+12	2.12E+12
<i>i45 – i47</i>	1.38E+07	2.69E+07	4.88E+07	8.35E+07	1.63E+08	2.13E+08
<i>i47 – i45</i>	6.79E+12	7.05E+12	7.28E+12	7.49E+12	7.76E+12	7.86E+12
<i>i4 – i42</i>	5.34E-01	1.80E+01	5.37E+02	9.55E+03	1.28E+05	3.00E+05
<i>i42 – i4</i>	1.00E+01	2.83E+02	7.17E+03	1.10E+05	1.21E+06	2.62E+06
<i>i11 – i33</i>	1.94E+09	2.28E+09	2.66E+09	3.09E+09	3.78E+09	4.10E+09
<i>i33 – i11</i>	3.84E+12	3.86E+12	3.88E+12	3.90E+12	3.92E+12	3.93E+12
<i>i54 – p22+H</i>	2.38E+07	5.52E+07	1.17E+08	2.32E+08	5.45E+08	7.63E+08
<i>i9 – i26</i>	1.36E+09	1.93E+09	2.67E+09	3.62E+09	5.37E+09	6.29E+09
<i>i26 – i9</i>	2.97E+09	4.10E+09	5.54E+09	7.34E+09	1.05E+10	1.22E+10
<i>i63 – i31</i>	4.12E+10	5.30E+10	6.70E+10	8.34E+10	1.11E+11	1.24E+11
<i>i31 – i63</i>	2.54E+12	2.57E+12	2.60E+12	2.63E+12	2.66E+12	2.67E+12
<i>i45 – i54</i>	2.42E+00	5.39E+01	7.07E+02	4.24E+03	2.82E+04	5.56E+04
<i>i54 – i45</i>	3.08E-01	7.52E+00	1.07E+02	6.95E+02	5.13E+03	1.06E+04
<i>i9 – i34</i>	1.00E+09	1.33E+09	1.74E+09	2.24E+09	3.10E+09	3.54E+09
<i>i34 – i9</i>	6.82E+12	6.84E+12	6.87E+12	6.90E+12	6.93E+12	6.94E+12
<i>i65 – i68</i>	8.49E+08	1.18E+09	1.61E+09	2.15E+09	3.13E+09	3.65E+09
<i>i68 – i65</i>	1.43E+12	1.53E+12	1.63E+12	1.73E+12	1.86E+12	1.91E+12
<i>i31 – i28</i>	3.08E-06	3.72E-04	3.91E-02	3.62E+00	1.60E+03	1.39E+04
<i>i28 – i31</i>	9.06E-07	1.10E-04	1.16E-02	1.08E+00	4.80E+02	4.20E+03
<i>i15 – i28</i>	3.20E+06	5.22E+06	8.24E+06	1.26E+07	2.21E+07	2.77E+07
<i>i28 – i15</i>	3.36E+12	3.70E+12	4.04E+12	4.38E+12	4.84E+12	5.04E+12
<i>i7 – i42</i>	1.42E+03	1.36E+04	6.66E+04	2.37E+05	9.94E+05	1.69E+06
<i>i42 – i7</i>	2.12E+05	1.56E+06	6.02E+06	1.71E+07	5.39E+07	8.14E+07
<i>i28 – i21</i>	4.60E+11	5.42E+11	6.27E+11	7.17E+11	8.47E+11	9.04E+11
<i>i21 – i28</i>	4.83E+11	5.35E+11	5.86E+11	6.37E+11	7.05E+11	7.33E+11
<i>i67 – p29+H</i>	0.00E+00	0.00E+00	7.37E+02	7.81E+03	8.67E+04	2.02E+05
<i>i48 – i62</i>	2.21E+12	2.43E+12	2.65E+12	2.86E+12	3.14E+12	3.26E+12

<i>i62 – i48</i>	2.05E+10	2.75E+10	3.59E+10	4.57E+10	6.21E+10	7.01E+10
<i>i2 – i42</i>	9.21E+08	1.21E+09	1.56E+09	1.97E+09	2.65E+09	2.99E+09
<i>i42 – i2</i>	1.23E+12	1.28E+12	1.33E+12	1.38E+12	1.44E+12	1.46E+12
<i>i8 – p22+H</i>	1.34E+08	2.93E+08	5.87E+08	1.10E+09	2.40E+09	3.26E+09
<i>i26 – i41</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.31E-01	5.90E+00
<i>i41 – i26</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.92E+10	3.77E+11
<i>i12 – i41</i>	2.13E+02	1.88E+03	9.12E+03	3.25E+04	1.38E+05	2.34E+05
<i>i41 – i12</i>	6.06E+13	8.36E+14	6.26E+15	3.41E+16	9.87E+15	5.31E+15
<i>i20 – i21</i>	1.50E+10	2.09E+10	2.86E+10	3.82E+10	5.55E+10	6.46E+10
<i>i21 – i20</i>	2.57E+14	2.57E+14	2.57E+14	2.57E+14	2.57E+14	2.56E+14
<i>i1 – p3+H</i>	1.03E+06	2.81E+06	6.79E+06	1.49E+07	3.92E+07	5.71E+07
<i>i8 – i41</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.85E+01	2.77E+02
<i>i41 – i8</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.12E+11	5.22E+11
<i>i7 – i57</i>	4.89E+08	7.42E+08	1.09E+09	1.55E+09	2.45E+09	2.93E+09
<i>i57 – i7</i>	9.90E+10	1.29E+11	1.65E+11	2.06E+11	2.74E+11	3.06E+11
<i>i67 – i37</i>	9.20E+09	1.19E+10	1.52E+10	1.91E+10	2.59E+10	2.93E+10
<i>i37 – i67</i>	6.08E+11	6.86E+11	7.69E+11	8.55E+11	9.81E+11	1.04E+12
<i>i21 – i37</i>	6.08E+08	1.27E+09	2.34E+09	3.97E+09	7.41E+09	9.39E+09
<i>i37 – i21</i>	2.19E+07	5.83E+07	1.35E+08	2.82E+08	6.89E+08	9.72E+08
<i>i62 – i64</i>	8.59E+11	9.25E+11	9.90E+11	1.05E+12	1.14E+12	1.18E+12
<i>i64 – i62</i>	5.74E+11	6.81E+11	7.99E+11	9.26E+11	1.12E+12	1.21E+12
<i>i4 – i18</i>	1.01E+10	1.53E+10	2.23E+10	3.14E+10	4.81E+10	5.69E+10
<i>i18 – i4</i>	9.12E+10	1.09E+11	1.28E+11	1.48E+11	1.76E+11	1.89E+11
<i>i16 – i17</i>	3.23E+09	4.58E+09	6.33E+09	8.56E+09	1.26E+10	1.47E+10
<i>i17 – i16</i>	1.44E+13	1.44E+13	1.44E+13	1.44E+13	1.44E+13	1.43E+13
<i>i15 – p4+H</i>	2.65E+07	5.17E+07	9.57E+07	1.69E+08	3.53E+08	4.73E+08
<i>i9 – p13+H</i>	0.00E+00	2.15E-10	4.72E-05	4.77E-02	2.59E+01	1.22E+02
<i>i26 – i28</i>	4.79E+06	8.44E+06	1.41E+07	2.26E+07	4.11E+07	5.20E+07
<i>i28 – i26</i>	5.79E+09	7.88E+09	1.04E+10	1.32E+10	1.79E+10	2.02E+10
<i>i24 – i28</i>	6.87E+09	9.02E+09	1.16E+10	1.48E+10	2.02E+10	2.29E+10
<i>i28 – i24</i>	1.93E+13	1.90E+13	1.87E+13	1.84E+13	1.81E+13	1.79E+13
<i>i27 – p5+H</i>	2.08E+08	4.13E+08	7.70E+08	1.36E+09	2.82E+09	3.76E+09
<i>i31 – i37</i>	9.55E+08	2.14E+09	4.20E+09	7.52E+09	1.50E+10	1.95E+10
<i>i37 – i31</i>	2.12E+07	5.74E+07	1.35E+08	2.84E+08	7.01E+08	9.93E+08
<i>i17 – i18</i>	3.19E+12	3.28E+12	3.37E+12	3.44E+12	3.54E+12	3.58E+12
<i>i18 – i17</i>	2.72E+12	2.81E+12	2.90E+12	2.98E+12	3.08E+12	3.12E+12
<i>i37 – p5+H</i>	2.07E+09	3.83E+09	6.66E+09	1.10E+10	2.04E+10	2.61E+10
<i>i27 – i37</i>	7.39E+09	9.11E+09	1.11E+10	1.34E+10	1.71E+10	1.89E+10
<i>i37 – i27</i>	6.32E+12	6.79E+12	7.25E+12	7.72E+12	8.37E+12	8.65E+12
<i>i26 – i37</i>	9.73E+07	1.42E+08	2.02E+08	2.79E+08	4.24E+08	5.02E+08
<i>i37 – i26</i>	8.89E+09	1.20E+10	1.59E+10	2.06E+10	2.87E+10	3.27E+10
<i>i37 – p13+H</i>	0.00E+00	4.38E+02	8.20E+04	1.02E+06	1.20E+07	2.79E+07
<i>i1 – i32</i>	3.92E-06	1.23E-04	3.66E-03	1.02E-01	6.49E+00	2.51E+01
<i>i32 – i1</i>	1.36E-03	3.76E-02	9.87E-01	2.44E+01	1.33E+03	4.84E+03
<i>i27 – p1+H</i>	9.24E+10	1.29E+11	1.75E+11	2.34E+11	3.42E+11	4.00E+11
<i>i20 – i18</i>	2.88E-01	8.07E+00	9.64E+01	6.22E+02	4.70E+03	9.72E+03
<i>i18 – i20</i>	2.25E+04	4.38E+05	3.75E+06	1.78E+07	9.02E+07	1.59E+08
<i>i30 – p12+H</i>	1.53E+04	8.06E+04	3.15E+05	1.00E+06	3.98E+06	6.71E+06
<i>i29 – i18</i>	7.63E+07	1.42E+08	2.47E+08	4.06E+08	7.57E+08	9.66E+08
<i>i18 – i29</i>	1.25E+10	1.77E+10	2.38E+10	3.11E+10	4.29E+10	4.86E+10
<i>i24 – p1+H</i>	1.63E+09	2.46E+09	3.62E+09	5.18E+09	8.22E+09	9.90E+09
<i>i2 – i23</i>	2.03E+06	4.48E+06	8.97E+06	1.66E+07	3.56E+07	4.79E+07
<i>i23 – i2</i>	1.69E+12	1.88E+12	2.05E+12	2.21E+12	2.40E+12	2.48E+12
<i>i10 – i31</i>	1.79E+09	2.43E+09	3.23E+09	4.22E+09	5.98E+09	6.88E+09
<i>i31 – i10</i>	9.98E+12	1.00E+13	1.00E+13	1.00E+13	1.00E+13	1.01E+13
<i>i56 – i57</i>	1.87E+04	1.57E+05	7.49E+05	2.55E+06	1.01E+07	1.68E+07
<i>i57 – i56</i>	4.53E+04	3.70E+05	1.72E+06	5.71E+06	2.20E+07	3.60E+07
<i>i63 – i60</i>	0.00E+00	0.00E+00	1.72E+02	2.03E+03	1.84E+04	3.88E+04
<i>i60 – i63</i>	0.00E+00	0.00E+00	7.84E+03	8.35E+04	6.65E+05	1.34E+06
<i>i60 – p29+H</i>	0.00E+00	0.00E+00	1.57E+04	2.72E+05	3.58E+06	8.27E+06
<i>i65 – p29+H</i>	0.00E+00	0.00E+00	3.68E+02	4.72E+03	5.59E+04	1.32E+05
<i>i60 – i57</i>	2.14E+04	2.08E+05	9.76E+05	3.31E+06	1.31E+07	2.17E+07
<i>i57 – i60</i>	9.28E+04	8.62E+05	3.90E+06	1.27E+07	4.81E+07	7.82E+07

<i>i63 – i7</i>	8.39E+04	2.79E+05	7.71E+05	1.86E+06	5.38E+06	8.08E+06
<i>i7 – i63</i>	1.02E+05	3.36E+05	9.24E+05	2.22E+06	6.40E+06	9.58E+06
<i>i7 – i68</i>	1.20E+06	2.69E+06	5.48E+06	1.04E+07	2.28E+07	3.10E+07
<i>i68 – i7</i>	3.90E+08	7.23E+08	1.24E+09	1.98E+09	3.52E+09	4.39E+09
<i>i65 – i45</i>	3.14E+07	5.98E+07	1.08E+08	1.84E+08	3.64E+08	4.77E+08
<i>i45 – i65</i>	8.37E+07	1.47E+08	2.45E+08	3.91E+08	7.02E+08	8.85E+08
<i>i67 – i60</i>	9.84E+01	6.63E+02	2.98E+03	1.05E+04	4.59E+04	8.01E+04
<i>i60 – i67</i>	2.68E+05	1.48E+06	5.52E+06	1.62E+07	5.63E+07	8.92E+07
<i>i2 – i10</i>	2.61E-02	2.08E+00	7.55E+01	5.79E+02	4.23E+03	8.46E+03
<i>i10 – i2</i>	2.14E-03	1.87E-01	7.46E+00	6.24E+01	5.11E+02	1.07E+03
<i>i67 – i60</i>	1.30E-02	1.71E-01	2.05E+00	1.80E+01	1.66E+02	3.65E+02
<i>i60 – i67</i>	3.55E+01	3.81E+02	3.80E+03	2.79E+04	2.04E+05	4.07E+05
<i>i58 – i62</i>	7.05E+04	1.83E+06	1.17E+07	4.16E+07	1.60E+08	2.58E+08
<i>i62 – i58</i>	5.67E+02	1.78E+04	1.36E+05	5.65E+05	2.66E+06	4.66E+06
<i>i15 – i51</i>	3.80E+08	4.86E+08	6.14E+08	7.67E+08	1.03E+09	1.16E+09
<i>i51 – i15</i>	8.27E+13	8.54E+13	8.79E+13	9.04E+13	9.37E+13	9.51E+13
<i>i43 – i16</i>	3.89E+13	3.78E+13	3.68E+13	3.59E+13	3.48E+13	3.44E+13
<i>i16 – i43</i>	1.81E+09	2.40E+09	3.14E+09	4.01E+09	5.53E+09	6.29E+09
<i>i65 – i67</i>	1.35E+05	3.86E+05	9.69E+05	2.19E+06	6.02E+06	8.91E+06
<i>i67 – i65</i>	2.40E+04	6.99E+04	1.79E+05	4.11E+05	1.15E+06	1.72E+06
<i>i37 – p6+H</i>	0.00E+00	0.00E+00	0.00E+00	1.46E+03	1.99E+05	7.35E+05
<i>i34 – i35</i>	1.85E+09	3.13E+09	4.94E+09	7.38E+09	1.20E+10	1.45E+10
<i>i35 – i34</i>	4.46E+11	5.61E+11	6.80E+11	8.01E+11	9.72E+11	1.05E+12
<i>i1 – i40</i>	6.91E+06	1.13E+07	1.78E+07	2.71E+07	4.63E+07	5.74E+07
<i>i40 – i1</i>	3.07E+12	3.06E+12	3.06E+12	3.06E+12	3.06E+12	3.06E+12
<i>i57 – i40</i>	5.76E+11	7.33E+11	9.11E+11	1.11E+12	1.43E+12	1.58E+12
<i>i40 – i57</i>	1.76E+12	1.69E+12	1.63E+12	1.58E+12	1.52E+12	1.50E+12
<i>i8 – i57</i>	1.01E+08	1.65E+08	2.59E+08	3.92E+08	6.62E+08	8.14E+08
<i>i57 – i8</i>	4.45E+10	6.21E+10	8.38E+10	1.10E+11	1.54E+11	1.76E+11
<i>i60 – i57</i>	2.66E-01	5.33E+00	9.90E+01	1.67E+03	4.04E+04	1.08E+05
<i>i57 – i60</i>	1.16E+00	2.21E+01	3.95E+02	6.41E+03	1.48E+05	3.90E+05
<i>i26 – i36</i>	1.44E+07	2.65E+07	4.60E+07	7.62E+07	1.44E+08	1.86E+08
<i>i36 – i26</i>	5.89E+12	6.50E+12	7.07E+12	7.62E+12	8.35E+12	8.66E+12
<i>i27 – i9</i>	5.39E+06	9.03E+06	1.46E+07	2.27E+07	4.02E+07	5.05E+07
<i>i9 – i27</i>	2.31E+07	3.73E+07	5.80E+07	8.74E+07	1.48E+08	1.82E+08
<i>i46 – i49</i>	8.35E+09	1.02E+10	1.23E+10	1.47E+10	1.85E+10	2.03E+10
<i>i49 – i46</i>	8.17E+12	8.16E+12	8.15E+12	8.14E+12	8.12E+12	8.12E+12
<i>i2 – i32</i>	1.25E+07	2.41E+07	4.31E+07	7.29E+07	1.40E+08	1.81E+08
<i>i32 – i2</i>	1.08E+08	2.01E+08	3.47E+08	5.67E+08	1.04E+09	1.32E+09
<i>i36 – p11b+CCH₂</i>	0.00E+00	0.00E+00	0.00E+00	1.17E-05	6.65E+03	8.51E+05
<i>i13 – i26</i>	1.34E+06	2.90E+06	5.71E+06	1.05E+07	2.20E+07	2.94E+07
<i>i26 – i13</i>	7.25E+06	1.68E+07	3.52E+07	6.84E+07	1.56E+08	2.15E+08
<i>i65 – i27</i>	9.50E+07	1.65E+08	2.72E+08	4.33E+08	7.82E+08	9.90E+08
<i>i27 – i65</i>	1.31E+06	2.31E+06	3.88E+06	6.28E+06	1.16E+07	1.48E+07
<i>i63 – i16</i>	2.71E+11	3.23E+11	3.80E+11	4.42E+11	5.39E+11	5.84E+11
<i>i16 – i63</i>	6.14E+09	7.51E+09	9.06E+09	1.08E+10	1.36E+10	1.50E+10
<i>i53 – i59</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.74E+02	1.73E+03
<i>i59 – i53</i>	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.90E+03	3.98E+04
<i>i61 – i59</i>	1.01E+12	1.14E+12	1.27E+12	1.40E+12	1.60E+12	1.68E+12
<i>i59 – i61</i>	3.84E+11	4.40E+11	4.99E+11	5.60E+11	6.48E+11	6.87E+11
<i>i6 – i32</i>	7.83E+09	9.65E+09	1.17E+10	1.41E+10	1.81E+10	1.99E+10
<i>i32 – i6</i>	9.83E+11	1.06E+12	1.14E+12	1.22E+12	1.33E+12	1.37E+12
<i>i9 – i54</i>	1.29E+12	1.34E+12	1.38E+12	1.43E+12	1.50E+12	1.53E+12
<i>i54 – i9</i>	1.49E+13	1.59E+13	1.68E+13	1.78E+13	1.92E+13	1.98E+13
<i>i44 – i32</i>	6.74E+11	7.15E+11	7.56E+11	7.97E+11	8.54E+11	8.78E+11
<i>i32 – i44</i>	2.83E+12	2.87E+12	2.91E+12	2.95E+12	3.00E+12	3.02E+12
<i>i63 – i31</i>	4.13E+10	5.32E+10	6.72E+10	8.37E+10	1.11E+11	1.24E+11
<i>i31 – i63</i>	2.55E+12	2.58E+12	2.61E+12	2.63E+12	2.67E+12	2.68E+12
<i>i5 – i56</i>	5.34E+06	1.04E+07	1.87E+07	3.18E+07	6.17E+07	7.99E+07
<i>i56 – i5</i>	1.13E+10	1.98E+10	3.22E+10	4.99E+10	8.55E+10	1.05E+11
<i>i30 – i40</i>	8.61E+05	1.75E+06	3.32E+06	5.94E+06	1.23E+07	1.65E+07
<i>i40 – i30</i>	8.91E+10	1.11E+11	1.33E+11	1.57E+11	1.90E+11	2.05E+11
<i>i49 – i59</i>	6.67E+12	6.59E+12	6.52E+12	6.45E+12	6.36E+12	6.33E+12

<i>i59 – i49</i>	6.40E+12	6.52E+12	6.64E+12	6.74E+12	6.89E+12	6.95E+12
<i>i45 – i51</i>	0.00E+00	0.00E+00	0.00E+00	7.69E+02	1.32E+04	3.31E+04
<i>i51 – i45</i>	0.00E+00	0.00E+00	0.00E+00	8.17E+03	1.33E+05	3.26E+05
<i>i20 – i62</i>	1.04E+08	1.37E+08	1.77E+08	2.25E+08	3.07E+08	3.48E+08
<i>i62 – i20</i>	2.01E+12	2.23E+12	2.45E+12	2.68E+12	3.01E+12	3.15E+12
<i>i67 – i20</i>	2.22E+09	3.13E+09	4.31E+09	5.83E+09	8.62E+09	1.01E+10
<i>i20 – i67</i>	1.19E+08	1.60E+08	2.10E+08	2.72E+08	3.80E+08	4.34E+08
<i>i67 – i62</i>	3.49E+09	4.38E+09	5.43E+09	6.66E+09	8.70E+09	9.70E+09
<i>i62 – i67</i>	7.18E+12	7.27E+12	7.35E+12	7.42E+12	7.51E+12	7.55E+12
<i>i67 – i24</i>	6.47E+06	1.16E+07	1.98E+07	3.24E+07	6.08E+07	7.81E+07
<i>i24 – i67</i>	4.01E+06	6.98E+06	1.16E+07	1.84E+07	3.33E+07	4.21E+07
<i>i11 – i7</i>	4.26E+05	6.54E+05	9.79E+05	1.43E+06	2.35E+06	2.88E+06
<i>i7 – i11</i>	8.07E+10	1.05E+11	1.34E+11	1.69E+11	2.27E+11	2.55E+11
<i>i36 – i35</i>	2.62E+12	2.79E+12	2.95E+12	3.09E+12	3.27E+12	3.34E+12
<i>i35 – i36</i>	4.81E+12	4.92E+12	5.01E+12	5.09E+12	5.19E+12	5.23E+12
<i>i54 – i48</i>	2.18E+03	9.12E+03	3.02E+04	8.41E+04	2.88E+05	4.61E+05
<i>i48 – i54</i>	6.34E+07	1.77E+08	4.02E+08	7.88E+08	1.71E+09	2.29E+09
<i>i63 – i35</i>	5.26E+06	1.12E+07	2.20E+07	4.00E+07	8.43E+07	1.13E+08
<i>i35 – i63</i>	5.93E+10	7.46E+10	9.04E+10	1.06E+11	1.29E+11	1.39E+11
<i>i27 – i39</i>	7.62E+09	9.20E+09	1.10E+10	1.31E+10	1.63E+10	1.79E+10
<i>i39 – i27</i>	4.09E+12	4.39E+12	4.69E+12	5.00E+12	5.43E+12	5.61E+12
<i>i39 – i37</i>	4.15E+12	4.34E+12	4.52E+12	4.70E+12	4.94E+12	5.04E+12
<i>i37 – i39</i>	6.61E+12	6.77E+12	6.92E+12	7.07E+12	7.26E+12	7.34E+12
<i>i27 – i29</i>	2.35E+03	6.49E+03	1.58E+04	3.50E+04	9.38E+04	1.38E+05
<i>i29 – i27</i>	7.71E+05	1.87E+06	4.02E+06	7.90E+06	1.81E+07	2.48E+07
<i>i63 – i9</i>	1.16E+11	1.39E+11	1.66E+11	1.95E+11	2.41E+11	2.62E+11
<i>i9 – i63</i>	7.95E+08	1.01E+09	1.26E+09	1.55E+09	2.03E+09	2.27E+09
<i>i4 – i10</i>	4.89E+11	5.72E+11	6.61E+11	7.56E+11	8.98E+11	9.62E+11
<i>i10 – i4</i>	5.64E+08	7.65E+08	1.02E+09	1.33E+09	1.88E+09	2.16E+09
<i>i1 – i9</i>	6.36E+07	9.90E+07	1.49E+08	2.19E+08	3.58E+08	4.36E+08
<i>i9 – i1</i>	1.30E+08	2.00E+08	2.99E+08	4.35E+08	7.04E+08	8.53E+08
<i>i3 – i24</i>	1.71E+05	3.71E+05	7.46E+05	1.41E+06	3.12E+06	4.26E+06
<i>i24 – i3</i>	3.68E+05	8.04E+05	1.63E+06	3.08E+06	6.88E+06	9.45E+06
<i>i10 – i16</i>	1.48E+10	1.99E+10	2.63E+10	3.42E+10	4.80E+10	5.51E+10
<i>i16 – i10</i>	3.03E+10	3.94E+10	5.02E+10	6.31E+10	8.49E+10	9.57E+10
<i>i68 – i69</i>	4.25E+12	4.37E+12	4.48E+12	4.58E+12	4.72E+12	4.78E+12
<i>i69 – i68</i>	4.36E+10	5.20E+10	6.12E+10	7.12E+10	8.67E+10	9.39E+10
<i>i54 – i55</i>	9.72E+09	1.24E+10	1.55E+10	1.92E+10	2.54E+10	2.85E+10
<i>i55 – i54</i>	1.23E+12	1.32E+12	1.40E+12	1.48E+12	1.60E+12	1.65E+12
<i>i44 – i50</i>	1.16E+11	1.25E+11	1.34E+11	1.43E+11	1.56E+11	1.61E+11
<i>i50 – i44</i>	9.81E+12	9.81E+12	9.80E+12	9.79E+12	9.78E+12	9.77E+12
<i>i8 – i66</i>	1.78E+08	2.66E+08	3.83E+08	5.36E+08	8.25E+08	9.80E+08
<i>i66 – i8</i>	2.82E+11	3.56E+11	4.40E+11	5.33E+11	6.79E+11	7.47E+11
<i>i54 – i60</i>	1.13E+10	1.50E+10	1.96E+10	2.51E+10	3.47E+10	3.96E+10
<i>i60 – i54</i>	8.06E+12	8.85E+12	9.65E+12	1.05E+13	1.16E+13	1.21E+13
<i>i50 – i55</i>	5.79E-04	1.41E-02	3.21E-01	6.89E+00	4.19E+02	1.82E+03
<i>i55 – i50</i>	2.47E-04	6.06E-03	1.39E-01	2.97E+00	1.82E+02	7.91E+02
<i>i6 – i9</i>	2.56E+04	7.94E+04	2.14E+05	5.14E+05	1.51E+06	2.30E+06
<i>i9 – i6</i>	1.88E+04	5.78E+04	1.54E+05	3.67E+05	1.06E+06	1.61E+06
<i>i67 – p30t+H</i>	0.00E+00	0.00E+00	0.00E+00	6.17E+00	2.59E+02	7.85E+02

Table S3. RRKM calculated statistical product branching ratios (%) for the pathways that include **i11** in reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3 , X^2A') at different collision energies (E_{col}).

<i>Channel</i>	E_{col} , kJ mol ⁻¹					
	0	10	20	30	44	50
<i>i1</i> → <i>i3</i> → <i>i11</i>	61.8	63.6	65.3	66.8	68.7	69.5
<i>i1</i> → <i>i3</i> → <i>i5</i> → <i>i8</i> → <i>i9</i> → <i>i11</i>	17.2	16.1	15.0	14.1	13.0	12.5
<i>i1</i> → <i>i3</i> → <i>i8</i> → <i>i9</i> → <i>i11</i>	12.3	11.5	10.9	10.3	9.5	9.3
<i>i1</i> → <i>i7</i> → <i>i11</i>	4.4	4.5	4.5	4.6	4.6	4.6
<i>i1</i> → <i>i2</i> → <i>i4</i> → <i>i7</i> → <i>i11</i>	3.4	3.3	3.2	3.2	3.0	3.0
<i>i1</i> → <i>i2</i> → <i>i4</i> → <i>i10</i> → <i>i11</i>	0.9	1.0	1.0	1.1	1.1	1.2

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) for all intermediates, transition states, reactants, and products involved in the C₃+C₂H₃ reactions at the ωB97X-D/6-311G(d,p) level.

Intermediates

i24 3122.1068 3220.1073 3235.0045

Cartesian coordinates

C -1.517626 0.613805 0.107823
C 1.006611 -0.102280 0.084914
C -0.342186 -0.467220 0.372723
C -1.439706 -0.393227 -0.663272
H 3.155683 0.473202 -0.347123
H -0.464910 -1.140369 1.218493
H -1.820997 1.537544 0.559929

Vibrational frequencies

193.9726 224.8692 468.2664
556.3718 638.1688 679.7369
685.8192 712.7092 855.6632
920.4692 934.2704 1057.8542
1351.4208 1788.6596 2200.5801
3145.0471 3363.8602 3485.4559

i30

Cartesian coordinates

C -1.864115 0.367516 0.000000
C 0.479462 -0.183284 0.000000
C 1.422675 0.848598 -0.000001
C 1.815913 -0.453858 0.000000
H -1.134725 -1.623486 0.000002
H -2.913845 0.098748 0.000000
H -1.608292 1.421744 -0.000001

Vibrational frequencies

74.6101 183.9098 353.5555
533.7864 590.5285 711.7885
781.7688 1006.5917 1022.1088
1073.0256 1316.4127 1360.6710
1440.0376 1682.3857 1749.0713
3161.2693 3197.1822 3261.5051

i44

Cartesian coordinates

C -1.901865 0.000020 0.016644
C 0.743566 0.744426 -0.006025
C 1.989489 0.000044 0.026149
C 0.743546 -0.744467 -0.006018
H -2.298658 -0.890711 -0.471703
H -2.298699 0.889500 -0.473968
H -2.241658 0.001371 1.057826

Vibrational frequencies

46.7031 121.2830 271.3626
474.4745 502.5224 710.5850
726.7537 1007.8015 1083.1332
1089.6915 1260.0318 1409.0685
1474.8622 1479.4366 1625.6701
3047.1873 3127.3206 3167.2735

i56

Cartesian coordinates

C -0.103294 -0.456514 0.653547
C 0.556943 0.846958 -0.038883
C -0.816461 0.638505 -0.229384
C -1.485586 -0.504087 -0.111391
H 1.031380 -1.007795 -1.174393
H 2.109718 -0.700172 0.280613
H 0.986203 1.659939 0.530642

Vibrational frequencies

273.5579 391.9930 557.1842
605.6581 715.1668 874.6185
913.9003 1027.8469 1071.7505
1132.0763 1133.9833 1191.0927
1316.9040 1496.2421 1583.6720

i4

Cartesian coordinates

C 0.353646 0.956764 0.000009
C 0.456328 -1.065008 -0.000022
C -0.725156 -0.200609 0.000007
C -2.011616 -0.048318 0.000028
H 2.489333 -0.123162 -0.000038
H 0.300512 1.558098 0.907657
H 0.300486 1.558126 -0.907619

Vibrational frequencies

182.8983 199.2139 503.0416
627.5857 752.9846 809.8959
910.1425 937.7043 979.4207
1097.2280 1174.3661 1191.1361
1452.8176 1611.9033 1805.9309
3088.0673 3170.5308 3287.7515

i54

Cartesian coordinates

C 1.867679 0.000072 0.086591
C -0.600190 -0.902296 -0.170350
C -1.586503 0.000045 0.198383
C -0.600241 0.902320 -0.170193
H 2.412498 -0.932746 0.154546
H 2.412149 0.933170 0.153421
H -2.654070 0.000002 0.331749

Vibrational frequencies

269.4215 348.8145 639.3264
683.1349 736.6208 778.7156
871.3501 922.3806 968.0282
970.9633 1063.6998 1156.4634
1440.1285 1460.2576 1821.1278
3178.9358 3277.2869 3312.1426

i53

Cartesian coordinates

C 1.733250 -0.361484 0.000140
C -0.673510 0.084315 0.733851
C -1.795340 -0.342765 0.000135
C -0.673498 0.083729 -0.733897
H 2.723558 0.071195 0.000209
H 1.614230 -1.436786 0.000286
H 0.752820 1.571792 -0.000601

Vibrational frequencies

146.9724 259.1970 370.2414
443.4390 562.7657 605.3876
865.3102 995.3169 1060.0616
1078.5937 1147.3316 1209.2892
1406.2883 1475.6241 1546.8068
3167.5571 3182.2749 3304.2947

i20

Cartesian coordinates

C 0.102914 0.604965 0.000001
C -1.202642 0.131688 0.000000
C 2.542707 -0.160700 -0.000001
C 1.230516 -0.252579 0.000000
H -3.346864 -0.627589 -0.000001
H 0.269710 1.675100 0.000000
H 1.101869 -1.353164 0.000002

Vibrational frequencies

120.4838 163.8962 234.8053
404.7301 542.3829 571.7409
661.9428 680.7837 688.6852

845.5100 1066.9046 1156.5724

1387.2594 1618.3960 2103.2637

3002.1434 3213.9687 3473.3758

i19

Cartesian coordinates

C 0.000000 0.737991 0.000000
C 1.196795 0.037392 0.000000
C -2.473795 -0.265319 0.000000
C -1.257522 0.120409 0.000000
H 3.168339 -1.096595 0.000000
H 0.007718 1.821744 0.000000
H -1.443373 -1.106027 0.000000

Vibrational frequencies

140.3945 225.8118 310.5400
376.9316 388.2088 540.5872
585.0178 634.6483 696.3214
717.6258 979.2016 1115.3762
1363.4592 1844.1384 2109.8054
2421.5097 3210.7532 3472.3384

i22

Cartesian coordinates

C -0.497558 0.931257 -0.000004
C 0.672304 -0.013332 0.000033
C -0.557011 -0.718802 0.000002
C -1.812744 -0.490437 -0.000011
H 2.776030 -0.769065 -0.000046
H -0.691630 1.451924 0.929528
H -0.691555 1.451904 -0.929564

Vibrational frequencies

199.5808 222.3731 385.6359
440.5913 656.6258 674.7749
756.6737 862.8634 994.0726
997.7412 1024.4593 1075.5268
1477.6416 1754.9079 1899.1931
3150.7674 3267.8820 3317.8695

i25

Cartesian coordinates

C 0.398526 0.922890 -0.056513
C -0.739409 -0.034305 0.342872
C 0.550333 -0.685640 0.143824
C 1.748891 -0.443407 -0.207465
H -1.090878 0.057440 1.385300
H 0.338127 1.323392 -1.060253
H 0.761354 1.578177 0.724759

Vibrational frequencies

161.2153 222.2039 313.1262
377.9026 671.6803 778.5676
896.9789 926.7010 978.8431
1050.4340 1063.1559 1097.7552
1303.7721 1484.2002 1893.1447
3007.1429 3157.6676 3273.7121

i23

Cartesian coordinates

C -1.133986 -0.355529 0.874663
C -0.234320 -0.512599 -0.393851
C 1.074672 -0.134371 -0.116148
C 2.236367 0.315755 0.163415
H -1.022878 1.611454 -0.097247
H -2.226025 0.405349 -0.792597
H -0.451431 -1.337769 -1.065320

Vibrational frequencies

96.0419 150.8807 317.8084

408.0648 601.4059 680.6243
738.7661 817.7058 959.3053
991.7670 1083.8397 1205.6585
1319.8690 1396.9278 2002.2239
3118.2649 3167.7877 3211.3862

i51

Cartesian coordinates

C -0.557665 0.831444 0.162290
C 0.627127 -0.044898 0.026910
C -0.610352 -0.819544 0.140101
C -1.581756 0.050932 -0.453496
H 2.765876 0.532619 -0.246626
H -0.687274 1.635361 0.881414
H -0.807391 -1.630501 0.835900

Vibrational frequencies

269.4155 331.2534 575.9378
595.4711 674.5747 719.7731
800.6971 894.5052 960.4497
1008.0593 1081.4832 1146.2856
1159.0157 1374.1457 1777.4322
3184.7253 3192.2435 3319.4378

i41

Cartesian coordinates

C -0.596975 -0.031207 0.418508
C 0.633288 0.770434 0.044742
C 0.532958 -0.792529 -0.243635
C -1.857441 0.135277 -0.297326
H -0.699283 -0.248771 1.485223
H 0.595646 1.693809 -0.531870
H -2.509014 -0.746171 -0.233772

Vibrational frequencies

202.1503 270.3698 322.4999
483.1296 657.5305 717.0813
792.8445 880.6903 957.3267
985.2201 1035.2611 1110.5728
1168.0344 1322.4151 1454.5808
3070.8309 3083.4818 3136.9975

i42

Cartesian coordinates

C -0.342689 -0.771867 -0.530518
C -0.374149 0.799201 -0.057353
C 0.800177 -0.066128 -0.013355
C 2.094775 -0.035116 0.224804
H -1.497014 -0.503985 1.325967
H -2.421211 0.024436 -0.156672
H -0.442581 1.596240 -0.787577

Vibrational frequencies

70.6662 221.5897 287.1989
545.4317 670.7157 841.5162
897.1213 954.3220 1041.0411
1069.7618 1123.2742 1209.2573
1296.5043 1504.8314 1658.5303
3117.2549 3198.6005 3208.8298

i68

Cartesian coordinates

C 1.163095 -0.035617 0.077174
C 0.106839 0.928450 -0.168503
C -0.925846 -0.201377 -0.702402
C 0.227130 -1.053680 -0.145061
H 2.220262 0.001294 0.311342
H 0.050855 1.979357 -0.408196
H -0.948359 -0.125583 1.718509

Vibrational frequencies

262.2917 399.5429 656.3572
713.0996 829.6970 841.0863
856.8818 903.1266 932.0714
954.1849 1031.3639 1095.1604
1277.9799 1341.6161 1381.7976
3220.8919 3256.5681 3302.8313

i47

Cartesian coordinates

C 0.405376 0.861967 0.004839
C -0.710930 -0.068266 0.278267
C 0.540855 -0.960470 -0.306075
C 1.472493 -0.042864 0.103556
H 0.322297 1.689271 -0.700612
H 2.547623 0.024399 0.076691
H -0.862278 -0.364244 1.330976

Vibrational frequencies

171.8555 288.4630 474.6554
540.2711 614.3712 783.6924
837.7884 860.4456 961.6490
1050.0529 1094.4273 1194.8706
1312.2916 1320.8084 1482.1403
3013.3789 3132.8955 3288.5955

i69

Cartesian coordinates

C -0.000108 0.925879 -0.318300
C -0.000102 -1.098091 -0.282279
C -1.034437 -0.095876 -0.179789
C 0.000336 0.062096 1.043143
H 2.104334 -0.096364 -0.073831
H -0.000168 2.003817 -0.349981
H -2.104362 -0.096348 -0.073077

Vibrational frequencies

224.2074 400.3402 433.0380
707.9763 850.7763 883.3737
931.5627 973.5822 982.5956
1056.2326 1095.5570 1138.7921
1296.5444 1315.0124 1319.8981
3266.6032 3312.7836 3317.0104

i63

Cartesian coordinates

C -1.126855 -0.468980 0.000222
C 1.303536 -0.178432 0.000041
C 0.471122 1.018912 0.000426
C -0.783811 0.998635 -0.000667
H -1.679460 -0.785405 0.886502
H -1.681564 -0.787001 -0.884162
H 2.373588 -0.290928 -0.000172

Vibrational frequencies

243.6857 352.1564 390.5368
672.9186 759.3770 854.3652
858.7456 1007.0563 1034.5506
1117.8559 1169.6022 1203.7170
1412.2887 1557.2161 1741.7668
3096.4776 3148.8764 3300.3983
858.7456 1007.0563 1034.5505

i61

Cartesian coordinates

C -0.029027 0.928443 -0.327032
C 0.269280 -1.056992 -0.253182
C -0.966243 -0.220588 -0.309371
C -0.075764 0.056275 0.881403
H -0.168455 0.086704 1.950052
H -0.131059 2.002352 -0.387273
H -2.031028 -0.399922 -0.322395

Vibrational frequencies

417.3369 493.4069 527.4031
640.4906 791.5820 829.3328
856.4582 914.3256 939.1350
1024.0887 1048.5827 1148.1104
1207.6358 1288.4793 1334.3669
3239.8521 3257.9321 3333.1112

i52

Cartesian coordinates

C 0.477763 -0.694994 -0.329405
C -0.776291 -0.013122 -0.009988
C 0.474518 0.704106 -0.329181
C 1.638995 0.003229 0.291358
H -3.076029 0.128464 0.234844

H 2.534525 0.006162 -0.315784
H 1.801085 0.002913 1.369416

Vibrational frequencies

149.2041 214.3648 351.5985
412.6790 461.7512 526.0686
746.8870 802.1069 996.3686
1076.6339 1082.4858 1209.7395
1344.9436 1528.3201 1834.3016
3100.8791 3228.6060 3454.3159

i31

Cartesian coordinates

C -1.432495 0.691905 -0.000010
C 1.203281 -0.338575 -0.000028
C -0.220479 -0.342548 -0.000002
C -1.418836 -0.795778 0.000029
H -1.632471 1.238937 0.920343
H -1.632498 1.238886 -0.920388
H 1.753241 -1.294642 -0.000031

Vibrational frequencies

140.8993 148.2729 274.0466
361.9669 622.6469 648.8015
785.2869 902.2344 1015.8692
1029.4372 1067.8122 1076.3773
1508.0849 1743.3107 1933.1953
3041.4939 3084.2396 3172.3708

i27

Cartesian coordinates

C 1.577467 -0.713563 -0.116759
C 0.288073 0.024650 -0.032105
C -1.095807 0.009731 -0.007394
C -2.300060 -0.031544 0.018643
H 1.911045 1.649082 0.135717
H -3.362682 -0.062923 0.041880
H 2.028409 -1.454594 0.540620

Vibrational frequencies

195.4203 202.4622 436.5003
469.4160 543.6760 639.6096
678.8888 778.6835 831.4371
963.3326 997.7252 1078.2595
1187.8340 1735.6512 2189.3464
3127.9964 3271.1042 3480.7093

i33

Cartesian coordinates

C 0.496683 1.513590 -0.000001
C -0.833102 -0.143271 0.000002
C 0.578146 0.162879 0.000004
C 1.618793 -0.763623 -0.000002
H -3.073254 -0.486537 -0.000009
H 2.645078 -0.423927 -0.000010
H 1.405272 -1.822720 0.000008

Vibrational frequencies

96.3934 224.6225 264.5708
447.4102 452.9294 550.4851
630.8760 677.4939 777.5653
818.8382 1018.7736 1240.8302
1410.6326 1472.1703 2206.8615
3184.7638 3300.0449 3477.9918
96.3934 224.6224 264.5708
1410.6325 1472.1703 2206.8615

i34

Cartesian coordinates

C 1.498205 -0.350811 0.353543
C -1.356583 -0.502227 -0.171616
C -0.014181 -0.015336 -0.312637
C 1.035081 0.731341 -0.518963
H 1.666583 -0.168644 1.413371
H 1.974077 -1.226254 -0.077320
H -1.807283 -1.412222 -0.530121

Vibrational frequencies

164.1807 218.2784 264.4129

321.9262 454.0628 712.2982
772.9522 907.2147 951.4265
1004.6959 1058.8397 1077.2047
1466.9435 1566.8713 1772.5099
3110.4684 3217.0660 3293.6577

i60

Cartesian coordinates

C -0.578679 0.811673 -0.346181
C 0.775115 0.725365 0.359238
C -0.018930 -0.450414 -0.529336
C -1.337521 -0.337049 0.280000
H 2.211243 -1.040090 0.186146
H -2.223701 -0.676029 -0.243253
H -1.322636 -0.491876 1.359328

Vibrational frequencies

343.6191 494.4256 554.5438
599.7829 664.5155 718.9644
853.3064 953.3937 1020.0054
1056.3627 1070.1874 1102.5579
1343.4483 1493.8396 1628.3927
3104.1630 3231.5840 3361.8004

i15

Cartesian coordinates

C 2.296480 -0.464514 -0.000003
C 0.000000 0.757089 0.000000
C -1.221547 0.092510 0.000002
C -2.296480 -0.464513 0.000002
H 3.237262 -0.960370 0.000014
H -3.237263 -0.960369 -0.000013
H -0.000001 1.842237 -0.000003

Vibrational frequencies

143.7428 346.0341 354.1235
382.1056 581.2933 582.4316
605.6107 662.1927 709.7113
711.8291 965.8882 1126.6954
1376.1202 2051.8767 2147.4588
3190.1563 3474.1000 3478.0282
143.7427 346.0341 354.1235

i28

Cartesian coordinates

C -0.215249 -0.308206 0.395760
C 1.052447 0.049447 -0.241949
C -1.457219 -0.616541 -0.396726
C -1.530522 0.564033 0.073289
H -0.114294 -0.706136 1.401753
H 1.070595 0.365211 -1.300943
H -1.884990 1.547473 0.314442

Vibrational frequencies

135.9572 145.3655 309.6634
425.5748 614.9295 652.8869
690.4702 813.7651 865.1658
953.3803 1035.1382 1071.9477
1373.2877 1741.8797 1790.8852
3021.0411 3155.7361 3356.3513

i48

Cartesian coordinates

C -0.567954 0.878053 0.264740
C -0.567952 -0.878074 0.264654
C 0.697143 -0.000005 0.492890
C 1.573357 0.000016 -0.590246
H -2.343701 0.000066 -0.881646
H 1.130131 -0.000139 1.493969
H 2.648181 0.000077 -0.706740

Vibrational frequencies

256.1315 334.7304 417.1854
513.2904 598.1304 717.1904
823.1957 896.9569 972.7297
1025.0055 1040.8104 1188.3207
1204.5842 1301.2127 1513.0262
3125.4352 3252.0102 3314.3189

i62

Cartesian coordinates

C -0.057314 -0.582168 0.400713
C 0.772238 0.730304 -0.416749
C -0.640221 0.742098 0.191723
C -1.276923 -0.492235 -0.381892
H 2.233761 -0.960231 -0.065677
H -0.961974 1.533930 0.850786
H -2.240294 -0.875307 -0.063258

Vibrational frequencies

215.9251 501.7167 549.6208
598.8385 689.8739 749.2505
834.5096 915.9031 938.6144
1010.0489 1086.3681 1096.3487
1181.0821 1330.0227 1573.7315
3202.1923 3251.4510 3327.3645

i11

Cartesian coordinates

C -2.521440 -0.000143 0.000079
C 0.062169 0.000291 -0.000020
C 1.415278 0.000133 -0.000204
C 2.625028 -0.000100 0.000211
H -3.074023 -0.932207 0.000143
H -3.074239 0.931786 0.000143
H 3.688454 -0.000761 -0.000061

Vibrational frequencies

138.5574 147.6883 342.5751
391.6672 502.5512 530.8890
624.9482 662.5452 733.4072
737.1396 1026.7803 1312.0226
1474.3282 2039.8998 2149.4373
3158.8778 3256.7341 3477.5776

i21

Cartesian coordinates

C 0.000000 0.608583 0.000000
C 1.209942 -0.123731 0.000000
C -2.282247 -0.778684 0.000000
C -1.243875 -0.034888 0.000000
H 0.033450 1.688822 0.000000
H 1.205261 -1.229003 0.000000
H -2.327634 0.555344 0.000000

Vibrational frequencies

147.5708 160.9632 238.9156
247.5979 395.1597 452.3326
655.1728 678.8953 754.9420
852.2263 1048.1113 1155.6952
1374.6022 1600.6920 1855.9106
2430.7968 3025.3496 3242.2778

i36

Cartesian coordinates

C -1.379004 0.665983 0.113917
C 1.115904 -0.403591 0.226845
C -0.336363 -0.148199 0.077832
C -1.599144 -0.668485 -0.306843
H -1.800762 1.640053 0.309071
H 1.374732 -1.464244 0.103145
H 1.434875 -0.117371 1.259449

Vibrational frequencies

52.8950 211.6091 317.3894
476.2556 511.9406 771.0526
903.1720 946.7805 994.2649
1104.9414 1157.0546 1257.3687
1313.5478 1361.9618 1787.1254
2896.3099 3035.4363 3268.2974
1313.5477 1361.9618 1787.1254

i8

Cartesian coordinates

C -1.852730 -0.030300 -0.081967
C 0.678616 0.792692 0.027916
C 1.716078 -0.201464 -0.302968
C 0.653331 -0.819294 0.261813

H -2.398119 0.883735 -0.276531
H -2.401269 -0.960139 -0.011872
H 0.878360 1.701646 0.593207

Vibrational frequencies

259.8387 342.6369 590.4312
645.2687 673.9321 771.8548
818.9667 892.3063 941.7399
974.3528 1097.0374 1131.2465
1403.5384 1446.9779 1832.4168
3143.2848 3177.7228 3274.6469

i64

Cartesian coordinates

C 1.031775 0.000115 -0.262601
C 0.000004 1.061594 -0.318440
C 0.000000 -1.061430 -0.318986
C -0.000004 -0.000343 0.877030
H -2.099729 0.000099 -0.118420
H 2.099735 0.000089 -0.118415
H -0.000033 -0.000500 1.950511

Vibrational frequencies

368.5753 531.7611 618.4892
783.9063 835.7247 843.6162
942.2106 966.1356 998.7342
1010.6755 1078.2317 1140.3506
1223.4761 1240.8886 1286.5890
3292.7076 3293.1467 3328.9029

i17

Cartesian coordinates

C 1.169746 0.030039 0.013687
C -1.293449 -0.001897 -0.020261
C -2.300857 -0.657659 -0.024871
C 2.274723 -0.552044 -0.140141
H -0.105902 1.479698 0.887584
H -0.042624 1.462061 -0.867323
H 1.521780 -0.764175 0.907569

Vibrational frequencies

127.1748 161.7602 220.4257
289.5995 300.1805 513.5998
633.1877 882.2635 929.0742
995.0742 1244.2746 1342.3980
1447.1238 2030.9269 2281.6407
2443.2023 3068.9938 3111.0463

i18

Cartesian coordinates

C -0.002037 0.750225 0.022572
C -1.155845 -0.184403 0.312671
C 1.276930 0.040949 -0.053062
C 2.327222 -0.544587 -0.091610
H -0.180593 1.276794 -0.917198
H 0.051758 1.505033 0.811900
H -1.143840 -0.802606 1.217445

Vibrational frequencies

88.1854 127.9952 172.2771
222.1863 426.2773 654.6413
830.3284 908.9816 1000.1761
1050.1450 1243.2979 1334.9836
1479.5430 1781.4166 2274.3986
3075.4648 3099.4808 3125.0717

i14

Cartesian coordinates

C -1.591609 -0.904662 0.000012
C 0.114189 0.848792 0.000010
C 1.201244 0.071650 -0.000003
C 2.251760 -0.651453 -0.000005
H -2.044961 1.131861 -0.000042
H -2.500503 -1.489129 0.000002
H 0.247022 1.930548 0.000039

Vibrational frequencies

143.6712 147.7608 263.0867
343.5023 609.1140 624.9237

858.9376 876.6465 952.4529
963.1276 1186.3914 1291.2814
1439.5032 1611.7953 2057.2467
3107.2621 3148.3004 3262.7281

i57

Cartesian coordinates

C 0.440617 0.963464 0.150771
C -0.875272 0.673095 -0.012274
C 0.005759 -0.580527 0.503255
C 1.225216 -0.246720 -0.314597
H 0.041246 -0.845512 1.552020
H 2.206214 -0.402068 0.124915
H 1.153864 -0.466981 -1.378283

Vibrational frequencies

289.9526 437.4132 536.3221
561.3618 728.1271 892.6572
991.4049 1020.0152 1064.9765
1135.6554 1166.7723 1213.1755
1314.1453 1445.1348 1489.5315
3112.0599 3205.9431 3215.4486

i40

Cartesian coordinates

C -0.336910 -0.669940 -1.280784
C -0.336910 -1.027797 0.000000
C -0.281541 0.562647 0.000000
C 0.993777 1.154637 0.000000
H -1.194718 1.141266 0.000000
H 1.108819 2.231634 0.000000
H 1.876868 0.529455 0.000000

Vibrational frequencies

52.9868 214.0822 273.0677
375.1048 430.9169 471.4126
786.6953 848.3804 978.1278
1056.2545 1188.8046 1230.2305
1332.3074 1486.7185 1645.9264
3169.0451 3229.1565 3286.5164

i29

Cartesian coordinates

C -1.296746 0.674797 -0.168366
C -0.191208 -0.076926 0.605273
C 1.127174 -0.080741 0.097878
C 2.312019 0.074017 -0.350568
H -1.736609 -1.513676 -0.670313
H -1.628720 1.680010 -0.351504
H -0.306331 -0.178352 1.681768

Vibrational frequencies

135.4473 191.1725 346.4181
522.5239 668.0093 720.0279
843.6990 897.4545 946.5544
971.3015 1029.9616 1032.7224
1358.4638 1786.3406 1914.3994
3137.1830 3299.9276 3358.2514

i49

Cartesian coordinates

C -0.469975 0.795316 0.213273
C -0.396594 -0.749693 0.282574
C 0.787513 0.093008 -0.048678
C 2.063305 -0.053013 -0.212665
H -2.459205 -0.134456 -0.338929
H -0.631559 1.515258 1.003079
H -0.456102 -1.427294 1.121894

Vibrational frequencies

91.1489 230.6629 516.8588
704.2351 752.7686 760.2508
809.7738 904.6237 989.1469
1015.7778 1094.9841 1151.9276
1195.9563 1344.7097 1829.2915
3198.9592 3235.0904 3251.8713

i32

Cartesian coordinates

C 1.699127 -0.472937 -0.000029
C 0.442795 0.295122 -0.000087
C -0.949253 0.026352 0.000044
C -1.876882 -0.908175 -0.000011
H 2.549460 0.208839 -0.002430
H 1.741097 -1.115656 -0.881739
H 1.743166 -1.111502 0.884629

Vibrational frequencies

67.7513 145.6016 312.8364
381.5946 428.6923 669.0808
828.3055 956.6871 1040.8247
1096.1141 1405.0591 1467.8840
1476.8719 1502.7710 1792.0670
3064.9231 3141.7036 3166.4187

i46

Cartesian coordinates

C -0.402856 1.017237 0.000010
C -0.403201 -1.017227 0.000004
C 0.700974 -0.000218 0.000013
C 2.005178 -0.000035 -0.000015
H -2.443817 0.000398 -0.000037
H -0.389301 2.095317 0.000005
H -0.390090 -2.095314 0.000021

Vibrational frequencies

129.7312 195.6623 486.8617
537.0793 640.7055 737.8691
894.4389 896.6396 930.3614
932.7371 1144.7527 1171.8827
1294.7307 1424.3320 1766.9970
3248.7789 3279.6399 3292.2376

i59

Cartesian coordinates

C 0.014350 -0.621369 0.469579
C 0.603801 0.823485 0.025960
C -0.808481 0.680410 -0.055006
C -1.500903 -0.394214 -0.288506
H 2.155458 -0.795744 -0.314747
H 0.056908 -0.913740 1.511505
H 1.119110 1.527258 0.669698

Vibrational frequencies

239.0664 370.4496 493.4703
647.5734 770.5625 832.4606
865.4827 888.0361 1009.8681
1100.9744 1122.6515 1159.8650
1234.5970 1296.1510 1690.3156
3204.1017 3206.1577 3223.4295

i7

Cartesian coordinates

C -0.958842 -0.713918 0.000020
C 0.453130 0.886647 -0.000011
C 1.571747 -0.031330 0.000037
C 0.553282 -0.808836 -0.000050
H -1.651126 1.552079 -0.000004
H -1.389049 -1.167829 0.894585
H -1.389061 -1.167821 -0.894535

Vibrational frequencies

265.0700 388.0649 440.6461
609.3709 614.9899 828.5249
916.4686 945.8117 1008.7597
1111.8198 1196.9916 1221.1363
1436.6055 1579.1640 1787.9878
3093.9399 3153.0859 3275.4672

i35

Cartesian coordinates

C -1.229974 0.683665 0.000158
C 1.209645 -0.556609 0.000161
C -0.238435 -0.203539 0.000037
C -1.588917 -0.675042 -0.000261
H -1.530979 1.719327 0.000404
H 1.429618 -1.152920 -0.897268
H 1.429530 -1.152255 0.898061

Vibrational frequencies

68.1837 131.2788 332.3283
367.5343 731.4277 837.0930
900.8916 938.5808 1046.8879
1074.0609 1117.7546 1215.3155
1319.0842 1426.1375 1740.2959
2988.8851 3033.4300 3276.3270

i67

Cartesian coordinates

C 1.028996 0.673944 0.000004
C -0.408437 -0.903089 0.000006
C -1.420117 -0.000013 0.000006
C -0.408422 0.903118 -0.000013
H 1.784283 -1.444870 -0.000043
H 1.784298 1.444842 0.000022
H -2.494650 0.000014 -0.000011

Vibrational frequencies

325.0843 374.7828 496.6606
606.9759 667.8719 787.0296
841.0317 859.3139 1029.8735
1068.2281 1160.4311 1174.2841
1317.0409 1572.8861 1655.0801
3244.9333 3270.3899 3307.5503
325.0843 374.7827 496.6606

i37

Cartesian coordinates

C -1.544061 -0.475500 0.000006
C -0.162207 -0.185864 -0.000030
C 1.173256 -0.515283 -0.000020
C 2.088387 0.534643 0.000032
H -1.426482 1.842467 -0.000065
H -2.345141 -1.196378 0.000107
H 1.431577 -1.578523 -0.000018

Vibrational frequencies

125.2013 220.7126 455.3101
526.5595 759.9038 821.9760
835.3330 968.2143 971.0186
1008.0573 1151.6568 1201.3740
1392.8332 1510.4160 1751.7916
3060.0091 3279.6876 3317.8238

i38

Cartesian coordinates

C -1.405924 0.412258 -0.230519
C 1.405987 -0.412164 -0.230589
C 0.000069 -0.000110 0.545843
C -1.196356 -0.824108 -0.099946
H -1.739002 1.401829 -0.469780
H 1.739481 -1.401538 -0.470108
H 0.000039 -0.000435 1.629944

Vibrational frequencies

217.8003 240.2892 332.2147
394.6595 474.3707 527.9096
669.9016 674.3295 826.1401
895.3820 918.7540 977.0550
1300.8221 1806.5761 1833.2438
3179.4849 3383.9765 3385.0565

i50

Cartesian coordinates

C 1.759412 0.000004 0.126980
C -0.753303 0.894567 -0.279488
C -1.629844 -0.000011 0.474813
C -0.753294 -0.894560 -0.279502
H 2.224903 -0.897808 -0.281146
H 1.910359 -0.000251 1.211125
H 2.224871 0.897998 -0.280774

Vibrational frequencies

88.6705 251.8799 341.9932
541.0539 612.5019 686.3880
876.9808 882.3815 1058.1270
1112.5218 1232.1110 1404.2472

1469.1091 1477.8984 1618.3714
3061.6066 3136.7447 3170.3299

i66

Cartesian coordinates

C	-1.318098	0.134896	-0.000004
C	1.002921	0.581846	0.000006
C	0.792181	-0.898617	-0.000017
C	-0.063715	-0.061973	0.826824
H	-1.767615	1.124417	0.000034
H	-2.025943	-0.691020	-0.000006
H	1.696190	1.401349	0.000001

Vibrational frequencies

430.8522 595.7496 734.5893
805.4186 851.3493 890.1792
911.8242 1006.6423 1025.7414
1082.6510 1125.5926 1146.1041
1161.6229 1409.4366 1491.3606
3134.2611 3223.2004 3329.7646

i55

Cartesian coordinates

C	1.722459	-0.000020	0.171971
C	-0.638927	1.046914	-0.358976
C	-1.237202	-0.000007	0.413537
C	-0.638972	-1.046878	-0.359043
H	2.246786	-0.938221	0.301097
H	-1.833290	-0.000020	1.319585
H	2.246882	0.938166	0.300821

Vibrational frequencies

209.3909 315.1637 356.5821
564.2128 588.1346 633.3339
768.5458 896.5195 976.6602
991.9471 1059.2720 1252.1731
1333.1826 1436.3074 1488.9067
3169.2231 3207.3018 3288.8243
564.2127 588.1346 633.3339

i45

Cartesian coordinates

C	0.543576	0.866821	0.054275
C	-0.646996	0.037322	0.033579
C	0.507424	-0.967585	0.330606
C	1.446304	-0.152233	-0.280635
H	-2.770734	-0.598063	-0.162773
H	2.499211	-0.218223	-0.501474
H	0.709933	1.721026	0.710678

Vibrational frequencies

265.9063 332.3610 527.6257
612.9592 670.8678 691.6617
761.1930 817.7058 903.1537
1010.7434 1051.0993 1202.0120
1303.6682 1447.9254 1754.7612
3139.5854 3287.4343 3308.6719

i9

Cartesian coordinates

C	1.635316	0.557678	0.065054
C	-0.920639	-0.003793	0.005289
C	0.407091	-0.039811	-0.007075
C	1.671797	-0.804921	-0.084097
H	-2.801261	-0.501256	0.754256
H	-2.774427	0.577161	-0.757363
H	2.138721	1.509899	0.125663

Vibrational frequencies

143.4991 191.6508 391.8711
406.3545 537.4519 683.6736
792.3845 878.9745 938.3619
960.1882 1010.9560 1073.3174
1411.9600 1596.5477 1880.0382
3107.3535 3185.2120 3266.8064

i10

Cartesian coordinates

C	1.612269	0.622078	0.000014
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C	-1.095555	-0.075018	-0.000070
C	0.270995	-0.284296	-0.000134
C	1.425881	-0.845110	0.000134
H	-3.325879	0.328642	0.000165
H	1.857061	1.146887	-0.921823
H	1.856520	1.147215	0.921806

Vibrational frequencies

186.8678 201.2541 465.3576
474.4932 618.3877 658.9393
727.9232 771.0977 912.7682
1014.2955 1067.8566 1073.2751
1504.3803 1872.1747 2239.5799
3090.9606 3182.6663 3480.3885

i16

Cartesian coordinates

C	1.128471	0.092408	0.000048
C	-1.315351	-0.037207	-0.000376
C	-2.308074	-0.715824	0.000196
C	2.170054	-0.497773	-0.000006
H	-0.171817	1.485924	0.878705
H	-0.171560	1.486314	-0.878283
H	3.092921	-1.026066	-0.000046

Vibrational frequencies

125.2706 186.7896 266.9195
324.9927 527.4563 700.1405
728.0507 893.2965 897.9373
1009.7637 1238.7743 1342.0743
1453.1402 2263.2168 2275.5363
3056.2749 3094.2410 3484.0166

i3

Cartesian coordinates

C	2.154030	-0.415323	0.000002
C	-0.189297	0.771788	0.000042
C	-1.364902	0.032100	-0.000182
C	-2.448218	-0.644366	0.000087
H	-0.227546	1.859431	0.000268
H	2.647320	-0.672242	0.932484
H	2.647483	-0.671881	-0.932494

Vibrational frequencies

132.5988 154.4170 316.4768
324.3500 503.3530 601.7629
867.2990 891.8251 961.4093
980.9346 1099.1818 1341.0871
1429.3257 1992.0901 2015.9885
3148.3158 3154.6416 3234.5533

i26

Cartesian coordinates

C	1.977583	0.448424	-0.000017
C	-0.374483	-0.152005	0.000006
C	-1.377402	0.717276	0.000010
C	-1.703821	-0.657622	-0.000026
H	1.300102	-1.532187	0.000051
H	3.058295	0.483024	-0.000032
H	-1.729288	1.737602	0.000031

Vibrational frequencies

80.8217 216.9771 375.8992
490.5391 696.4408 713.3401
877.1776 878.6038 920.0382
980.1148 1156.4830 1252.0651
1337.9935 1656.9373 1793.1055
3091.0649 3261.3434 3265.4819

i12

Cartesian coordinates

C	-2.287162	0.070620	0.000120
C	0.097527	0.526886	-0.000069
C	1.364777	0.106016	-0.000112
C	2.573426	-0.302540	0.000160
H	-0.832016	-1.439811	-0.000257
H	-3.282726	-0.350260	0.000203
H	-0.118664	1.594652	0.000016

Vibrational frequencies

104.5040 155.4076 252.5983
370.1205 548.9622 663.7255
794.7772 882.5880 932.9780
1109.2124 1191.9741 1243.0774
1413.9513 1623.1596 2056.2737
3111.9902 3151.6023 3268.7660

i6

Cartesian coordinates

C	-2.402652	-0.001021	-0.006221
C	0.266873	0.005534	0.007418
C	1.601571	0.001012	0.012164
C	2.882288	-0.005453	-0.013352
H	-2.815379	0.997767	-0.161972
H	-2.768632	-0.387300	0.950094
H	-2.769935	-0.669138	-0.790221

Vibrational frequencies

92.3257 139.3728 252.9042
289.7840 465.9046 492.9940
691.3936 1047.1821 1177.7277
1355.3601 1407.9574 1467.8211
1706.3033 1960.6270 2249.0073
3045.1756 3125.3739 3138.7823
92.3257 139.3728 252.9043
289.7840 465.9045 492.9940
1355.3603 1407.9574 1467.8211
1706.3052 1960.6270 2249.0073
3045.1756 3125.3740 3138.7823

i65

Cartesian coordinates

C	0.406154	1.014442	0.000024
C	0.227834	-1.231738	0.000124
C	-0.996800	-0.802036	-0.000161
C	-1.010728	0.601183	0.000053
H	2.258997	-0.171223	-0.000399
H	0.755167	2.039327	-0.000164
H	-1.865935	1.263120	0.000076

Vibrational frequencies

419.9251 518.8172 597.0594
692.4969 705.8522 758.3980
895.1863 932.1237 1054.4386
1079.0852 1122.0647 1199.9405
1309.3995 1394.3937 1544.6383
3221.3284 3240.5157 3270.9171
419.9251 518.8172 597.0595
895.1863 932.1237 1054.4387

i39

Cartesian coordinates

C	1.267458	-0.659700	0.043191
C	-0.019259	-0.000008	-0.091863
C	-1.456848	0.000172	0.510658
C	-1.349400	-0.000204	-0.779828
H	1.855870	1.562692	0.095245
H	1.855787	-1.562712	0.095779
H	-1.968229	0.000203	1.458321

Vibrational frequencies

274.4394 361.4290 398.3779
566.4335 623.8164 682.0658
702.0235 855.6631 920.8038
933.1263 948.9441 1094.8209
1405.8682 1652.8283 1704.3602
3243.8109 3284.9531 3297.1990

i58

Cartesian coordinates

C	-0.577552	0.765637	0.287534
C	0.823080	0.612034	-0.270861
C	-0.006471	-0.672877	0.036249
C	-1.341735	-0.323396	-0.326836
H	-0.702124	1.082605	1.319841
H	1.112494	1.057249	-1.222438
H	-2.252718	-0.772064	0.051506

Vibrational frequencies
282.9573 344.0068 588.7650
614.2529 722.5812 759.4373
868.0717 944.0669 1014.8264
1080.6183 1129.8619 1181.7556
1201.0541 1220.7952 1444.8769
3127.9119 3156.2005 3212.6807

i5
Cartesian coordinates
C 1.708418 -0.516228 0.000000
C -0.276409 1.238611 0.000000
C -0.984689 0.037678 -0.000003
C -1.676186 -1.059392 0.000002
H 1.710199 -1.596185 0.000000
H 2.651846 0.016006 0.000001
H -0.442135 2.301145 0.000007

Vibrational frequencies
84.6211 286.7041 346.3801
360.6970 436.5371 582.3068
624.3711 812.4157 844.2003
1043.0478 1065.9717 1104.5147
1436.1613 1556.3277 1831.7286
3173.9451 3281.5634 3303.2473

i13
Cartesian coordinates
C -2.356019 0.587376 0.000000
C 0.000000 -0.074098 0.000000
C 1.201348 -0.542712 0.000000
C 2.330392 -1.082873 0.000000
H -0.764047 1.908363 0.000000
H -3.255416 1.187075 0.000000
H 3.298969 -1.522131 0.000000

Vibrational frequencies
67.5935 117.9869 320.3295
351.6126 359.7057 415.1739
428.4596 549.8245 736.7886
776.6148 934.7548 1249.7678
1487.5340 1570.1167 1729.0740
3038.2235 3250.8387 3460.5489

i1
Cartesian coordinates
C 2.137263 -0.447858 -0.000002
C -0.200025 0.217248 0.000010
C -1.440925 0.000539 0.000002
C -2.728216 -0.235496 -0.000006
H 1.397350 1.543076 -0.000010
H 3.173761 -0.139321 -0.000007
H 1.918716 -1.508057 0.000005

Vibrational frequencies
131.4290 147.5913 277.9476
361.3323 561.2959 605.6420
790.2844 851.8732 918.0121
1057.8123 1263.4022 1364.2835
1506.2430 1557.0570 1929.6182
3157.1289 3177.6963 3281.1150

i2
Cartesian coordinates
C -1.445462 -0.684354 0.005068
C -0.133337 0.064200 -0.011153
C 1.217605 0.001113 -0.022096
C 2.491474 -0.072951 0.018165
H -1.720532 1.761194 0.020281
H -1.762685 -1.176767 0.924195
H -1.782754 -1.175541 -0.907483

Vibrational frequencies
98.1435 180.0320 243.7640
453.6743 491.5648 665.3013
905.4562 938.2563 991.7631
1033.8396 1080.2926 1143.2844
1461.5334 1571.7162 2042.2409
3079.1882 3157.0231 3288.8398

98.1434 180.0320 243.7640

i43
Cartesian coordinates
C -0.616250 0.961420 0.000000
C -0.514299 -1.140043 0.000000
C 0.558235 -0.009835 0.000000
C 1.839841 0.066806 0.000000
H -0.707484 1.559267 -0.904910
H -0.707484 1.559267 0.904910
H 2.766478 -0.475903 0.000000

Vibrational frequencies
143.1389 321.8543 425.6536
434.9670 609.5573 651.8274
718.4136 815.1902 913.0563
990.3071 1090.9928 1145.1359
1456.8543 1631.7437 1708.5124
3108.8842 3187.2271 3338.5216

Transition states

i10 – i24
Cartesian coordinates
C -1.748003 0.484448 -0.047298
C 1.083785 -0.017191 0.033137
C -0.280846 -0.090270 0.303963
C -1.399949 -0.847144 -0.120119
H 3.330464 0.130123 -0.255838
H -0.749805 1.065312 0.614334
H -2.182860 1.213435 -0.726481

Vibrational frequencies
-1117.3503 182.8301 227.7508
441.3825 549.5380 640.4538
648.8716 695.4134 730.7960
817.5640 985.4365 1064.9951
1248.1626 1482.5733 2127.8437
2163.2493 3177.7292 3477.8949

i26 – i30
Cartesian coordinates
C -1.552845 -0.568049 0.000000
C 0.419803 0.501057 0.000005
C 1.044084 -0.830873 0.000001
C 1.767821 0.312678 -0.000004
H -1.443534 1.655183 -0.000004
H -2.640950 -0.665913 -0.000006
H 0.031425 -1.454602 0.000002

Vibrational frequencies
-1209.1923 206.0269 375.0742
463.8433 500.3477 672.2032
706.8443 869.3603 953.2312
1053.7423 1118.5635 1134.8108
1330.1808 1484.3394 1683.5037
2103.2656 3124.0591 3181.6631

i26 – i24
Cartesian coordinates
C 2.261686 0.037897 -0.089873
C -0.347886 -0.040957 0.057837
C -1.578577 0.568686 -0.023397
C -1.627663 -0.799606 -0.098571
H 0.337403 -0.213400 1.196713
H 3.325113 0.050731 -0.073553
H -2.090569 1.516600 -0.064747

Vibrational frequencies
-1218.7305 180.5956 277.0393
396.8895 438.8041 522.9091
617.2907 644.9841 699.8626
788.9792 970.1815 1046.8110
1266.2645 1592.8995 1688.1704
2000.0208 3270.9209 3468.1476

i9 – i24
Cartesian coordinates

C -1.590598 0.537891 0.063638
C 1.014900 0.056486 -0.638561
C -0.204623 -0.136307 0.102809
C -1.536017 -0.749050 -0.015574
H 3.075631 0.131457 0.288944
H -2.000161 1.531076 0.084700
H 0.822692 -0.178519 1.143060

Vibrational frequencies
-2790.9930 168.8933 341.1320
364.1185 541.1571 645.1324
682.0599 701.9873 736.8521
893.4489 910.7080 933.6995
1239.8712 1449.1784 1630.2491
1719.4815 3260.5166 3335.2821

i6 – i30
Cartesian coordinates
C -1.936620 0.186966 0.239446
C 0.463859 -0.128685 -0.099249
C 1.701557 0.701788 -0.115420
C 1.676611 -0.555542 0.329831
H -1.607132 -1.066059 -0.021260
H -2.930516 0.119136 -0.198080
H -1.876633 0.619194 1.241765

Vibrational frequencies
-1243.0864 143.6206 177.8166
256.5499 510.7881 613.9137
726.9990 828.3040 1049.8764
1103.7360 1253.9648 1299.5551
1464.7640 1548.3097 1767.1544
2206.7337 3070.7959 3183.6361

i6 – i44
Cartesian coordinates
C 1.991177 0.074498 0.000092
C -0.621455 -0.628122 -0.000079
C -1.976528 -0.228760 0.000181
C -1.139492 0.889966 -0.000070
H 2.270550 0.653299 -0.884786
H 2.541306 -0.869390 -0.001496
H 2.270640 0.650327 0.886887

Vibrational frequencies
-390.5357 57.4035 139.2463
242.6507 408.7944 707.1112
779.6914 1012.2326 1016.6355
1106.8105 1357.9071 1407.1808
1454.0072 1462.7640 1897.8139
3042.6835 3115.7662 3137.2426

i1 – i30
Cartesian coordinates
C 2.060945 -0.225911 -0.169385
C -0.344250 -0.095388 0.168050
C -1.549294 -0.619096 0.233583
C -2.073830 0.418316 -0.373311
H 0.935902 1.485781 0.455405
H 3.010158 0.289262 -0.129412
H 2.050460 -1.264436 -0.472915

Vibrational frequencies
-1043.7187 146.5044 193.9562
256.3954 501.1719 579.1602
774.0293 862.5349 895.8548
1066.5346 1215.0768 1365.3505
1487.4418 1554.9934 1740.4868
3158.6346 3180.4953 3287.7014

i1 – i30
Cartesian coordinates
C -1.874226 0.485356 -0.089255
C 0.378590 -0.423790 -0.033172
C 1.756512 0.809425 0.247503
C 1.673406 -0.393148 -0.269103
H -1.305305 -1.504250 0.456736
H -2.931199 0.300075 0.038650
H -1.552791 1.471542 -0.397768

Vibrational frequencies
-1173.9012 146.1805 213.2693
247.8786 555.2562 590.6236
789.2280 847.3063 888.5310
1031.8901 1215.1276 1373.2440
1478.3784 1554.6197 1746.1433
3161.7244 3182.2778 3290.4517
789.2280 847.3063 888.5311

i22 – i16
Cartesian coordinates
C -0.288144 1.132029 -0.000055
C -0.681809 -0.391749 0.000466
C 0.693570 0.051500 0.000038
C 1.920286 -0.350271 -0.000159
H -0.483723 1.659562 -0.926882
H -0.483218 1.660058 0.926599
H 2.489743 -1.264036 0.000024

Vibrational frequencies
-141.4093 211.8758 345.8988
360.3312 670.9611 683.0465
730.2159 831.1008 952.9800
977.5310 1002.8840 1066.9024
1459.7214 1759.8619 1925.5523
3137.4451 3242.9196 3302.8937

i56 – i42
Cartesian coordinates
C -0.185614 -0.646313 -0.630766
C -0.500710 0.839585 0.044839
C 0.795471 0.248758 0.046281
C 2.009140 -0.215934 0.188531
H -1.334490 -0.817164 1.240213
H -2.363692 -0.314483 -0.182631
H -0.736409 1.671263 -0.608441

Vibrational frequencies
-157.3727 241.3301 357.7854
531.5577 676.0589 814.5220
878.4665 973.8016 1032.2240
1060.5561 1117.7598 1195.7795
1303.1643 1490.6249 1753.1768
3120.4265 3199.8416 3213.0262
-157.3727 241.3301 357.7855

i2 – i4
Cartesian coordinates
C 0.527261 -0.895958 -0.000008
C 0.385486 0.883413 -0.000018
C -0.853590 0.242668 -0.000015
C -2.116346 -0.020131 -0.000009
H 2.569886 0.360664 -0.000465
H 0.359728 -1.434243 -0.928866
H 0.359542 -1.434316 0.928776

Vibrational frequencies
-438.4700 212.3008 286.4275
502.4674 598.3003 616.6484
889.2906 951.4632 1034.4446
1064.2085 1087.1247 1153.0597
1472.5252 1679.5181 1839.4823
3117.6066 3229.6959 3346.1100

i67 – i20
Cartesian coordinates
C 0.724407 0.932576 -0.000002
C -0.682042 0.718359 -0.000002
C 0.192566 -1.307874 -0.000001
C 1.216374 -0.364228 0.000000
H -2.526222 -0.618076 -0.000003
H 1.230431 1.885424 0.000005
H 2.251347 -0.689358 0.000006

Vibrational frequencies
-338.8217 309.1236 434.2933
463.4994 606.2297 638.7921
690.8510 797.7848 843.6145

998.6704 1039.7665 1148.9477
1360.0969 1405.5170 2070.2925
3197.9399 3261.7976 3466.8839

i8 – i54
Cartesian coordinates
C -1.906622 0.104322 0.002843
C 0.702758 0.741555 -0.103059
C 1.832783 -0.012899 -0.091046
C 0.510870 -0.916594 0.042913
H -2.291329 1.112718 -0.035242
H -2.591491 -0.731582 0.041144
H 1.504004 0.836882 0.899955

Vibrational frequencies
-1184.2190 225.0241 298.1169
455.1997 471.0069 567.5469
610.5035 721.8931 785.7831
1010.4836 1031.5834 1084.2877
1422.9163 1475.0426 1598.8907
2180.1193 3193.7638 3303.4905

i8 – i53
Cartesian coordinates
C -1.887339 -0.110093 -0.073880
C 0.641209 0.825181 -0.159763
C 1.907875 -0.138796 -0.032673
C 0.721214 -0.972117 0.043114
H -2.520585 0.763455 -0.146254
H -2.324717 -1.097287 -0.056639
H -0.225000 0.986939 0.941719

Vibrational frequencies
-1729.1442 236.7985 313.0947
447.3494 471.1504 518.9428
681.6302 734.5071 751.9290
981.4556 1057.3340 1084.8027
1417.4763 1510.6447 1679.3897
1818.4488 3192.0802 3308.2410

i4 – i47
Cartesian coordinates
C 0.567574 0.883191 -0.039701
C -0.770635 -0.145446 0.127520
C 0.409871 -0.916888 -0.213535
C 1.485058 -0.145774 0.122868
H 0.478176 1.621941 -0.831021
H -0.563682 0.635161 1.011134
H 2.553425 -0.255751 0.167424

Vibrational frequencies
-1161.0890 183.8745 301.6609
429.2111 594.6453 654.5609
744.4398 807.5588 936.0818
1053.4722 1079.0258 1102.4605
1273.2123 1481.6329 1514.7324
2318.8365 3178.9116 3316.6556

i24 – i20
Cartesian coordinates
C 0.272337 -0.449771 -0.357481
C -1.056638 -0.138278 -0.047648
C 1.921862 -0.247003 0.582482
C 1.319842 0.585350 -0.219593
H -3.219553 0.395709 0.397505
H 0.473933 -1.430340 -0.767656
H 1.239079 1.628624 -0.486521

Vibrational frequencies
-235.1557 197.2523 211.9945
470.6773 548.7815 596.3998
677.1552 706.0213 730.5279
916.8776 1031.9569 1088.5627
1340.2453 1632.4542 2130.8816
3219.7902 3257.3432 3476.9992

i27 – i10
Cartesian coordinates
C -1.468846 -0.824972 -0.170521

C 1.085525 0.002606 0.042568
C -0.257841 -0.032368 0.208958
C -1.497009 0.589666 -0.065396
H 3.357472 0.057833 -0.142777
H -2.253233 -0.151046 0.663399
H -2.067867 1.476182 -0.307342

Vibrational frequencies
-1249.2155 91.6924 201.4661
380.5694 492.4871 521.5289
656.9024 675.1835 801.0626
876.2274 909.4800 1145.6912
1316.5086 1574.2491 2037.3120
2116.2497 3231.5615 3479.0759

i3 – i23
Cartesian coordinates
C 1.168271 0.438358 0.777034
C 0.164513 0.516433 -0.335126
C -1.129885 0.125740 -0.082093
C -2.287510 -0.351149 0.141163
H 1.318719 -1.612891 0.153958
H 2.039148 -0.412803 -1.050494
H 0.408666 1.103232 -1.218371

Vibrational frequencies
-431.2961 144.9855 168.1190
377.3335 448.6879 736.5645
782.1515 880.0559 907.0865
980.1821 1089.7642 1239.1578
1321.4961 1437.5335 2032.5368
3122.3610 3138.3567 3222.3647

i20 – i19
Cartesian coordinates
C 0.074738 0.660921 0.000000
C -1.205722 0.125692 0.000000
C 2.531936 -0.283913 0.000000
C 1.242990 -0.127494 0.000000
H -3.311163 -0.735174 -0.000001
H 0.198599 1.736999 0.000000
H 1.211182 -1.264024 0.000003

Vibrational frequencies
-188.2105 189.7314 190.3710
394.7548 526.6141 556.3013
570.7564 660.8816 705.9926
740.9650 1039.2123 1142.3916
1381.6666 1729.3894 2105.5769
2783.5545 3212.7420 3473.8083

i67 – i45
Cartesian coordinates
C 0.499683 0.877930 0.010029
C -0.716759 0.063747 0.189945
C 0.524758 -0.918471 0.441696
C 1.351527 -0.175429 -0.362523
H -1.414302 0.270874 1.082238
H 0.759614 1.748511 0.612225
H 2.360262 -0.264471 -0.731180

Vibrational frequencies
-203.7310 337.3235 444.4552
491.8993 588.1474 774.8166
833.6079 884.7565 950.9147
967.1800 1056.7989 1217.7591
1307.2376 1393.4675 1480.0555
2649.1818 3127.3114 3289.0430

i47 – i21
Cartesian coordinates
C 0.330208 0.836745 -0.003040
C -0.763929 -0.058066 0.299416
C 0.687642 -0.982185 -0.317073
C 1.483385 0.025508 0.113850
H 0.210181 1.648457 -0.720639
H -0.832957 -0.512046 1.297508
H 2.543948 0.214627 0.123588

Vibrational frequencies

-312.5986 156.6781 352.1312
481.2120 616.4361 781.3464
802.6310 872.4208 939.0884
1035.5300 1137.4379 1209.0411
1290.7836 1371.1134 1513.3077
3063.3210 3135.4630 3289.4349

i2 – i22

Cartesian coordinates

C 0.353089 1.143554 0.000008
C 0.454489 -0.326439 -0.000125
C -0.919894 -0.496952 -0.000025
C -2.161806 -0.201571 0.000058
H 2.672907 -1.004398 0.000211
H 0.318359 1.676984 0.942426
H 0.318371 1.677107 -0.942345

Vibrational frequencies

-781.9199 142.2244 185.4146
372.1087 419.9913 471.9313
502.2735 581.3392 838.6919
905.9300 1006.6153 1094.9493
1436.4597 1777.7650 2031.3619
3162.3553 3301.9852 3376.4061

i38 – i28

Cartesian coordinates

C -1.357132 0.534448 -0.194468
C 1.301054 -0.435955 -0.241295
C -0.048476 -0.191455 0.528818
C -1.280616 -0.722968 -0.162440
H -1.595399 1.566167 -0.352370
H 1.586090 -1.384464 -0.657539
H -0.033960 -0.193066 1.612035

Vibrational frequencies

-176.2045 165.3723 256.1690
397.7633 468.3849 681.9635
703.0985 794.6125 877.5006
922.4338 956.1794 993.9693
1311.5059 1779.6684 1830.5068
3181.6039 3328.1976 3388.1462

i22 – i25

Cartesian coordinates

C 0.491186 0.902598 -0.003347
C -0.713356 -0.086141 0.019600
C 0.549401 -0.752686 0.018380
C 1.775923 -0.390636 -0.043822
H -1.465578 -0.101472 1.048290
H 0.580579 1.434856 -0.942054
H 0.639554 1.453761 0.917171

Vibrational frequencies

-498.8917 200.1906 265.0728
402.9171 555.1988 563.2378
598.1952 810.8528 957.8537
1012.1699 1023.3575 1056.3578
1475.9812 1487.8733 1828.8533
2259.3012 3149.4988 3270.9968

i3 – i10

Cartesian coordinates

C -1.404785 -0.805099 0.105935
C -0.168859 -0.306876 0.025723
C 1.170863 0.009408 0.103588
C 2.422950 0.210386 -0.028494
H -1.459159 1.311144 0.808652
H -1.955622 1.051772 -0.953700
H 0.525561 -0.799664 -0.855139

Vibrational frequencies

-1254.0098 160.1284 173.6630
247.0216 357.2691 414.3845
535.5447 651.1993 822.9701
990.9625 1033.5841 1103.8831
1465.8863 1602.6044 1933.4016
2333.7889 3091.3127 3187.3808

i29 – i23

Cartesian coordinates

C 1.288470 -0.348492 -0.783673
C 0.185099 -0.438057 0.461944
C -1.109340 -0.108899 0.078618
C -2.288339 0.259015 -0.243315
H 1.538234 1.576371 0.532039
H 2.247696 -0.200980 0.072583
H 0.350823 -1.156888 1.256456

Vibrational frequencies

-756.7303 168.9651 182.7523
394.6224 475.7706 564.6866
849.1358 924.1075 948.1569
1005.1071 1053.0455 1137.0896
1330.6888 1524.9966 2013.2072
2310.5628 3180.2537 3238.5043

i27 – i20

Cartesian coordinates

C 1.433725 0.612505 0.028682
C -1.099841 0.009704 -0.036158
C 0.248486 0.004022 -0.338686
C 1.839378 -0.668166 0.197514
H -3.353770 -0.021151 0.257769
H 1.821922 1.592692 0.239784
H 0.804765 -1.238574 -0.265793

Vibrational frequencies

-882.6176 171.2047 212.3881
440.6967 528.2258 608.4377
660.2471 701.1267 738.9057
899.3297 1012.6493 1084.9865
1360.5970 1585.7137 2127.0233
2300.0328 3315.4597 3475.2194

i7 – i56

Cartesian coordinates

C 1.121143 -0.525677 -0.201964
C 0.580131 0.868212 -0.047848
C -0.173498 -0.568057 0.626103
C -1.429013 -0.479299 -0.180144
H 1.022685 -0.997468 -1.177661
H 2.063022 -0.732817 0.299188
H 1.072362 1.643374 0.527430

Vibrational frequencies

-344.9270 399.7753 548.3346
591.9385 726.7945 854.6616
911.6419 1014.0284 1076.1066
1121.8109 1161.3620 1196.2296
1326.7603 1491.5482 1514.0941
3111.5016 3202.0580 3213.7292

i39 – i58

Cartesian coordinates

C 0.726088 0.711978 -0.305310
C -1.039748 0.534076 0.294679
C 0.047837 -0.497827 -0.238526
C 1.367738 -0.383469 0.402341
H 0.837214 1.568865 -0.947022
H -1.200516 1.097371 1.203858
H 2.275370 -0.912581 0.136015

Vibrational frequencies

-575.4839 307.1554 427.6677
529.3563 648.5425 721.7441
824.5939 845.1381 893.7216
972.3651 1013.8037 1072.9436
1133.5378 1376.5466 1542.1755
3203.3180 3249.8885 3302.3698
972.3651 1013.8038 1072.9436

i24 – i51

Cartesian coordinates

C -0.755696 -0.823714 -0.174789
C 0.722052 0.182014 -0.041074
C -0.526711 0.799209 -0.150185

C -1.603502 -0.017016 0.484857
H 2.818110 -0.642358 0.202451
H -0.747286 -1.610970 -0.914985
H -0.756674 1.590954 -0.859504

Vibrational frequencies

-699.5095 248.0378 307.3527
455.5070 501.1299 622.8341
693.2101 754.5721 911.2211
968.8614 1030.3968 1066.8498
1235.4090 1467.5960 1880.8043
3164.6683 3264.8496 3406.7117
3164.6682 3264.8496 3406.7117

i58 – i41

Cartesian coordinates

C -0.603960 0.230133 0.493541
C 0.694354 0.754578 -0.082283
C 0.356401 -0.775092 -0.101756
C -1.697500 -0.026864 -0.429147
H -0.692544 0.267290 1.578998
H 0.757114 1.555533 -0.816415
H -2.413305 -0.709061 0.058419

Vibrational frequencies

-340.8615 290.0495 415.1305
579.5432 667.5297 713.3330
811.4786 946.3197 968.4006
1009.0866 1105.6739 1107.4261
1144.8241 1320.9060 1438.7347
3030.0385 3125.6756 3150.7907

i23 – i42

Cartesian coordinates

C 0.765788 -0.551218 0.842858
C 0.304765 0.762128 0.051096
C -0.981012 0.280741 -0.084795
C -2.078672 -0.383139 -0.110432
H 1.070030 -0.817592 -1.366136
H 2.369391 0.025277 -0.376138
H 0.558581 1.778130 0.325247

Vibrational frequencies

-197.2127 175.3976 234.4374
421.5542 595.0515 754.1738
793.4422 841.8124 969.5490
1002.0294 1093.3193 1182.5551
1309.1935 1426.7174 1969.8445
3103.6672 3201.8758 3206.6995

i44 – i53

Cartesian coordinates

C 1.897552 0.000004 -0.147989
C -0.728618 -0.738162 0.006155
C -1.940277 -0.000005 -0.120323
C -0.728632 0.738164 0.006168
H 2.373600 0.945297 -0.363520
H 2.373596 -0.945298 -0.363489
H 1.349208 -0.000032 1.119369

Vibrational frequencies

-2093.0156 192.7259 236.0245
339.2278 554.5060 588.9578
699.7505 780.8045 790.6503
1025.4261 1101.3633 1132.6267
1395.7994 1414.5329 1587.2307
2220.9722 3183.8643 3318.8928

i29 – i46

Cartesian coordinates

C 0.599858 0.844814 -0.189261
C 0.349425 -0.838416 -0.157962
C -0.881270 -0.212261 0.074834
C -2.109513 0.178575 0.153171
H 2.506983 -0.107194 0.546302
H 0.459812 1.722596 -0.799981
H 0.514400 -1.534526 -0.981138

Vibrational frequencies

-472.0294 185.7852 278.1831
442.6000 626.3463 679.3283
858.3048 893.2729 934.2828
1012.2537 1053.9443 1157.9083
1277.5509 1660.9940 1833.0057
3131.2056 3281.8456 3324.1439

i68 – i69

Cartesian coordinates

C -1.111637 0.211951 -0.010148
C 0.066232 0.982625 -0.064861
C 1.086494 0.077463 0.663825
C -0.582011 -1.081512 0.277495
H -2.148626 0.501714 -0.173943
H 0.279482 2.006680 -0.349605
H 0.993148 -0.760924 -1.520037

Vibrational frequencies

-381.5118 204.3406 407.5313
535.0996 754.8832 802.7689
874.5955 911.5150 918.2508
980.8493 1024.0174 1095.7843
1305.1006 1357.6296 1392.0084
3153.2933 3197.4424 3293.2800

i25 – i47

Cartesian coordinates

C 0.363727 0.871286 0.007283
C -0.714670 -0.077207 0.299571
C 0.547105 -0.830107 -0.313205
C 1.649775 -0.236991 0.043578
H 0.298543 1.470146 -0.899277
H 1.741141 0.856499 0.497108
H -0.831614 -0.412520 1.344480

Vibrational frequencies

-1336.5017 159.5216 267.0404
411.2325 523.9397 599.7444
680.1055 873.8135 933.6443
957.6320 1029.2922 1122.0842
1205.4363 1308.9672 1645.3059
2550.7114 3013.4933 3144.6371

i65 – i45

Cartesian coordinates

C 0.275583 1.015373 -0.012231
C 1.361952 0.158455 -0.123746
C -0.612805 -0.536563 0.077702
C -1.708642 -0.005298 -0.096036
H 0.000810 1.725526 0.761173
H 2.410620 0.385010 -0.268505
H -2.643605 0.494726 -0.197910

Vibrational frequencies

-481.1986 252.0021 337.4611
510.9105 535.5668 596.0215
647.3220 717.7415 838.2102
893.3317 1054.3018 1105.6820
1306.8777 1356.1503 1986.6074
3182.4317 3219.9193 3463.3448

i4 – i56

Cartesian coordinates

C 1.227168 0.418627 0.103422
C 0.418654 -0.702986 -0.483479
C -0.249858 0.453580 0.384669
C -1.409490 0.740060 -0.298001
H 1.812904 0.168145 0.982075
H 1.678698 1.141426 -0.573089
H 0.320996 -0.854996 -1.557416

Vibrational frequencies

-258.4664 224.5125 426.5130
622.0460 727.8150 793.6260
959.0251 989.5838 1005.4087
1081.2476 1116.7326 1140.6989
1234.7378 1451.1247 1492.8928
3117.7539 3154.8832 3216.0875

i14 – i20

Cartesian coordinates

C -0.134805 0.861492 -0.001788
C -1.282617 -1.105692 -0.055796
C 0.935058 -0.051905 0.072762
C 2.208847 -0.236768 -0.047670
H -2.327313 0.818135 0.000460
H 0.037062 1.925480 -0.143089
H 0.310847 -1.122717 0.158455

Vibrational frequencies

-1072.1032 175.6683 180.1215
265.3452 557.4324 687.9692
813.0760 905.9013 1010.0471
1028.6138 1123.8202 1182.3136
1383.9029 1462.9295 1802.0376
1843.3951 3187.5963 3208.8862

i58 – i47

Cartesian coordinates

C 0.283124 -0.935272 -0.188163
C 0.484554 0.866115 -0.066846
C -0.695543 0.140853 0.480593
C -1.839851 -0.114048 -0.362167
H 2.467056 -0.319696 -0.115832
H 0.424938 1.612388 -0.858144
H -0.737765 0.015783 1.562762

Vibrational frequencies

-151.7644 315.4226 477.8829
583.6779 686.9601 815.5297
926.4955 966.3085 1056.7589
1063.0450 1112.8676 1213.2054
1296.7746 1328.9722 1475.8930
3108.3815 3140.5219 3266.9498

i67 – i69

Cartesian coordinates

C 0.150242 0.782226 0.391156
C -0.735290 -0.980750 -0.080771
C 0.708709 -0.672280 0.211052
C 1.109611 0.414397 -0.699453
H -2.061690 0.797261 -0.451095
H 0.366041 1.465986 1.205212
H 1.412614 -1.255021 0.789450

Vibrational frequencies

-553.4156 449.1229 635.6359
695.9393 749.1319 823.7871
848.8559 906.1587 1010.5141
1044.2336 1104.5568 1139.3364
1189.4014 1263.8946 1500.5576
3183.0081 3226.0824 3265.0210

i48 – i21

Cartesian coordinates

C -0.093252 0.589355 0.536160
C -0.648375 -0.765042 -0.452435
C 0.750837 -0.545411 0.325485
C 1.542448 0.410115 -0.477603
H -2.371914 0.687603 -0.145030
H 0.559474 1.371743 -0.212529
H 1.054969 -1.369590 0.952743

Vibrational frequencies

-544.3786 214.7340 461.8493
527.6247 612.5818 723.1834
807.7082 839.8003 934.5470
972.3069 1058.8663 1081.4026
1144.0922 1310.1362 1641.2973
2153.1072 3251.5703 3349.3753

i3 – i63

Cartesian coordinates

C 0.591274 -1.193270 -0.000037
C 0.508145 1.136576 -0.000013
C -0.784905 0.503607 -0.000008
C -1.815298 -0.257060 0.000038
H 0.435063 -1.742105 0.926915

H 0.434893 -1.741795 -0.927146
H 0.759126 2.184574 -0.000103

Vibrational frequencies

-558.9605 190.0160 238.7299
346.5807 588.1091 652.1359
845.1458 931.5706 964.1163
1013.4539 1134.5481 1243.0908
1474.2798 1691.7415 1906.3715
3128.9739 3225.1681 3276.8629
845.1457 931.5706 964.1163

i56 – i53

Cartesian coordinates

C 1.376929 -0.465620 -0.206911
C -0.326063 -0.303276 0.737545
C -1.581450 -0.477337 -0.094746
C -0.769445 0.543932 -0.445528
H 0.914938 1.619715 0.527039
H 1.185235 -1.089007 -1.068372
H 2.277296 -0.619245 0.374212

Vibrational frequencies

-579.9333 307.6925 403.6626
554.4140 644.9204 761.2706
824.7568 875.3510 997.4854
1033.4722 1129.4549 1199.8362
1342.5603 1467.0210 1584.1521
3178.1461 3214.9184 3304.0755

i61 – p33+H

Cartesian coordinates

C 0.861202 -0.614340 -0.185822
C 0.245358 0.648109 -0.597590
C -1.176111 0.458025 -0.156508
C -0.572835 -0.909646 -0.182609
H 0.173532 0.309694 1.899003
H 1.810205 -1.121147 -0.215474
H 1.534869 2.783161 -0.077260

Vibrational frequencies

-326.5377 91.7854 95.7596
243.9298 326.1104 531.5868
731.6902 781.6651 815.0652
877.5545 921.7465 965.8572
1092.3876 1105.7153 1207.1565
1328.6742 3306.0255 3324.1706

i67 – i68

Cartesian coordinates

C 1.019647 -0.559917 0.122644
C 0.770402 0.785114 0.041900
C -0.613902 0.565106 -0.645772
C -0.359347 -0.886498 -0.385900
H -1.295076 0.149759 1.549325
H 1.904111 -1.132611 0.372165
H 1.305609 1.674842 0.356502

Vibrational frequencies

-336.5715 365.8182 657.2283
782.8259 800.7507 826.8862
879.7074 891.1966 978.2831
1037.5247 1066.3741 1112.1569
1234.7422 1410.4599 1479.6210
3187.4667 3197.6193 3229.8646

i69 – p27+H

Cartesian coordinates

C 0.000009 0.574556 -0.815130
C -0.000019 -1.131519 -0.162868
C -1.043096 -0.094075 -0.001227
C 0.000004 0.289163 0.980580
H 2.117619 -0.092984 -0.000640
H 0.000066 2.921804 0.000516
H -2.117623 -0.092915 -0.000641

Vibrational frequencies

-268.1946 93.4674 142.9806
545.9980 555.5185 709.4004

721.4306 854.8196 861.6005
868.9911 1028.7925 1031.1981
1140.0779 1144.7455 1287.0173
1328.2038 3328.2391 3331.2047

i15 – i19

Cartesian coordinates

C	0.049972	0.751722	0.000002
C	-1.186429	0.123549	-0.000004
C	2.419845	-0.468116	-0.000015
C	1.264960	0.061542	0.000004
H	-3.220553	-0.893383	-0.000003
H	0.111387	1.834188	0.000021
H	1.432919	-1.246197	0.000078

Vibrational frequencies

-489.8772 152.3818 181.9382
327.6707 376.0426 403.6919
574.1436 622.7111 623.7059
729.9689 955.5457 1111.1860
1363.7950 1849.0834 2113.9923
2434.1611 3204.2101 3474.9621

i69 – i61

Cartesian coordinates

C	0.072159	0.806529	-0.493481
C	-0.028552	-1.146851	-0.114286
C	-1.036495	-0.157276	-0.072949
C	0.015222	0.523912	0.929897
H	1.190170	0.019394	1.103408
H	0.062736	1.709428	-1.082509
H	-2.116338	-0.127908	-0.034104

Vibrational frequencies

-1227.8629 133.7425 607.5176
723.0478 789.3426 837.2529
885.9061 902.7239 963.5810
987.5743 1063.3503 1108.1433
1199.2526 1292.6327 1327.5717
2161.5971 3241.7549 3269.2799

i45 – i52

Cartesian coordinates

C	0.530739	-0.950231	-0.328267
C	-0.656262	0.036332	-0.098434
C	0.464365	0.969621	-0.230833
C	1.455452	0.101013	0.240443
H	-2.790811	0.456036	0.384710
H	2.530388	0.115498	0.347547
H	0.981774	-0.804076	0.961455

Vibrational frequencies

-887.3862 234.5623 255.9320
459.2663 636.5546 663.8335
718.0806 729.8381 807.9980
906.8138 976.9388 1076.2461
1190.2177 1390.9340 1671.6919
2077.0778 3262.0583 3299.9530

i54 – i33

Cartesian coordinates

C	-0.258276	1.196280	-0.000011
C	-0.679666	-0.578423	-0.000045
C	0.586348	0.110443	0.000001
C	1.902440	-0.270317	0.000012
H	-2.929304	-0.166019	-0.000061
H	2.677324	0.483130	0.000023
H	2.174837	-1.315671	-0.000006

Vibrational frequencies

-257.5678 254.9742 358.8992
477.7928 516.5411 556.0040
556.0222 731.8150 819.0821
874.6539 1008.2356 1169.3713
1428.3769 1517.9895 2038.9258
3190.2782 3299.9025 3461.8669

i11 – p3+H

Cartesian coordinates

C	-2.486237	0.089220	0.000006
C	0.083554	-0.079169	-0.000007
C	1.377755	-0.165129	-0.000005
C	2.650857	-0.292984	0.000000
H	-3.046880	0.125292	0.930096
H	-3.046895	0.125429	-0.930070
H	3.399132	2.410037	0.000047

Vibrational frequencies

-270.0433 49.9585 81.1724
142.7508 143.8603 273.7561
281.8605 472.7987 604.8258
775.6597 985.5578 1035.6523
1378.3757 1527.4738 2005.9149
2239.3495 3135.8223 3225.2632

i25 – i31

Cartesian coordinates

C	0.674432	0.859557	-0.014292
C	-0.809457	-0.122232	0.327458
C	0.438481	-0.739366	0.063885
C	1.656124	-0.442159	-0.204213
H	0.481541	1.400690	-0.933124
H	0.875569	1.428249	0.887719
H	-1.126903	0.016909	1.377902

Vibrational frequencies

-537.6458 169.8634 292.5044
358.3492 498.2076 794.5079
846.1186 925.7645 954.6742
1014.7723 1034.2840 1060.1711
1335.2675 1477.7393 1820.3046
2992.1805 3129.5332 3252.9739

i1 – i27

Cartesian coordinates

C	-1.258551	0.846237	-0.115380
C	-0.195954	-0.365850	0.083099
C	1.178800	-0.299397	0.048116
C	2.348708	0.174223	-0.032221
H	-2.274333	-1.291383	0.011336
H	0.393134	0.815711	-0.244002
H	-1.569251	1.616136	0.593365

Vibrational frequencies

-1696.5850 120.8414 174.7474
299.5677 395.5822 501.2887
624.7159 742.5586 857.0434
912.9379 948.2490 1064.4716
1188.9684 1715.8479 1844.7889
2019.3937 3106.7271 3276.8356

i10 – i52

Cartesian coordinates

C	0.473363	-0.409736	-0.592604
C	-0.802927	-0.114601	-0.074372
C	0.541589	0.867894	-0.061767
C	1.612691	-0.183855	0.310806
H	-3.045635	0.099989	0.395378
H	2.557825	0.004756	-0.180663
H	1.668225	-0.619559	1.306183

Vibrational frequencies

-341.0106 213.6811 303.1867
399.9662 533.8531 566.3046
634.2100 775.2641 936.7278
1024.5209 1068.1327 1224.8142
1350.0828 1512.1273 1899.8000
3116.7529 3239.0054 3459.4291

i10 – i33

Cartesian coordinates

C	-1.096470	1.358497	0.056488
C	0.931744	-0.009425	-0.014188
C	-0.488209	0.146064	-0.055235
C	-1.410031	-0.910961	-0.016679
H	3.185303	-0.212335	0.018668
H	-2.463058	-0.717025	-0.179540
H	-1.102128	-1.888812	0.332522

Vibrational frequencies

-167.1662 183.3970 254.2265
489.3307 502.5560 580.5776
703.2377 727.9271 755.7323
808.2177 954.9707 1205.9437
1425.4896 1496.0922 2250.0792
3158.8917 3273.5984 3484.6413

i34 – p18at+H

Cartesian coordinates

C	-1.339007	0.030528	0.457206
C	1.376113	0.573430	-0.145231
C	0.075508	-0.183500	-0.069991
C	-1.175830	-0.437484	-0.762518
H	-1.866842	0.206366	1.378865
H	-2.051824	2.144621	0.066302
H	1.750036	1.526726	-0.479354

Vibrational frequencies

-492.0716 145.9976 214.8669
332.7323 375.8649 383.0631
618.0824 647.0655 700.6432
718.1781 739.2265 904.8073
937.5016 1267.6168 1589.7589
1670.3923 3295.5684 3301.8834

i10 – i34

Cartesian coordinates

C	1.648565	0.506066	-0.089483
C	-1.151714	0.174578	0.094070
C	0.216802	-0.186034	0.071210
C	1.263862	-0.923851	0.047936
H	1.895064	0.921233	-1.065852
H	2.062399	1.041049	0.763804
H	-1.503236	1.153496	0.535126

Vibrational frequencies

-199.1619 50.4328 272.3954
276.8691 509.3404 598.3220
781.2354 893.3186 935.1602
1022.4056 1064.9021 1081.8107
1509.3053 1809.4005 1972.7025
2832.9634 3080.3571 3169.5162

i10 – i60

Cartesian coordinates

C	0.576112	-0.839794	-0.135291
C	-0.765325	-0.559149	0.242251
C	0.291827	0.395504	-0.783511
C	1.365488	0.348361	0.341349
H	-2.504761	0.923497	0.102649
H	2.368431	0.466204	-0.052717
H	1.187639	0.767569	1.328278

Vibrational frequencies

-353.9267 280.7280 483.6054
556.8956 588.4557 683.0525
760.0907 817.9858 881.5833
1006.0551 1055.1934 1172.2719
1260.2537 1486.0279 1992.6974
3122.3632 3228.1304 3452.9373

i45 – i47

Cartesian coordinates

C	0.461258	0.877205	-0.046685
C	-0.711094	0.002785	0.010348
C	0.561114	-0.957219	-0.345786
C	1.446236	-0.096482	0.237399
H	0.541871	1.700786	-0.754899
H	-1.205017	-0.247741	1.102943
H	2.500827	-0.092859	0.457740

Vibrational frequencies

-221.3504 357.8510 376.5784
441.2889 610.3283 645.1980
696.5267 834.5547 889.0063
989.2914 1053.0603 1204.9760
1306.3165 1464.1243 1500.0773

2365.9418 3140.4278 3290.0740

i4 – i42

Cartesian coordinates

C	0.392324	-0.843606	0.302723
C	0.305521	0.918948	0.060716
C	-0.781545	-0.020349	-0.003807
C	-2.103218	-0.128053	-0.130452
H	1.149694	0.684493	-0.979059
H	2.511758	-0.247908	0.128850
H	0.494872	1.578101	0.902325

Vibrational frequencies

-1410.4767 184.7557 327.9400
505.2684 525.9400 629.4441
773.2882 803.9228 943.0834
1012.4733 1043.4707 1119.8273
1279.2192 1459.9410 1566.7991
2212.9355 3183.5137 3243.4264

i11 – i33

Cartesian coordinates

C	-0.152845	1.454462	-0.000005
C	0.799366	-0.053551	0.000027
C	-0.652133	0.222989	0.000001
C	-1.709753	-0.674855	-0.000004
H	2.938021	-0.828078	-0.000026
H	-2.720074	-0.290611	-0.000026
H	-1.533768	-1.739927	0.000017

Vibrational frequencies

-161.5308 230.6847 286.9913
406.8309 406.9447 489.0511
544.1253 645.5982 764.5905
802.1551 1024.7445 1104.3102
1459.6745 1575.5103 2103.0264
3192.0208 3308.6052 3471.4329

i54 – p22+H

Cartesian coordinates

C	-1.958354	-0.000069	0.122111
C	0.569781	0.746620	-0.117674
C	1.767122	0.000121	-0.235307
C	0.569823	-0.746495	-0.118002
H	-2.499326	0.934782	0.173011
H	-2.499260	-0.934981	0.172597
H	3.202728	-0.000865	1.748158

Vibrational frequencies

-344.0491 100.5862 118.3992
268.9209 340.5754 593.7855
599.2683 724.0625 820.1679
916.3671 988.8946 1058.4819
1115.5714 1430.7641 1489.1788
1871.9752 3187.2560 3290.3707

i9 – i26

Cartesian coordinates

C	-1.592870	-0.845393	-0.034458
C	-0.390222	-0.021951	-0.026117
C	0.968084	0.050470	-0.216543
C	2.231978	-0.080386	0.055870
H	-2.166911	1.445081	0.248370
H	1.669158	1.012195	-0.548192
H	2.838461	-0.270607	0.941969

Vibrational frequencies

-1555.9795 168.3901 187.5220
359.0908 485.6714 579.0260
661.5068 711.9370 858.6556
893.2598 966.3011 1060.6539
1292.1134 1643.5630 1911.3783
2386.0208 3116.4509 3274.4457
-1555.9796 168.3901 187.5220

i3 – i15

Cartesian coordinates

C	-1.514971	-0.474379	0.050228
C	0.408991	1.075559	0.033709

C	1.272203	0.026761	-0.156956
C	1.092161	-1.210967	0.056221
H	-2.437028	-0.981661	-0.165989
H	-0.342317	-1.227259	0.382799
H	0.652965	2.008044	0.529979

Vibrational frequencies

-1971.5150 321.9809 384.9614
431.1367 495.0596 595.2728
693.8855 830.5997 836.6256
1067.5460 1112.1975 1190.0415
1359.5977 1371.9226 1769.8311
1898.1596 3204.7933 3337.2104

b160

Cartesian coordinates

C	-1.231752	0.695034	-0.000003
C	1.300202	-0.448890	-0.000003
C	-0.122500	-0.533222	0.000001
C	-1.379962	-0.764510	0.000004
H	-1.326503	1.265754	0.922183
H	-1.326500	1.265749	-0.922193
H	1.983293	-1.290318	-0.000010

Vibrational frequencies

-174.3842 166.8277 317.5120
364.9127 516.6942 733.1706
745.8260 962.1031 999.8955
1044.5072 1064.0287 1105.3506
1501.2332 1638.9086 1928.6886
3087.9945 3180.8760 3206.0760

i45 – i54

Cartesian coordinates

C	-0.516163	0.412771	-0.438393
C	0.879828	0.945027	-0.059952
C	0.041939	-0.881379	-0.336746
C	-1.610369	0.039629	0.241844
H	2.214776	-0.692149	0.719914
H	-1.087602	-1.360738	0.070570
H	-1.936181	0.505218	1.174306

Vibrational frequencies

-1506.1505 255.4450 390.2868
549.2684 593.9502 733.2232
784.7574 832.1903 927.8784
985.5738 1038.7195 1101.9483
1311.0186 1541.4622 1571.9688
2068.3022 3141.5874 3293.8895

i9 – i34

Cartesian coordinates

C	1.524114	0.344989	-0.348815
C	-1.365911	0.511195	0.157105
C	-0.044178	-0.008313	0.306878
C	1.036947	-0.706890	0.531089
H	1.754309	0.128525	-1.390020
H	1.921452	1.264008	0.068932
H	-1.809666	1.427268	0.509100

Vibrational frequencies

-249.0279 190.5408 223.5385
315.1202 450.8549 715.7995
744.4221 902.0402 913.2519
993.3503 1051.9645 1091.9555
1454.9707 1543.9654 1769.1664
3111.6206 3221.3497 3291.7358

i65 – p30t+H

Cartesian coordinates

C	0.552336	-0.631073	0.332707
C	-1.052452	0.622238	-0.184653
C	0.367056	0.941560	-0.216640
C	1.499951	0.289202	0.078935
H	-1.573956	-1.464993	0.499339
H	0.678562	-3.178075	-1.685836
H	-1.890556	1.246562	-0.448214

Vibrational frequencies

-160.7788 35.5545 63.0638
271.6255 450.3623 607.1931
660.2374 697.0215 776.3028
826.5269 1028.6032 1049.5313
1136.9731 1267.2144 1499.1697
1696.6212 3260.6905 3283.8881

i5 – p8+H

Cartesian coordinates

C	1.694919	-0.519708	0.098189
C	-0.270071	1.202295	-0.424077
C	-0.962924	-0.009741	-0.098511
C	-1.682110	-1.041304	0.180377
H	1.724779	-1.561616	0.384915
H	2.624598	0.022143	-0.032372
H	-0.380842	2.972052	1.739480

Vibrational frequencies

-298.5216 67.7621 78.9506
135.5164 238.8916 359.0537
384.9222 589.4843 602.1126
839.7373 919.6074 1036.3964
1046.8819 1437.5011 1718.9000
1867.9358 3176.3190 3282.2031
-298.5217 67.7621 78.9506
1046.8819 1437.5011 1718.8999

i65 – i68

Cartesian coordinates

C	1.170381	0.272567	0.236779
C	-0.103966	0.852279	-0.274809
C	-0.669016	-0.565556	-0.590269
C	0.732652	-0.990609	-0.026085
H	-1.579582	-0.064231	1.464373
H	2.111053	0.665150	0.593604
H	-0.272593	1.696153	-0.929374

Vibrational frequencies

-400.6470 474.0515 597.8976
723.4239 738.3063 788.1579
830.8811 877.9810 923.2806
1010.2390 1032.5369 1152.5637
1204.0208 1447.2557 1537.9725
3221.8732 3227.3740 3252.9200

i46 – p23+H

Cartesian coordinates

C	0.523161	0.800422	0.444169
C	0.337823	-0.975258	0.004585
C	-0.745831	0.000810	0.105690
C	-2.000620	0.042757	-0.211230
H	2.400925	-0.120305	-0.503190
H	0.473415	3.305320	-0.384503
H	0.351255	-1.943182	0.498508

Vibrational frequencies

-295.8062 69.4571 84.4742
200.4297 251.8002 535.2944
669.7803 679.8707 839.6533
879.2971 999.1532 1049.8066
1184.8981 1300.4622 1463.0731
1824.0865 3175.6404 3286.5399

i69 – p33t+H

Cartesian coordinates

C	-0.126318	0.980955	-0.217022
C	-0.103853	-1.080306	-0.285228
C	-1.138813	-0.056692	-0.101882
C	0.085206	-0.118318	0.932227
H	4.549478	-0.004707	0.247357
H	-0.085266	2.040164	-0.020258
H	-2.168231	-0.094354	0.216160

Vibrational frequencies

-80.2835 17.1015 25.6540
276.2336 461.8406 464.2012
710.8368 857.6819 921.6322
927.6393 996.1882 1046.8679
1179.4975 1242.8339 1258.3512

1318.4964 3263.6034 3279.5732

i31 – i28

Cartesian coordinates

C	-0.216624	-0.206081	0.312181
C	1.182195	-0.334924	0.010801
C	-1.413078	-0.757805	-0.183683
C	-1.568642	0.600955	0.002108
H	-0.547506	0.997840	0.704369
H	1.561427	-1.358206	-0.117598
H	-1.915520	1.432120	-0.605144

Vibrational frequencies

-1100.5167 113.3316 215.3882
295.8330 414.4200 619.6529
659.0357 695.5206 813.6079
901.2059 1042.3046 1106.1211
1244.4474 1478.9801 1665.2104
2142.7613 3080.4367 3190.6552
901.2059 1042.3046 1106.1212

i15 – i28

Cartesian coordinates

C	-0.087025	-0.551952	0.239964
C	1.095538	0.097882	-0.185860
C	-1.386482	-0.442714	-0.490077
C	-1.793725	0.526369	0.175274
H	-0.047181	-1.196918	1.107360
H	1.098555	0.713077	-1.110578
H	-2.194035	1.356858	0.718520

Vibrational frequencies

-586.2977 163.0150 165.2038
210.4274 436.0317 621.3658
636.4139 674.0203 840.0257
861.8380 1043.6838 1169.3626
1329.8337 1625.3299 1842.7555
2978.6062 3222.4298 3417.1068

i3 – i12

Cartesian coordinates

C	-2.326222	-0.244052	0.080712
C	0.143495	0.676367	0.002786
C	1.372723	0.079315	-0.011401
C	2.508512	-0.490923	-0.033282
H	-3.057072	-0.395684	-0.711872
H	-0.978589	-1.182315	0.250225
H	0.037558	1.758306	0.022139

Vibrational frequencies

-1011.6272 140.9486 183.8143
283.0950 399.0723 484.4443
597.8770 690.4683 775.0929
875.1269 1049.5703 1154.1623
1374.7377 1781.5806 2049.3981
2661.8978 3163.4966 3175.8965

i41 – i48

Cartesian coordinates

C	-0.602871	0.360587	-0.749109
C	-0.584309	0.223160	0.841781
C	0.717979	0.496748	0.034854
C	1.579477	-0.581463	-0.068590
H	-1.415783	-0.848347	0.919021
H	1.136771	1.496757	0.147639
H	2.652912	-0.704723	-0.063528

Vibrational frequencies

-1218.7171 239.0250 285.3923
402.8551 461.0354 506.5352
571.9378 685.0681 796.7766
880.1684 984.7761 1022.0716
1194.7440 1304.2079 1514.3884
2478.5665 3123.5441 3260.6563
571.9378 685.0680 796.7766

i7 – i42

Cartesian coordinates

C	0.134249	0.949052	-0.194228
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C	0.480847	-1.154592	-0.167012
C	-0.691309	-0.268234	-0.278412
C	-1.838235	-0.015138	0.313310
H	2.265409	0.238477	-0.293306
H	-0.085284	2.000700	-0.310763
H	1.487300	0.068643	1.293327

Vibrational frequencies

-212.6575 216.4645 294.1640
423.9129 672.7696 779.0387
846.1662 875.3257 920.4231
1024.3634 1055.6158 1215.3417
1216.3891 1415.6464 1629.0618
3033.9255 3087.9689 3238.7632

i28 – i21

Cartesian coordinates

C	-0.146893	-0.522709	-0.214843
C	1.027578	0.144729	0.208190
C	-1.467026	0.851250	-0.341838
C	-1.519254	-0.276650	0.299965
H	-0.021149	-1.340192	-0.919360
H	0.967702	0.969163	0.938788
H	-2.187995	-1.004761	0.734095

Vibrational frequencies

-224.9567 160.9132 181.7956
284.9012 404.8730 646.6494
720.5190 795.6012 873.2333
982.1041 1089.1890 1175.2651
1332.4507 1578.8619 1678.3801
3034.8916 3166.1434 3251.2725

i45 – p23+H

Cartesian coordinates

C	0.656977	0.806897	0.125702
C	-0.636331	0.130612	0.070521
C	0.386748	-0.998445	0.282427
C	1.426707	-0.259481	-0.300397
H	-3.260123	-1.998510	0.139572
H	0.890650	1.645468	0.776629
H	2.466783	-0.443433	-0.514478

Vibrational frequencies

-214.3856 57.4266 81.5731
201.6163 256.0893 551.8301
666.6938 680.7278 845.4568
881.4080 1002.0802 1058.5105
1187.4368 1303.5344 1464.8509
1823.4672 3176.6788 3288.5906

i67 – p29+H

Cartesian coordinates

C	-0.821639	-0.521985	-0.184963
C	0.341778	0.786968	-0.003485
C	1.433849	-0.038312	-0.124685
C	0.428400	-0.955817	0.194361
H	-1.777992	1.566454	-0.086991
H	-2.839012	-2.220456	-0.020559
H	2.482795	0.069421	0.084749

Vibrational frequencies

-292.2725 54.3920 92.2102
375.4291 462.5580 636.1613
655.3308 738.3439 747.3211
893.7614 1071.4173 1095.7551
1152.5791 1160.4451 1309.2369
1627.7811 3302.8057 3304.2170

i48 – i62

Cartesian coordinates

C	0.317144	-0.451195	0.876320
C	0.624288	0.841591	-0.369724
C	-0.730589	0.600787	0.155425
C	-1.234257	-0.559426	-0.406236
H	2.156023	-0.832891	-0.516902
H	-1.300417	1.326646	0.726224
H	-2.207563	-1.032699	-0.470724

Vibrational frequencies

-418.7822 322.7846 414.1933
537.3542 657.5996 774.8177
788.5364 847.8370 983.9535
1004.5707 1074.7072 1153.3106
1220.6691 1344.5108 1517.0974
3194.7195 3220.3610 3315.7439

i34 – p6+H

Cartesian coordinates

C	-1.299614	0.432455	-0.102348
C	1.321600	0.566676	-0.074695
C	0.039759	-0.017518	-0.046443
C	-1.237355	-0.912068	-0.090281
H	-1.712653	1.026482	1.598651
H	-1.768959	1.335213	-0.461339
H	1.685165	1.572607	-0.201872

Vibrational frequencies

-967.2174 181.0996 230.3685
265.3577 302.8949 418.9845
531.3929 613.7682 800.9604
912.0246 955.4476 978.7174
1028.0375 1063.0072 1553.7052
1677.5814 3266.5602 3295.7963

i2 – i42

Cartesian coordinates

C	-0.371890	-0.383775	-0.728578
C	-0.528601	0.815250	-0.061947
C	0.938131	-0.267007	-0.244534
C	2.021380	-0.020501	0.393673
H	-1.234384	-0.752214	1.369138
H	-2.431922	-0.251938	0.053650
H	-0.253331	1.854334	0.008556

Vibrational frequencies

-500.5955 174.4616 255.0525
500.5931 692.5938 786.3201
888.7658 931.6070 1041.4273
1080.6409 1094.2774 1175.4019
1362.8615 1498.7331 1909.0272
3122.3993 3226.7115 3299.4488

i63 – p34+H

Cartesian coordinates

C	1.334739	-0.015842	0.025013
C	-0.778164	-0.427172	0.031582
C	-1.135736	1.001771	0.020406
C	0.163244	0.903536	-0.065978
H	2.027706	0.002126	-0.812579
H	1.839601	0.034238	0.987150
H	-2.948962	-1.968497	-0.014261

Vibrational frequencies

-238.6342 63.1967 71.4417
134.1158 350.1197 412.2385
644.2408 763.7662 866.2523
874.7121 1023.2933 1073.2144
1140.6019 1440.9808 1638.4277
1716.1851 3137.8045 3213.5315

i8 – p22+H

Cartesian coordinates

C	-1.885452	-0.023901	-0.016123
C	0.672265	0.616690	-0.272688
C	1.854453	-0.144570	-0.057979
C	0.634324	-0.800796	0.211140
H	-2.402166	0.877841	-0.314889
H	-2.454850	-0.891100	0.289082
H	0.632967	2.520820	0.989787

Vibrational frequencies

-481.8984 158.6403 170.1007
265.8228 339.0211 594.4555
599.0180 722.6692 814.8570
914.4661 971.4574 1058.1017
1097.4424 1429.2008 1483.9117
1870.7874 3188.0822 3291.3034

-481.8985 158.6402 170.1007

i3 – i11

Cartesian coordinates

C	2.443392	-0.000085	0.006218
C	-0.138346	-0.000096	-0.052696
C	-1.495967	-0.000324	-0.099759
C	-2.778670	-0.000186	-0.001058
H	3.000159	-0.931164	0.021157
H	3.000590	0.930807	0.015854
H	-0.907737	0.004542	1.039198

Vibrational frequencies

-1286.6722 142.9828 163.7646
289.3186 345.2406 424.3926
454.7494 524.9405 735.7074
870.2677 1024.7590 1331.4341
1492.2813 1890.9546 2033.9748
2251.0417 3147.6358 3240.8991

i26 – i41

Cartesian coordinates

C	-0.696668	-0.194549	0.352097
C	0.755858	0.730993	0.053000
C	0.518543	-0.699330	-0.318190
C	-1.878777	0.149733	-0.322204
C	0.548781	1.769020	-0.169771
H	-2.816559	-0.185950	0.127150
H	-0.705662	-0.376918	1.427677

Vibrational frequencies

-735.4313 247.5845 300.1381
409.8250 535.3251 622.8589
756.1098 810.8641 933.7346
974.5178 1022.7480 1090.6330
1200.0919 1313.0634 1446.6885
3105.0484 3131.8496 3225.1549

i12 – i41

Cartesian coordinates

C	-0.634650	-0.031558	0.385231
C	0.548378	0.766253	0.003473
C	0.719599	-0.887782	-0.260273
C	-1.892128	0.112221	-0.234712
H	-0.689591	-0.371326	1.422934
H	0.470200	1.706942	-0.541103
H	-2.515531	-0.774617	-0.370883

Vibrational frequencies

-546.7694 261.7127 284.6980
356.1359 504.2141 606.1554
748.6874 840.4301 893.2626
1047.9356 1108.4510 1157.6364
1191.2177 1315.5092 1518.0722
3093.4043 3137.9428 3140.3077

i20 – i21

Cartesian coordinates

C	-0.072448	0.583927	0.000000
C	-1.199763	-0.271799	0.000000
C	2.376208	-0.469568	0.000000
C	1.228713	0.076605	0.000000
H	-0.214287	1.655642	0.000000
H	-1.079143	-1.369019	0.000001
H	2.344014	0.783664	0.000000

Vibrational frequencies

-528.9275 28.2500 155.2927
159.9414 274.6565 388.3170
601.1722 635.8814 680.0446
868.1075 1054.4977 1154.5459
1378.2332 1596.1318 1863.5868
2442.3053 3036.6684 3238.4884

i1 – p3+H

Cartesian coordinates

C	-2.332963	-0.200154	0.000025
C	0.223935	-0.050468	-0.000039
C	1.515700	-0.039035	-0.000034

C	2.797258	-0.045810	0.000052
H	-3.087679	0.578451	0.000067
H	-2.668547	-1.234339	0.000022
H	-1.193697	2.211332	0.000010

Vibrational frequencies

-667.3387 115.1520 142.5516
235.3960 277.9768 325.2046
398.4940 501.5189 621.7184
782.8641 1001.3261 1034.3196
1381.3230 1523.1353 1977.7009
2166.3191 3141.6941 3240.3437

i8 – i16

Cartesian coordinates

C	0.303120	1.004966	0.129676
C	0.901488	-1.014679	0.215227
C	-0.368021	-0.288494	0.376957
C	-1.612222	-0.108473	-0.158906
H	0.606036	1.741321	0.865973
H	-2.473864	-0.715020	-0.414565
H	-0.940512	1.194134	-0.506863

Vibrational frequencies

-2571.5653 207.6385 343.0816
497.7378 528.3640 595.4041
722.7502 866.3789 874.5156
945.5960 1018.1570 1079.0166
1159.6755 1235.2744 1415.5385
1665.7470 3200.3864 3207.0083

i8 – i41

Cartesian coordinates

C	-0.597934	-0.022674	0.158504
C	0.646564	0.786036	-0.001573
C	0.624076	-0.832080	-0.250208
C	-1.969064	0.136322	-0.100048
H	-0.947524	-0.164777	1.239457
H	0.712247	1.695086	-0.597979
H	-2.402318	-0.868188	-0.248877

Vibrational frequencies

-295.9228 355.8355 398.6154
594.6539 640.6200 704.5339
785.3248 850.4629 916.7848
967.2121 1018.0282 1095.2466
1117.3165 1424.1657 1463.7976
2686.6657 3027.6523 3142.1957
-295.9229 355.8355 398.6154

i7 – i57

Cartesian coordinates

C	-0.799683	1.041883	-0.137084
C	0.563148	0.783530	-0.171124
C	0.319329	-0.881229	-0.195562
C	-1.097994	-0.427681	0.193196
H	0.480402	-1.411369	-1.131098
H	-1.940495	-0.861322	-0.347681
H	-1.268279	-0.527256	1.269515

Vibrational frequencies

-2418.2360 257.3243 477.6468
498.9255 617.2992 733.0002
867.9173 911.5519 970.4601
1092.9252 1118.5440 1190.1990
1237.5691 1408.1524 1445.2598
3064.3568 3135.5440 3162.3798

i28 – i36

Cartesian coordinates

C	-1.315844	0.665428	0.039247
C	1.220767	-0.482365	0.025815
C	-0.234718	-0.159472	0.151701
C	-1.559616	-0.663851	-0.241821
H	-1.678884	1.677114	0.120612
H	1.487554	-1.528331	-0.081990
H	0.375024	-0.387578	1.221015

Vibrational frequencies

-1232.0224 141.9573 194.2180
352.6665 473.2067 622.8966
734.6295 791.8481 900.3105
957.5525 997.9657 1067.4599
1265.4942 1479.7868 1595.1496
1920.0742 3196.0968 3276.1121

i67 – i37

Cartesian coordinates

C	-0.069717	-0.395083	0.012011
C	1.384075	0.795423	-0.039124
C	-1.027953	0.822127	-0.106493
C	-1.390107	-0.527280	-0.006898
H	1.974937	-1.388796	0.066493
H	-1.128874	1.667220	0.570344
H	-2.173809	-1.263994	0.041471

Vibrational frequencies

-182.4829 276.1942 355.3859
388.6918 638.2541 710.4676
768.4437 854.7583 935.9499
974.7189 1007.3216 1085.7346
1241.5207 1556.7562 1781.3562
3139.0559 3283.1340 3287.2243

i21 – i37

Cartesian coordinates

C	1.437176	-0.515432	-0.076364
C	-1.187858	-0.358296	0.016013
C	0.186566	-0.142744	0.359332
C	1.606296	0.826667	-0.128217
H	1.996774	-1.379833	-0.385863
H	-1.526023	-1.396304	-0.112536
H	0.555095	1.218228	0.375807

Vibrational frequencies

-871.4853 61.8282 215.1273
256.7142 370.9340 638.8618
665.2471 737.8227 836.5921
995.0011 1013.6656 1086.3914
1356.6513 1564.9407 1642.8710
2413.3162 3063.7276 3307.6991

i3 – i8

Cartesian coordinates

C	-1.852635	-0.195476	-0.072047
C	0.550085	0.890463	0.104763
C	1.517613	-0.021745	-0.423498
C	1.073737	-1.057562	0.242362
H	-2.586238	0.451334	-0.544227
H	-2.158920	-1.179129	0.260773
H	0.764388	1.739990	0.746789

Vibrational frequencies

-457.1197 263.4101 268.4840
375.2569 517.3879 630.1575
831.9453 865.1141 965.0764
1044.6211 1166.2813 1317.7607
1424.0881 1591.8634 1909.7888
3153.5793 3176.4331 3252.8473

i62 – i64

Cartesian coordinates

C	0.711037	0.735921	-0.111934
C	-0.677101	0.894398	0.350627
C	0.192329	-0.561199	-0.764033
C	0.912715	-0.680330	0.399225
H	-2.058082	-0.893575	0.142173
H	1.444355	1.436827	-0.473481
H	0.912395	-1.173605	1.364598

Vibrational frequencies

-511.7324 429.7267 523.7969
691.5604 733.7492 801.9894
840.6425 910.4838 947.1104
987.1377 1083.9779 1111.3951
1184.5680 1338.3569 1476.8007
3216.9216 3277.2932 3290.9012

i4 – i18

Cartesian coordinates

C	-0.206730	0.919810	-0.000186
C	-1.445186	0.014895	0.000321
C	0.983700	0.062775	-0.000190
C	2.172233	-0.369166	0.000267
H	-0.226742	1.546659	-0.896239
H	-0.226302	1.546840	0.895761
H	-2.451802	0.410636	0.000786

Vibrational frequencies

-272.5365	123.0064	208.5363
272.3614	465.4523	652.3516
857.2814	932.8618	979.4571
1034.0726	1200.3809	1261.0255
1458.0265	1683.5667	1721.7141
3052.7666	3110.8658	3248.0322

i16 – i17

Cartesian coordinates

C	1.169576	0.043544	-0.010643
C	-1.294234	-0.006082	-0.016677
C	-2.302447	-0.660487	-0.022056
C	2.261963	-0.559075	-0.134298
H	-0.101380	1.468916	0.900609
H	-0.055886	1.476798	-0.852927
H	1.642091	-0.763566	0.924126

Vibrational frequencies

-511.9604	127.0389	166.1042
227.0070	277.0396	397.9573
531.8404	877.6074	897.5890
994.0580	1240.1339	1342.2999
1440.1668	2038.3830	2281.5597
2473.6313	3065.3017	3106.5506

i7 – p34+H

Cartesian coordinates

C	-0.712615	-1.004257	0.060931
C	0.233321	0.915516	-0.044070
C	1.583208	0.369053	0.127636
C	0.729292	-0.623964	-0.034349
H	-3.256598	2.048479	0.610990
H	-0.990539	-1.240571	1.085316
H	-1.100401	-1.719683	-0.659539

Vibrational frequencies

-307.1670	37.1217	54.9298
146.2192	290.1075	454.6117
635.2190	775.4021	877.1197
905.0608	1026.9280	1064.4156
1161.7589	1447.6386	1565.6116
1722.2061	3132.5604	3211.0907
-307.1669	37.1217	54.9298

i15 – p4+H

Cartesian coordinates

C	-0.029054	-0.704757	0.206620
C	1.223240	-0.069585	0.050994
C	-2.322172	0.346058	-0.466520
C	-1.192596	-0.149805	-0.130186
H	3.252292	0.913628	-0.180240
H	-0.011059	-1.708371	0.631959
H	-3.136190	1.594218	1.989615

Vibrational frequencies

-254.4737	49.1103	74.7217
137.5945	233.9699	315.7783
324.1326	600.3558	725.0671
777.5305	907.5543	975.0312
1173.1104	1409.0669	2058.1818
2229.5667	3142.9942	3475.9363

i12 – trans-p7+H

Cartesian coordinates

C	-2.237774	0.309229	-0.000003
C	0.169800	0.572852	0.000002
C	1.391530	0.043710	0.000003
C	2.566638	-0.455935	-0.000001

H	-0.983588	-1.317002	-0.000008
H	-4.147104	-1.791739	0.000019
H	0.046015	1.653928	0.000007

Vibrational frequencies

-220.2368	50.5756	89.3116
106.3402	163.8309	226.2700
246.0838	527.8378	721.0447
911.0846	930.6166	1092.0915
1202.7538	1416.1327	1708.8214
2064.8572	3147.3924	3165.4571
106.3402	163.8308	226.2700

i14 – cis-p7+H

Cartesian coordinates

C	-1.673648	-0.855179	0.000433
C	0.212904	0.813556	-0.000012
C	1.288869	0.027861	-0.000069
C	2.345846	-0.688938	-0.000159
H	-1.988090	1.070328	0.000011
H	-4.444037	-0.846155	-0.001805
H	0.345659	1.894131	-0.000082

Vibrational frequencies

-305.3705	41.9325	96.6893
125.4986	149.6123	244.1564
252.9995	563.0593	633.8729
917.3069	936.3928	1023.5101
1199.8524	1434.3272	1736.7746
2065.1566	3088.6995	3158.0905

i52 – p25+H

Cartesian coordinates

C	0.572742	-0.730897	-0.220423
C	-0.747488	-0.183700	0.037991
C	0.377194	0.613604	-0.410584
C	1.643187	0.193039	0.262907
H	-3.202454	2.356527	0.100168
H	2.518737	0.229983	-0.371933
H	1.817074	0.368370	1.325481

Vibrational frequencies

-209.5490	51.8593	73.7275
195.6804	220.7322	419.6641
476.7426	774.8235	847.8269
998.2233	1079.3018	1126.2243
1236.3367	1389.3043	1533.0780
1841.0307	3100.1273	3238.0532

i42 – p25+H

Cartesian coordinates

C	-0.318330	-0.597464	-0.562346
C	-0.359164	0.549510	0.419809
C	0.859054	-0.051122	0.004043
C	2.220869	-0.066730	0.076553
H	-1.947580	-0.904494	0.886334
H	-2.338310	0.255887	-0.476881
H	-0.702160	3.008857	-0.757943

Vibrational frequencies

-300.6491	84.9637	112.8237
146.0891	342.2768	383.3925
580.6918	692.6102	942.5086
982.6046	1030.9984	1058.4628
1099.8961	1288.5385	1500.7552
1633.7292	3099.4104	3196.1599
-300.6492	84.9637	112.8237

i51 – p24+H

Cartesian coordinates

C	-0.421417	0.829217	0.197543
C	0.601222	-0.222009	0.055900
C	-0.774388	-0.743825	0.137284
C	-1.552039	0.282225	-0.484393
H	3.245549	2.012377	-0.131445
H	-0.382315	1.633571	0.924553
H	-1.095380	-1.538024	0.803086

Vibrational frequencies

-282.2490	46.1515	84.2001
212.3295	251.7566	532.4013
680.2416	779.6148	871.6169
950.5725	983.3299	1084.5417
1134.4054	1162.7183	1372.8595
1803.1967	3205.6052	3213.2975

i3 – p4+H

Cartesian coordinates

C	-2.144389	-0.301519	-0.231745
C	0.238691	0.721383	0.090292
C	1.375066	0.021561	0.016758
C	2.476204	-0.624087	-0.046461
H	0.270959	1.788426	0.311117
H	-3.104376	-0.693174	-0.475167
H	-2.623285	-0.974089	1.817321

Vibrational frequencies

-612.6129	91.0454	138.7318
226.0000	237.7415	316.3172
378.1248	601.3879	683.9561
787.9725	898.8723	980.8228
1165.1815	1407.1349	2036.4745
2159.2869	3133.7792	3466.8394
-612.6114	91.0442	138.7323
226.0000	237.7414	316.3176
378.1249	601.3880	683.9565
787.9729	898.8725	980.8228
1165.1816	1407.1350	2036.4747
2159.2871	3133.7792	3466.8396

i44 – p22+H

Cartesian coordinates

C	-1.791292	-0.000004	-0.186538
C	0.747300	0.746368	-0.008223
C	1.949758	0.000001	0.093621
C	0.747300	-0.746368	-0.008212
H	-2.326996	-0.934739	-0.277854
H	-2.327003	0.934724	-0.277880
H	-2.450282	0.000035	1.893347

Vibrational frequencies

-589.9988	197.5814	220.2039
318.6004	340.6276	595.6324
598.0482	775.7957	816.5062
926.3152	966.8723	1065.0345
1117.2659	1431.7049	1479.4711
1806.1174	3191.4778	3297.2610

i22 – p17+H

Cartesian coordinates

C	0.971321	-0.496690	0.000000
C	0.000000	0.675701	0.000000
C	-0.628564	-0.568943	0.000000
C	-0.616851	-1.844974	0.000000
H	-2.486735	3.032461	0.000000
H	1.484441	-0.688347	-0.933462
H	1.484441	-0.688347	0.933462

Vibrational frequencies

-184.2825	54.2827	65.6207
110.5782	170.3849	184.6677
396.0833	669.9794	815.7395
955.3139	1001.6231	1029.6795
1075.6204	1477.8886	1767.0301
1999.0781	3162.1091	3285.8031
-148.4234	58.3793	68.5285
116.8075	173.9387	184.5513
396.7818	669.4844	815.3100
956.0422	1001.5423	1030.0186
1076.5367	1478.2321	1766.7882
1998.7860	3161.6929	3285.3857

i9 – p13+H

Cartesian coordinates

C	-1.269853	0.438878	-0.111240
C	1.383376	-0.457405	0.099445
C	0.030851	-0.087473	-0.034129
C	-1.268556	-0.908316	-0.075072

H -1.674694 1.067778 1.572500
H -1.664077 1.375767 -0.472666
H 1.850796 -1.415004 0.254607

Vibrational frequencies

-989.3052 166.5031 214.7164
258.4625 370.8531 422.5029
538.8024 614.2672 798.4479
838.9774 944.3980 965.9787
1059.5750 1146.0653 1566.8403
1708.0924 3265.6812 3298.9687

i26 – i28

Cartesian coordinates

C 0.047250 0.105071 -0.070662
C -1.175209 -0.591333 -0.183451
C 1.390903 0.294087 -0.710012
C 1.469513 -0.187140 0.487341
H -0.469479 1.165635 0.323189
H -1.529025 -1.564355 -0.476319
H 1.932046 -0.614315 1.359349

Vibrational frequencies

-501.9569 271.4139 295.4525
539.2540 643.9995 670.9345
768.3194 780.1396 927.0481
983.0231 1027.2135 1035.5230
1408.6758 1560.1295 1706.8260
2257.6089 3303.5063 3318.4199

i24 – b205for

Cartesian coordinates

C -0.249478 -0.346763 0.403742
C 1.053953 0.017460 -0.126626
C -1.453313 -0.572800 -0.470123
C -1.529302 0.575108 0.073837
H -0.203876 -0.812079 1.384836
H 1.182148 0.402918 -1.179830
H -1.874882 1.548617 0.363318

Vibrational frequencies

-182.6475 149.8624 295.4279
403.5210 550.6312 635.6386
673.9427 736.9971 871.5288
959.7403 1015.3045 1064.2359
1357.1875 1779.3558 1845.1748
2844.9104 3157.1212 3356.0163

i47 – p23+H

Cartesian coordinates

C 0.420084 0.854779 -0.029056
C -0.713290 -0.067520 0.069252
C 0.504602 -0.937755 -0.399815
C 1.433696 -0.060353 0.177307
H 0.402561 1.790349 -0.581678
H 2.508755 -0.035964 0.249364
H -0.651503 -0.514402 1.858674

Vibrational frequencies

-1079.0896 158.0665 339.9268
365.3129 550.7248 615.9232
640.4238 687.7291 846.3731
873.7771 1005.1902 1052.0346
1193.8318 1309.4374 1464.2415
1668.3593 3174.2735 3286.7347

i28 – b205for

Cartesian coordinates

C -0.297333 -0.453409 0.378847
C 1.054709 -0.065619 0.080412
C -1.397019 -0.419360 -0.646308
C -1.508436 0.582769 0.129965
H -0.363964 -1.125507 1.231989
H 1.478681 0.390730 -1.050279
H -1.857786 1.486483 0.590371

Vibrational frequencies

-224.8948 196.3139 230.4934
316.2638 457.8718 597.3771

643.7145 690.5912 866.4140
919.1851 940.0669 1053.2519
1341.6020 1781.6131 1966.5445
2435.9222 3140.6363 3355.7254

i27 – p5+H

Cartesian coordinates

C 1.504026 0.664778 0.074477
C 0.265896 -0.000133 -0.047644
C -2.314160 -0.000972 -0.317186
C -1.060830 -0.000546 -0.179150
H 2.060877 -1.585892 0.133387
H 2.060378 1.586732 0.128620
H -3.516275 0.006073 2.096146

Vibrational frequencies

-237.7250 30.8921 63.7017
160.8559 172.1974 472.8718
503.8873 744.4690 789.2925
957.7479 973.6482 974.9683
1148.2497 1478.8889 1699.5385
2110.6196 3266.8566 3305.3112

i31 – i37

Cartesian coordinates

C -0.285025 -0.125827 -0.055176
C 2.151577 0.443649 -0.016061
C -1.218247 0.890101 -0.107315
C -1.407834 -0.879079 0.043379
H 1.508434 -1.392391 0.128940
H -1.451813 1.666969 0.620712
H -2.285930 -0.058780 -0.097226

Vibrational frequencies

-803.4168 117.3020 140.1858
359.9037 404.2825 629.7495
676.0900 826.6601 871.0515
910.0276 939.4242 981.0111
1286.6632 1661.5454 1809.5292
2477.0111 3067.1437 3126.6406

i17 – i18

Cartesian coordinates

C 0.048379 0.783568 0.010252
C -1.157320 -0.084540 0.165981
C 1.298236 0.019751 -0.036190
C 2.327841 -0.601370 -0.055465
H -0.060477 1.359650 -0.911068
H 0.094959 1.498856 0.836231
H -1.254876 -0.824318 1.011137

Vibrational frequencies

-212.1187 105.7580 169.4870
217.5625 392.5966 549.3776
697.0776 893.9427 981.5636
1024.2115 1248.6147 1336.3020
1467.3100 1909.4359 2279.5971
2859.5713 3076.4990 3126.0970

i37 – p5+H

Cartesian coordinates

C 0.195507 0.006948 0.000073
C -2.366584 -0.278414 -0.000238
C 1.396701 -0.725202 0.000079
C 1.465377 0.604407 -0.000177
H -1.244036 2.094710 0.000717
H 1.902997 -1.677069 0.000214
H 2.065564 1.499972 -0.000423

Vibrational frequencies

-564.4528 85.9767 195.5557
232.6062 429.5623 480.6591
516.8964 754.9008 799.5773
963.5485 974.7040 979.2382
1164.0170 1468.4556 1691.5280
2040.5157 3272.1809 3311.2701
-564.4527 85.9767 195.5557

i12 – i14

Cartesian coordinates

C 1.999463 -0.532760 -0.296545
C -0.145266 0.683526 -0.187843
C -1.291008 0.032927 -0.059736
C -2.408009 -0.576892 0.083096
H 1.354689 0.511535 1.395694
H 2.960189 -0.994138 -0.125324
H -0.130226 1.646454 -0.701104

Vibrational frequencies

-247.5663 159.7333 199.3230
321.7549 461.9513 665.4308
775.4464 834.4695 901.1729
1016.9900 1174.4426 1229.8692
1390.4046 1695.1428 2066.9740
3063.4350 3130.8707 3271.2333

i27 – i37

Cartesian coordinates

C 0.215418 0.069226 -0.283247
C -2.366732 -0.272213 0.076515
C 1.521616 0.581480 0.063758
C 1.386301 -0.722575 0.042574
H -1.637449 1.203208 0.138385
H 2.155166 1.436780 0.227357
H 1.823162 -1.696940 0.176582

Vibrational frequencies

-254.7250 152.9144 280.3441
312.0589 535.6883 645.6402
691.1172 753.8951 900.5895
935.1677 970.6661 1051.4044
1413.6458 1658.1268 1747.2049
2792.5022 3274.7330 3321.8680
1413.6458 1658.1268 1747.2050

i26 – i37

Cartesian coordinates

C -0.276765 0.448687 -0.000027
C 1.707164 -0.596236 0.000022
C -1.616781 0.237434 0.000017
C -0.831610 -0.868086 -0.000018
H 1.604951 1.616273 0.000001
H -2.622519 0.634503 0.000063
H 0.325065 -1.426424 -0.000005

Vibrational frequencies

-1349.0570 141.0510 472.8256
492.7707 670.9893 798.8321
832.5039 888.4910 991.6034
1048.7992 1112.4237 1179.1560
1413.1418 1449.6416 1690.1317
1785.9864 3208.0062 3249.2831

i37 – p13+H

Cartesian coordinates

C -0.045070 -0.047978 0.052078
C -1.514013 -0.670931 -0.210110
C 1.162163 -0.740716 -0.006348
C 1.382583 0.534348 0.292479
H -1.580335 1.612277 0.292334
H 1.440877 -1.759588 -0.215981
H 2.020817 2.142167 -1.385875

Vibrational frequencies

-331.8070 58.3991 123.1202
190.5781 245.2839 396.2657
451.5376 573.9281 784.7836
844.5287 854.0134 969.1105
1065.6956 1158.0461 1633.3139
1727.9874 3300.8218 3305.2543

i1 – i32

Cartesian coordinates

C 1.677106 -0.518471 -0.122242
C 0.489292 0.248063 0.078613
C -0.983238 0.085436 -0.004722
C -1.735953 -0.969477 -0.014704
H 1.013167 0.218996 1.139392

H 2.615674 0.014231 -0.216121
H 1.661147 -1.589253 0.025111

Vibrational frequencies

-1482.6324 108.7315 271.6339
294.1655 415.9996 452.4612
706.5345 738.3934 810.1380
883.3050 982.6594 1071.5423
1433.4027 1474.5432 1748.9244
2423.4615 3166.3334 3296.6289

i27 – p1+H

Cartesian coordinates

C -1.529739 0.550039 -0.423450
C -0.290574 -0.071726 -0.064729
C 1.099993 0.002044 -0.001886
C 2.297911 0.075771 0.048111
H -1.913257 -1.620251 0.517946
H -2.363057 2.522020 1.126976
H 3.358969 0.143477 0.091590

Vibrational frequencies

-297.0148 59.1643 95.9123
200.5046 215.6782 534.8213
537.2223 661.7953 711.9997
781.5713 911.0539 949.7898
1142.3486 1293.9616 1754.5176
2239.2085 3269.9041 3480.6777

i67 – p28+H

Cartesian coordinates

C 0.985346 -0.711622 0.048424
C -0.393572 0.941459 -0.183701
C -1.171763 -0.000031 0.401637
C -0.393558 -0.941448 -0.183802
H 1.818235 1.377285 -0.138035
H 1.818255 -1.377246 -0.138183
H -3.707225 0.000042 -0.510137

Vibrational frequencies

-309.0419 69.5411 97.7371
293.7327 363.4833 679.7288
785.4722 860.0149 894.9547
928.8372 1030.7683 1198.8231
1205.4305 1271.3800 1342.7592
1383.3156 3220.5202 3237.2776

i7 – p28+H

Cartesian coordinates

C -0.893582 -0.559144 -0.274901
C 0.619859 0.872315 0.303347
C 1.403514 -0.156575 -0.181482
C 0.403110 -0.971107 0.129296
H -1.456145 1.628891 -0.082801
H -1.753117 -0.779345 1.691474
H -1.796926 -1.139086 -0.395165

Vibrational frequencies

-780.1909 149.7303 243.7994
332.0319 424.7180 651.6281
779.1253 824.4229 855.8597
912.3643 991.9592 1124.9350
1207.3210 1266.4815 1331.6460
1413.4012 3232.3802 3253.4506

i20 – i18

Cartesian coordinates

C -0.040539 0.560511 0.050465
C -1.190536 -0.311986 0.001557
C 1.290015 0.081338 0.089669
C 2.490357 -0.357673 0.011090
H 0.847519 0.402027 -1.024278
H -0.211203 1.628732 0.133922
H -1.058480 -1.404234 -0.003678

Vibrational frequencies

-1381.1200 133.5582 145.8980
226.2442 315.2252 481.3771
539.9361 687.3232 855.2124

869.5485 1057.2829 1146.5548
1367.6342 1690.7715 1897.5089
2275.4349 3069.1400 3192.5532

i30 – p12+H

Cartesian coordinates

C -1.709374 0.771326 0.000172
C 0.826708 -0.066038 0.000003
C -0.472734 -0.073516 -0.000017
C -1.786561 -0.568899 -0.000188
H 2.864118 -0.546752 -0.000061
H 2.420628 1.262028 -0.000059
H 0.972662 -2.429004 0.000554

Vibrational frequencies

-537.9829 112.0382 131.8372
212.6991 288.0257 396.5188
453.3670 578.8870 585.5580
776.7808 970.6387 1000.2003
1265.5853 1432.9562 1581.0127
1987.0285 3130.5847 3223.4752

i29 – i18

Cartesian coordinates

C 0.159488 -0.104939 0.605787
C 1.291780 0.600589 -0.129400
C -1.144159 0.085984 0.079009
C -2.326001 -0.012929 -0.374723
H 0.267855 -0.152256 1.687903
H 1.547049 1.637284 -0.234098
H 0.551913 -1.229210 0.215773

Vibrational frequencies

-782.2003 182.1422 185.0014
442.3289 471.7013 717.1680
766.3881 919.7873 940.3420
1018.2350 1074.2890 1187.7303
1318.8262 1678.2001 1788.1257
2166.3297 3136.4324 3346.7768

i65 – i14

Cartesian coordinates

C -0.983678 -0.944767 0.146666
C 0.143825 1.081257 0.008340
C 1.218750 0.255334 0.202145
C 1.309780 -0.959987 -0.216831
H -2.050272 0.858643 -0.318508
H -1.622549 -1.813795 0.074828
H 0.197847 2.162750 -0.084993

Vibrational frequencies

-451.4475 200.9449 267.2844
437.3155 636.0245 684.5461
839.8656 898.4767 952.9380
1033.8416 1163.5579 1246.2200
1385.5298 1524.2943 1745.1696
3171.2027 3186.1227 3263.8155

i24 – p1+H

Cartesian coordinates

C 1.530238 0.597580 0.023289
C -1.041789 0.004620 -0.000903
C 0.357534 -0.055057 -0.096650
C 1.571293 -0.784684 0.239094
H -3.297222 0.092252 0.194020
H 2.048997 1.543301 0.011266
H 0.174449 -0.526618 -1.791614

Vibrational frequencies

-1042.7910 169.7937 228.2290
271.5451 467.8200 524.7257
549.0215 664.7158 723.6086
756.6836 867.8835 958.1539
1107.1182 1280.1931 1667.3082
2229.4318 3268.1641 3482.0620

i21 – trans-p7+H

Cartesian coordinates

C 0.041090 0.551821 0.000063

C -1.231089 0.133038 0.000040
C 2.422934 -0.022085 -0.000261
C 1.160230 -0.366605 0.000218
H 0.272694 1.613533 -0.000059
H 0.993943 -1.448436 0.000576
H -2.083640 1.938739 0.000220

Vibrational frequencies

-712.7846 111.5127 134.7671
162.1965 256.1608 288.6516
483.1161 555.2541 722.4787
917.0839 941.6334 1091.8224
1192.6385 1411.2796 1727.0140
1972.8868 3111.3493 3175.6561

i2 – i23

Cartesian coordinates

C 1.449131 0.758371 0.260716
C 0.160012 0.284334 -0.122043
C -1.175546 0.085935 -0.012672
C -2.417850 -0.185327 0.074226
H 1.390313 -1.298211 0.877731
H 1.695735 -1.178132 -0.940976
H 0.583359 0.983839 -0.982276

Vibrational frequencies

-620.4661 136.4865 200.4139
359.7411 583.4539 646.9773
789.4241 874.9333 931.5170
998.8417 1024.4967 1168.0683
1432.4968 1511.8016 2035.2277
2427.7652 3127.9803 3229.9645

i20 – trans-p7+H

Cartesian coordinates

C -0.106802 -0.503432 -0.223854
C -1.229332 0.326759 0.167965
C 2.370044 0.042754 0.384130
C 1.157167 -0.213170 0.075656
H -0.337827 -1.402848 -0.790565
H -1.066979 1.246267 0.740033
H 3.198211 1.650931 -1.806914

Vibrational frequencies

-264.0053 50.5219 74.2040
128.3820 132.8015 207.0514
265.4710 525.8112 710.0740
906.6610 920.2909 1091.1850
1199.5810 1410.8960 1731.2335
2061.2006 3107.2193 3162.0223

i10 – i31

Cartesian coordinates

C 1.510704 -0.660468 0.000002
C -1.167327 0.203469 -0.000004
C 0.240630 0.302759 -0.000002
C 1.411996 0.822132 -0.000001
H 1.737743 -1.196145 0.920448
H 1.737748 -1.196147 -0.920443
H -1.827374 1.126546 0.000021

Vibrational frequencies

-176.5571 133.5277 235.0788
270.4591 534.8783 611.0670
783.5680 803.2350 975.7590
1028.8818 1071.6209 1078.3284
1510.6165 1810.0229 1992.2632
2803.9141 3082.5777 3171.6536

i56 – i57

Cartesian coordinates

C 0.031070 -0.439097 0.610309
C 0.510303 0.897171 0.003322
C -0.838701 0.522608 -0.306912
C -1.619720 -0.483561 -0.083073
H 1.164957 -0.803530 -1.258235
H 2.241387 -0.507083 0.214364
H 0.425492 0.614787 1.300740

Vibrational frequencies

-1786.9387 272.7400 305.1645
563.6559 610.1395 755.7778
815.4814 999.4391 1044.4131
1083.2800 1146.0625 1169.4357
1367.2173 1486.0298 1754.9482
2142.3529 3154.8502 3260.2398

i63 – i60

Cartesian coordinates

C -0.528766 0.874935 -0.231619
C 0.792856 0.536469 0.422738
C -0.045709 -0.379545 -0.635695
C -1.327364 -0.303241 0.249360
H 1.799317 0.615721 -0.313803
H -2.244159 -0.528629 -0.279892
H -1.282931 -0.611632 1.292350

Vibrational frequencies

-730.9384 300.8020 416.9918
497.9914 677.2106 714.3798
766.2819 933.3255 1035.2982
1049.4913 1094.8435 1124.2876
1324.1414 1421.2861 1509.4863
2298.1476 3118.0015 3241.1075

i60 – p29+H

Cartesian coordinates

C 0.042351 -0.731435 -0.141340
C -0.553527 0.910720 -0.261271
C 0.710890 0.824580 0.273457
C 1.361455 -0.367372 -0.065243
H -2.180825 -0.685816 -0.492923
H -1.863446 -0.507956 1.963338
H 2.272940 -0.867835 0.207261

Vibrational frequencies

-469.8909 199.5240 223.5594
393.1509 477.2460 631.5894
677.3026 744.1287 798.9536
881.9440 1084.0387 1087.3521
1153.5935 1155.4429 1292.1104
1621.8959 3294.3700 3306.8657

i65 – p29+H

Cartesian coordinates

C 0.025136 0.680648 -0.156463
C -0.710581 -0.933740 -0.052203
C 0.614546 -0.925207 0.308291
C 1.303042 0.167435 -0.221882
H -2.234132 0.778045 -0.237814
H 0.337503 2.727871 0.906166
H 2.278779 0.602243 -0.098936

Vibrational frequencies

-497.0761 84.1518 192.3195
372.5627 459.2576 613.0700
654.5282 735.5003 748.4763
894.8039 1070.4048 1104.3206
1159.9102 1165.3908 1315.7126
1610.4591 3301.5985 3308.2749

i60 – i57

Cartesian coordinates

C -0.508736 0.854794 -0.298382
C 0.811334 0.652265 0.171098
C -0.173824 -0.515966 -0.636926
C -1.303171 -0.269291 0.357216
H 1.110945 -1.166042 -0.587138
H -2.286758 -0.478897 -0.049289
H -1.170459 -0.436823 1.423426

Vibrational frequencies

-1366.7076 257.8071 350.9185
538.2106 600.9667 673.0832
740.9270 844.7304 950.7930
1047.2969 1066.2141 1165.5382
1256.7248 1486.5568 1787.0803
2176.9713 3119.2627 3227.2829

i12 – i15

Cartesian coordinates

C -2.055792 -0.083226 0.120632
C 0.368761 0.810979 -0.111332
C 1.533334 0.235006 0.384939
C 1.400068 -0.924062 -0.191092
H -0.034379 -1.129503 -0.193155
H -2.952322 -0.671290 0.132713
H 0.345392 1.757099 -0.651809

Vibrational frequencies

-1769.6226 209.0485 301.2840
373.5817 478.2293 567.2900
614.7462 701.4203 851.8129
941.5968 1000.1331 1210.3475
1372.0300 1600.8972 1676.3689
1804.3937 3152.4879 3360.8210

i63 – i7

Cartesian coordinates

C -0.340048 -0.784583 0.061205
C 0.795583 0.947769 -0.150420
C -0.567192 0.846500 -0.054875
C -1.559236 -0.377477 -0.042477
H 1.635522 -0.993417 -0.845268
H 1.662474 -0.788284 0.935824
H -0.024708 1.370972 0.932437

Vibrational frequencies

-1323.6667 307.7680 390.2867
434.2494 608.4869 689.1623
774.0476 870.5205 970.3694
1003.8913 1099.5394 1151.2377
1375.0702 1431.0038 1768.0851
2250.8569 3113.7521 3181.9366

i7 – i68

Cartesian coordinates

C -0.821113 -0.100764 0.810716
C 1.155094 0.169866 0.001748
C 0.118657 1.072981 -0.029361
C -1.040610 0.214156 -0.528342
H -0.401223 -0.740768 -1.215463
H 0.300694 -2.014116 0.007010
H 2.223905 0.235123 0.145385

Vibrational frequencies

-1045.1580 343.3928 495.5234
639.8217 797.1464 844.5892
870.5953 932.5528 947.7514
1029.3069 1120.4369 1249.0056
1307.6770 1354.6114 1451.6351
2085.8196 3213.5300 3254.2225

i65 – i45

Cartesian coordinates

C 0.318096 -0.891441 0.294665
C -1.005573 0.745228 0.020154
C 0.468825 0.553235 0.228120
C 1.653860 0.263642 -0.278176
H -1.943197 -1.239733 -0.438676
H 1.775516 -0.940732 -0.172819
H -1.632035 1.623149 -0.046438

Vibrational frequencies

-1280.2326 182.9697 407.8405
444.3384 590.1642 703.5833
746.0023 857.3148 896.6097
916.7755 997.6658 1118.5743
1227.4034 1556.4706 1708.4608
2359.8436 3220.6707 3256.1229

i67 – i60

Cartesian coordinates

C -0.484713 0.967007 -0.372932
C 0.858663 0.652404 0.590376
C -0.151156 -0.404189 -0.525776
C -1.321104 -0.573264 0.211690

H 2.083910 -1.114983 -0.163074
H -1.662732 0.773901 0.085535
H -1.413106 -0.966491 1.223016

Vibrational frequencies

-1127.1101 187.6544 415.8952
476.8856 642.4040 657.1608
736.6017 814.8855 905.1676
963.6792 1039.0409 1078.6301
1178.8149 1389.2018 1516.3787
2243.6686 3161.0744 3319.0758

i2 – i10

Cartesian coordinates

C 1.335630 -0.229927 0.362960
C 0.125171 -0.493470 -0.406795
C -1.255361 -0.676397 -0.178544
C -1.278760 0.448543 0.491663
H -0.644873 1.433747 0.094325
H 2.291148 -0.485132 -0.088659
H 1.295265 -0.250916 1.451325

Vibrational frequencies

-1110.7531 282.0690 424.3641
489.5280 518.9879 624.3776
892.8462 928.6419 943.4810
1030.9774 1052.4117 1177.5788
1412.0521 1460.3379 1555.0502
2114.6474 3094.9413 3193.0902

i67 – i60

Cartesian coordinates

C -0.673921 0.656966 -0.585412
C 0.541457 0.772045 0.358039
C 0.032683 -0.562499 -0.509051
C -1.198256 -0.358501 0.373129
H 2.136215 -0.861438 0.429332
H -2.129175 -0.902621 0.515341
H -0.315247 0.401194 1.342260

Vibrational frequencies

-1918.0809 414.7880 595.7420
652.8595 722.9512 778.5940
838.4205 905.6524 909.4463
951.0440 1061.9979 1090.7246
1177.5056 1332.3476 1444.7818
1832.3994 3171.8755 3307.9906

i49 – p24+H

Cartesian coordinates

C 0.441129 0.805310 -0.310040
C 0.441129 -0.805307 -0.310048
C -0.766926 0.000000 -0.059356
C -2.012545 -0.000002 0.313813
H 1.447488 -0.000015 2.812298
H 0.502040 1.625415 -1.017370
H 0.502040 -1.625405 -1.017386

Vibrational frequencies

-299.0678 83.3825 108.7546
196.7154 254.0937 524.9790
676.5225 777.5280 866.9096
947.2692 980.8249 1081.7085
1132.3180 1161.1649 1370.7150
1805.7957 3200.8745 3208.6570

i65 – p28+H

Cartesian coordinates

C -0.050750 1.080709 -0.073952
C 0.661720 -0.941322 0.215176
C -0.581734 -1.148942 -0.274933
C -0.943224 0.036729 0.271852
H 2.175531 0.714106 -0.016838
H -0.174487 2.146260 0.070461
H -3.508117 0.937942 -0.166735

Vibrational frequencies

-278.4043 63.2423 90.6753
293.5929 368.0794 676.8749

786.1362 860.1219 892.8926
925.2079 1027.6386 1195.4091
1206.7137 1272.2128 1342.1848
1385.3875 3221.5214 3238.1493

i58 – i62

Cartesian coordinates

C -0.647464 0.775198 0.124851
C 0.757243 0.654811 -0.268093
C -0.067169 -0.568669 0.557794
C -1.181590 -0.517903 -0.383603
H -1.057078 1.637781 0.630209
H 1.250627 -0.176990 -1.177836
H -2.184676 -0.893862 -0.223003

Vibrational frequencies

-1218.2252 323.6968 435.2500
503.3004 707.6761 741.0036
787.1725 856.8136 906.1037
1014.3439 1065.1412 1077.0624
1192.1816 1262.1729 1498.5137
2183.2528 3211.8304 3239.3096

i15 – i51

Cartesian coordinates

C 0.633457 -1.100623 -0.000023
C 0.581039 1.041366 0.000015
C -0.596217 0.229516 0.000002
C -1.854663 0.030117 -0.000002
H 0.504050 -2.168846 0.000113
H 0.725903 2.109800 -0.000006
H -2.620456 -0.721281 -0.000016

Vibrational frequencies

-769.9560 260.2631 281.0355
405.3475 509.2005 615.9166
620.8177 655.5947 730.9662
854.8171 1008.4976 1128.9624
1244.0006 1438.2684 1768.3290
3268.2662 3315.5680 3349.5660

i3 – i15

Cartesian coordinates

C 1.736240 -0.594387 0.000003
C -0.211995 1.108459 0.000000
C -1.192391 0.133573 -0.000004
C -1.721406 -1.022943 0.000002
H 0.268111 -0.829564 0.000003
H 2.433319 -1.400190 -0.000007
H -0.298523 2.183044 0.000011

Vibrational frequencies

-1386.7161 169.4779 306.6789
347.9205 362.4686 455.4564
599.3106 702.0403 719.8643
737.3223 1037.3700 1059.4324
1309.5521 1546.7407 1905.6416
2053.8720 3264.6817 3456.1951

i43 – i16

Cartesian coordinates

C -0.541169 -0.051156 -0.000005
C 1.429592 0.344647 0.000023
C 0.493418 1.202694 -0.000015
C -1.820239 -0.074700 0.000006
H 0.760437 -1.573193 0.903721
H 0.760454 -1.573166 -0.903749
H -2.731094 0.492629 0.000017

Vibrational frequencies

-466.3305 100.9544 362.6559
394.7621 492.2123 649.7433
681.2284 852.1393 931.3026
1007.3364 1094.0474 1162.7268
1470.4676 1640.2228 1752.1860
3107.1060 3181.0199 3346.9966

i65 – i67

Cartesian coordinates

C -0.328623 1.020784 0.015377
C 0.996417 0.528861 -0.025123
C -0.329890 -0.915109 0.007956
C -1.381732 -0.105450 -0.192389
H -0.664172 2.014260 0.299222
H 1.883147 1.153752 0.022045
H -1.172631 -0.861138 0.957904

Vibrational frequencies

-1329.0843 206.4825 450.8648
539.0746 621.3135 717.2642
882.5695 905.5319 958.5315
1033.7267 1084.0216 1128.2118
1277.9600 1313.6943 1428.5118
2190.5338 3175.5979 3193.7205

i37 – p6+H

Cartesian coordinates

C -1.202495 0.725607 0.009591
C 1.404448 0.433858 0.143968
C 0.044385 0.102240 -0.040565
C -1.352562 -0.561677 -0.294948
H -1.574009 1.715364 0.216183
H 1.920026 1.345462 0.394955
H -1.862373 -2.166129 1.427340

Vibrational frequencies

-381.5872 60.9308 129.2548
223.3060 253.1126 294.7031
444.1404 612.3454 784.8333
815.2494 966.9396 998.6034
1050.9669 1079.5753 1620.9908
1698.9846 3290.1093 3295.0093

i65 – p32+H

Cartesian coordinates

C -0.703335 0.786123 -0.061061
C 0.781433 0.596511 -0.315012
C 0.096711 -0.740572 -0.000256
C -1.282638 -0.426529 -0.192884
H -0.808274 1.567303 2.226404
H 1.210211 1.146370 -1.147292
H -2.212234 -0.882220 0.102133

Vibrational frequencies

-361.5198 106.0333 151.7923
357.9602 470.7185 552.3463
619.6525 723.7748 761.5214
868.9876 1032.9359 1120.8413
1130.9140 1151.1681 1419.2481
1565.9784 3174.5687 3292.6807

i34 – i35

Cartesian coordinates

C 1.406051 0.512113 -0.000408
C -1.284486 0.562250 0.000364
C 0.145556 0.043227 0.000053
C 1.307901 -0.866863 0.000574
H 1.998976 1.413036 -0.000891
H -1.486104 1.149729 -0.907973
H -1.486206 1.148408 0.909553

Vibrational frequencies

-308.0785 55.2115 258.5896
365.6149 655.1113 848.5041
857.0514 935.5601 953.1095
1000.1036 1094.5923 1225.8221
1271.0109 1443.1679 1636.1213
2965.2679 3008.3229 3275.1525

i1 – i40

Cartesian coordinates

C -0.641751 1.295953 -0.097505
C -1.050883 0.027147 -0.239008
C 0.351009 0.090497 0.525376
C 1.505443 -0.110405 -0.253345
H 0.373484 0.078560 1.606727
H 2.476781 -0.223884 0.211941
H 1.434465 -0.105556 -1.333065

Vibrational frequencies

-77.6179 208.3619 281.9559
397.7366 433.0525 478.0883
777.4273 842.3086 980.9615
1044.2749 1185.0848 1218.2381
1329.5811 1483.6766 1662.4386
3169.3805 3222.6650 3286.4629

i57 – i40

Cartesian coordinates

C -0.351681 1.382390 0.025385
C -1.014310 0.241301 -0.196458
C 0.292566 -0.281483 0.537366
C 1.426089 -0.151737 -0.268117
H 0.333339 -0.353679 1.615554
H 2.419644 -0.098267 0.162583
H 1.321954 -0.157272 -1.344915

Vibrational frequencies

-255.3757 236.6056 328.7571
355.5928 463.2456 574.1731
858.6021 890.7303 976.3393
1051.9823 1186.8220 1234.5614
1322.9007 1494.3488 1590.9538
3166.3357 3228.2213 3285.9638

i8 – i57

Cartesian coordinates

C 0.495774 -0.397495 -0.569047
C -0.827589 -0.801054 -0.254293
C -0.379608 0.791710 -0.205675
C 1.488751 -0.013609 0.311924
H -0.441986 1.679063 -0.826332
H 2.284847 0.643097 -0.027367
H 1.581492 -0.453100 1.305146

Vibrational frequencies

-730.8880 304.8287 383.0843
526.3333 627.8073 754.9794
779.5162 942.8278 974.2505
983.5534 1080.0048 1112.0796
1318.8050 1407.4340 1509.5536
3104.7041 3189.9075 3218.7740

i60 – i57

Cartesian coordinates

C 0.085873 -0.593318 -0.431494
C -0.648230 0.957244 -0.234511
C 0.632355 0.726531 0.136345
C 1.529733 -0.300648 0.272708
H -1.258158 -0.593020 1.296504
H -2.140132 -0.739078 -0.301779
H 1.315814 -0.998112 -0.794083

Vibrational frequencies

-1638.2656 266.5544 384.7439
396.1921 609.9019 663.9241
818.7048 864.5597 998.7096
1027.9451 1099.2249 1141.4469
1201.9760 1480.8738 1513.1723
2205.7128 3100.8428 3210.1011

i26 – i36

Cartesian coordinates

C -1.457207 0.614666 0.047775
C 1.085211 -0.237082 0.354366
C -0.340195 -0.095627 0.124422
C -1.546304 -0.744071 -0.301310
H -1.942273 1.570258 0.173974
H 1.348774 -0.833523 1.242349
H 1.849554 0.894515 0.487022

Vibrational frequencies

-980.4308 132.3008 207.0940
279.8058 536.7621 614.8619
781.4942 909.5007 943.8096
965.7788 1108.7656 1205.7391
1294.8416 1391.0743 1765.8952

2282.0733 2991.3996 3270.0205

i14 – i29

Cartesian coordinates

C 1.622769 0.723194 -0.048030
C 0.035361 -0.542336 -0.436275
C -1.172223 -0.062812 -0.072926
C -2.321136 0.367278 0.272344
H 1.637752 -1.086226 1.173067
H 1.687434 1.644819 -0.585628
H 0.179444 -1.019313 -1.403014

Vibrational frequencies

-606.7862 102.7584 184.3438
270.0353 338.8097 523.5522
679.1287 762.4610 842.1432
969.4869 1139.4609 1176.4377
1332.7761 1710.1059 2036.9753
3155.1901 3190.3470 3416.9873

i27 – i9

Cartesian coordinates

C 1.687433 -0.166152 0.000012
C 0.366738 -0.468437 -0.000010
C -1.018614 -0.765701 -0.000010
C -1.766545 0.320401 0.000010
H -0.388997 1.321974 -0.000004
H 2.718394 -0.493312 0.000039
H -2.853115 0.364782 0.000033

Vibrational frequencies

-1421.3043 98.0340 461.9469
471.9411 642.2797 738.0243
801.1567 849.2380 978.4537
1029.9573 1065.7606 1093.2866
1383.4771 1552.0229 1616.0145
1758.1439 3183.8125 3239.1173

i46 – i49

Cartesian coordinates

C -0.456849 -0.888517 -0.117997
C -0.381381 0.775554 -0.221457
C 0.784206 -0.167942 0.048491
C 2.051226 0.111767 0.167660
H -2.478517 0.252023 0.242993
H -0.656455 -1.552637 -0.954269
H -0.337676 1.520711 -1.006435

Vibrational frequencies

-580.6638 210.9173 299.9844
528.2955 659.0311 772.3101
858.2710 882.7500 976.9449
995.9019 1102.0289 1144.1047
1192.9907 1391.1045 1741.8397
3172.7901 3217.6428 3258.5788

i2 – i32

Cartesian coordinates

C 1.379092 0.735223 0.000124
C 0.183751 -0.107980 -0.000308
C -1.173742 0.003085 -0.000984
C -2.445099 0.120532 0.000730
H 2.176848 -0.419188 0.000644
H 1.691010 1.203312 0.930070
H 1.691858 1.203083 -0.929654

Vibrational frequencies

-804.6701 115.8889 180.1579
366.8494 517.2747 636.3970
770.5770 865.7991 988.6596
1039.3947 1070.7174 1213.1922
1448.1172 1501.4843 2047.0183
2368.8166 3109.3677 3220.8100

i36 – p13b+CCH2

Cartesian coordinates

C -1.675500 0.595926 0.128784
C 1.608459 -0.339258 0.277377
C -0.583400 -0.137284 0.282621

C -1.632793 -0.706928 -0.443724
H -2.269815 1.487960 0.257037
H 1.517589 -1.351139 -0.116891
H 1.710923 -0.221713 1.355982

Vibrational frequencies

-451.0487 42.3898 104.1030
135.1103 310.6041 345.4523
598.2029 782.3630 885.2404
900.7865 1058.8630 1194.3431
1212.6553 1521.2673 1671.3260
3112.3396 3202.3574 3263.0382

i13 – i26

Cartesian coordinates

C 1.865512 -0.689385 0.049279
C -0.202724 0.520693 0.018225
C -1.724521 -0.730132 -0.099717
C -1.483756 0.618906 0.057541
H 1.705050 1.410245 -0.135385
H 2.897054 -0.991574 -0.042879
H -2.502709 -1.423738 0.196124

Vibrational frequencies

-811.0019 107.5792 147.8038
209.5824 380.6006 494.8418
555.0342 737.9873 774.9507
831.7180 966.7269 1158.3995
1228.1222 1594.8505 1731.9689
3074.9075 3200.9174 3276.1054

i65 – i27

Cartesian coordinates

C -0.543953 0.819450 0.225519
C -0.389100 -0.618733 0.265292
C 1.038558 -0.771311 0.218129
C 1.444973 0.354390 -0.309019
H -2.250829 -0.326516 -1.020296
H -0.457752 1.528365 1.035976
H 2.342914 0.801184 -0.716132

Vibrational frequencies

-697.6579 278.9606 374.8472
458.2154 622.1218 709.5707
725.6196 771.4271 886.1080
962.5676 998.1014 1096.8057
1188.7835 1545.2760 1703.2892
3220.7599 3241.5343 3243.4153

i63 – i16

Cartesian coordinates

C -1.151143 -0.477765 -0.000004
C 0.629905 0.548270 0.000010
C 1.840010 0.140475 -0.000006
C -0.216880 -1.313743 0.000001
H -1.106171 1.504669 -0.896687
H -1.106189 1.504669 0.896679
H 0.315207 -2.242990 0.000006

Vibrational frequencies

-606.6953 195.3438 237.2823
328.9403 598.1232 676.0381
823.4162 883.1261 964.8699
1035.8582 1131.2216 1234.8503
1471.3340 1796.2445 1922.5273
3102.2514 3159.7607 3399.3184

i53 – i59

Cartesian coordinates

C -0.712065 -0.712609 -0.005210
C 0.027311 0.189016 0.946166
C 0.670850 -0.498136 -0.401902
C -1.214425 0.597573 -0.347260
H -1.199633 -1.648487 0.220460
H -0.902856 1.170268 -1.221228
H -0.427457 1.263761 0.808962

Vibrational frequencies

-816.6514 227.1277 254.2469

478.1450 564.1747 666.5708
801.9056 864.9555 926.2851
979.4369 1019.7594 1060.8558
1206.3868 1276.4474 1831.8026
2573.4067 3151.7979 3246.7834

i14 – i46

Cartesian coordinates

C -0.726737 -1.110498 -0.151843
C -0.239496 1.062958 -0.045136
C 0.952508 0.376520 -0.087389
C 1.883491 -0.472045 0.129198
H -2.302192 0.286822 0.384534
H -0.944852 -2.155237 0.027651
H -0.355298 2.136798 -0.128644

Vibrational frequencies

-756.8052 126.5877 211.8296
432.3765 649.7544 708.1756
818.4546 874.0120 897.0777
1023.7056 1045.6837 1232.0722
1354.5468 1482.0808 1940.8319
3184.1006 3219.6934 3251.6374

i61 – i59

Cartesian coordinates

C 0.007370 -0.389046 -0.750566
C -0.631743 0.808307 0.092895
C 0.805329 0.770192 0.166129
C 1.169638 -0.548709 0.325553
H -1.648361 -1.287579 0.663218
H -0.055012 -0.481781 -1.823060
H -1.296631 1.577703 -0.279164

Vibrational frequencies

-536.9738 420.1854 483.8237
605.4398 676.3916 795.0713
843.0185 874.6193 982.0138
1018.1244 1096.4634 1132.5416
1255.4426 1328.1064 1365.4595
3213.4963 3258.1365 3275.3804

i32 – p8+H

Cartesian coordinates

C -1.620921 -0.342791 -0.304384
C -0.463018 0.284151 -0.092398
C 1.025978 0.070749 0.036901
C 1.764504 -0.985708 -0.029400
H -2.528773 0.248625 -0.322105
H -2.311357 -1.139706 2.211765
H -1.677030 -1.407198 -0.483999

Vibrational frequencies

-317.8532 77.5068 115.5093
134.0261 257.8640 362.3867
389.4147 596.0537 609.9546
824.4086 903.7828 1023.9767
1053.1312 1437.1046 1576.2361
1799.9496 3171.2891 3282.0699

i6 – i32

Cartesian coordinates

C 1.707790 -0.492281 0.004252
C 0.568436 0.405647 -0.024664
C -1.142811 0.122723 0.044698
C -1.803242 -0.979918 -0.022930
H 2.616618 0.111927 0.064664
H 1.744601 -1.115776 -0.890579
H 1.645082 -1.132410 0.887672

Vibrational frequencies

-3250.9820 144.2594 156.0858
303.9228 337.8756 380.4614
818.9577 930.6857 1027.2745
1051.8279 1394.6980 1453.0388
1473.3519 1636.2244 1885.1620
3052.3718 3138.3783 3143.8694

i9 – i54

Cartesian coordinates
 C -1.706040 -0.123663 -0.083269
 C 0.727073 -0.225949 0.038765
 C -0.447721 -0.739720 0.134841
 C -0.978489 0.981215 0.009373
 H 2.331294 1.106233 0.220134
 H 2.742765 -0.616433 -0.382932
 H -2.714033 -0.483604 -0.171174

Vibrational frequencies
 -267.0383 215.8953 304.7504
 420.1476 452.1859 607.0582
 739.4365 742.8814 892.6937
 986.4661 1069.6088 1262.0084
 1442.2752 1582.3444 1824.1704
 3169.7738 3271.4710 3325.6361

i44 – i32
 Cartesian coordinates
 C -1.847988 -0.285067 0.000001
 C -0.440203 0.164345 -0.000009
 C 0.822171 -0.383798 0.000008
 C 2.126116 -0.486484 -0.000004
 H -2.517247 0.574110 0.000051
 H -2.040834 -0.898108 0.882951
 H -2.040874 -0.898035 -0.882992

Vibrational frequencies
 -136.9823 86.8131 245.0791
 351.0097 438.1288 576.5729
 827.2360 997.2478 1033.6329
 1170.2367 1408.4662 1479.1286
 1480.8938 1563.8296 1833.1416
 3063.1002 3137.9027 3167.9067

i63 – i31
 Cartesian coordinates
 C 1.231804 0.695018 -0.000003
 C -1.300213 -0.448890 -0.000002
 C 0.122503 -0.533147 0.000002
 C 1.379949 -0.764537 0.000003
 H 1.326590 1.265731 -0.922190
 H 1.326601 1.265733 0.922181
 H -1.983231 -1.290376 -0.000011

Vibrational frequencies
 -174.3386 166.8034 317.4952
 364.8901 516.7402 733.1828
 745.8331 962.0986 999.9140
 1044.4999 1064.0381 1105.3435
 1501.2413 1638.9230 1928.6740
 3087.9848 3180.8615 3206.0827

i5 – i56
 Cartesian coordinates
 C 0.281596 -0.123871 0.597926
 C -0.012519 1.145247 -0.023060
 C -1.054536 0.256349 -0.326478
 C -1.263734 -0.950751 0.080153
 H 1.309220 -1.163139 -1.013174
 H 2.379823 -0.149670 0.143562
 H 0.246393 2.187122 -0.043415

Vibrational frequencies
 -749.6832 170.9343 223.8317
 320.6137 397.4475 553.4110
 691.0548 934.5486 949.8179
 1016.7959 1053.4012 1222.7811
 1310.8363 1465.5919 1692.4945
 3119.5300 3240.3571 3323.6275

i30 – i40
 Cartesian coordinates
 C -0.612434 -1.323283 0.247642
 C 0.639754 0.487449 0.322976
 C -0.721571 -0.028948 -0.073661
 C -1.897343 0.686468 -0.260927
 H 2.720935 0.387447 0.051840
 H 1.703058 -0.697120 -1.060585

H 0.651267 1.205585 1.135385
 Vibrational frequencies
 -470.7908 128.1028 248.7427
 280.3653 505.1610 623.1135
 811.6856 992.8025 1009.7703
 1033.7949 1078.5708 1280.4185
 1333.6997 1422.8173 1671.6620
 3162.8577 3203.4706 3261.2599

i49 – i59
 Cartesian coordinates
 C 0.211065 -0.640961 0.422770
 C 0.586543 0.824069 0.091494
 C -0.793615 0.463631 -0.063383
 C -1.835534 -0.261213 -0.237361
 H 2.305241 -0.612837 -0.378173
 H 0.149332 -1.130192 1.382493
 H 0.969374 1.568225 0.776260

Vibrational frequencies
 -110.7310 286.9699 471.9770
 707.8750 750.4785 762.7594
 784.3014 884.1431 988.6321
 1037.7739 1101.9973 1138.3488
 1214.9291 1331.5565 1893.9127
 3211.0062 3229.0030 3262.4633

i65 – i7
 Cartesian coordinates
 C 0.884388 -0.697244 -0.045037
 C -0.384629 0.884111 -0.003555
 C -1.482607 0.176970 0.002298
 C -0.593192 -0.879825 -0.091174
 H 1.797194 1.409145 0.088696
 H 1.604129 -1.480452 -0.234200
 H 0.164550 -1.120849 0.990704

Vibrational frequencies
 -1339.5585 439.0134 527.9337
 625.2328 672.3305 736.7400
 885.6095 944.4757 1034.0856
 1163.0348 1212.7163 1266.6524
 1342.7979 1380.2345 1760.9559
 2037.2893 3247.4382 3302.2073

i45 – i51
 Cartesian coordinates
 C 0.617430 0.772740 0.140905
 C -0.635123 -0.019293 0.063002
 C 0.468527 -0.891987 0.447447
 C 1.578585 0.029820 -0.501521
 H -2.794467 -0.422162 -0.298938
 H 0.844872 1.540221 0.877166
 H 1.111790 -1.356712 -0.385700

Vibrational frequencies
 -843.7922 228.3633 265.1602
 447.6548 571.6823 587.3943
 629.3377 691.8369 736.6959
 884.3210 990.9409 1032.3092
 1135.1272 1420.3596 1760.5190
 2699.1853 3156.0272 3306.1153

i20 – i62
 Cartesian coordinates
 C -0.663710 0.789043 0.071353
 C 0.720951 0.666316 -0.183817
 C -0.258765 -0.689474 0.638395
 C -1.194357 -0.494551 -0.430213
 H 2.397054 -0.875129 -0.264018
 H -1.110638 1.594384 0.635802
 H -2.218359 -0.836965 -0.475936

Vibrational frequencies
 -469.6364 321.0610 394.5678
 541.0060 578.8710 587.1157
 716.0878 789.3405 821.9769
 921.2037 1061.4708 1117.0154

1204.8341 1290.8962 1957.2858
 3228.7358 3247.3431 3433.2410

i67 – i20
 Cartesian coordinates
 C 1.203510 -0.544298 0.321966
 C -0.700751 0.668096 0.290477
 C 0.680138 0.775718 -0.081404
 C 0.257372 -0.601867 -0.723897
 H -2.355892 -0.892928 0.194065
 H 1.665960 -1.038458 1.161438
 H 1.139347 1.638753 -0.539386

Vibrational frequencies
 -448.5444 208.3846 356.6942
 508.4120 584.9827 593.2145
 713.9998 800.7233 836.5565
 924.4752 1040.4310 1095.3997
 1193.9459 1269.5138 1917.4282
 3234.7062 3261.6877 3421.5965

i67 – i62
 Cartesian coordinates
 C -1.313114 -0.449848 -0.353611
 C 0.820191 0.739766 -0.418315
 C -0.602839 0.767434 0.187098
 C -0.082256 -0.610769 0.325258
 H 2.194095 -1.019210 -0.029077
 H -2.282089 -0.820884 -0.046753
 H -0.854679 1.473505 0.965211

Vibrational frequencies
 -352.8996 384.3423 492.0027
 591.0215 656.6545 759.0517
 801.5328 901.6284 941.5950
 1013.3881 1106.0322 1140.0147
 1166.6980 1372.5673 1529.6082
 3223.1470 3234.1709 3294.8446

i67 – i24
 Cartesian coordinates
 C 0.758103 0.756174 0.000312
 C -0.631490 0.748622 -0.117566
 C 0.248585 -0.611106 0.498536
 C 1.226101 -0.677789 -0.562070
 H -2.275373 -0.761233 -0.506882
 H 1.339652 1.456645 0.582185
 H 0.135308 -0.817841 1.554973

Vibrational frequencies
 -610.9617 303.7781 434.7417
 499.6220 533.5325 587.7870
 751.8386 805.5343 867.9251
 981.2158 1058.2466 1079.6004
 1201.8097 1229.9037 1865.0204
 3217.5079 3236.0619 3387.6156

i11 – i7
 Cartesian coordinates
 C -0.174729 -1.255596 0.000070
 C -0.964933 1.072472 0.000092
 C 0.402155 0.841974 0.000017
 C 1.456770 0.154305 -0.000085
 H 0.027938 -1.796115 0.922725
 H 0.027805 -1.797063 -0.922054
 H 2.518122 0.037175 -0.000070

Vibrational frequencies
 -933.3832 175.4750 288.9972
 469.8719 489.9742 545.6344
 601.6112 665.7561 905.1243
 998.2697 1055.2210 1100.9279
 1444.8451 1641.7085 1860.9315
 3120.0912 3218.5335 3409.8438

i36 – i35
 Cartesian coordinates
 C -1.283602 0.705266 0.071743
 C 1.148785 -0.527051 0.088436

C	-0.294835	-0.174525	0.028944
C	-1.624115	-0.650320	-0.145538
H	-1.618394	1.724998	0.182256
H	1.356007	-1.367404	-0.589201
H	1.337882	-0.861137	1.123218

Vibrational frequencies
-631.9032 64.8226 255.5504
365.7111 623.8697 775.3110
894.4688 945.3953 997.6789
1087.6594 1126.3813 1233.5124
1342.0904 1406.1559 1768.0349
2977.3956 3025.7930 3268.9789

i54 – i48
Cartesian coordinates
C 0.577470 -0.903934 0.247896
C 0.603664 0.907525 0.165449
C -0.622279 0.064388 0.240980
C -1.884101 0.111810 -0.390992
H 2.529802 -0.070087 -0.595325
H -1.230708 0.153730 1.206623
H -2.303730 -0.908979 -0.338087

Vibrational frequencies
-586.7658 333.9396 399.2709
570.5115 671.7887 722.2417
860.9029 880.8186 947.3548
990.2371 1034.8127 1064.1737
1169.8782 1414.5003 1486.9247
2694.9141 3009.8318 3302.8004

i65 – i67
Cartesian coordinates
C -0.902753 0.737462 -0.010938
C 0.335752 -0.929951 -0.071681
C 1.443098 -0.188359 -0.057750
C 0.497857 0.925275 -0.081026
H -1.850285 -1.333567 0.099485
H -1.670709 1.492050 -0.086285
H 1.307056 0.570121 0.946728

Vibrational frequencies
-1416.6291 330.9865 420.6650
580.4001 673.4095 747.4994
839.6355 869.8854 944.0236
1037.2873 1162.1463 1180.8021
1350.0715 1374.3427 1610.6104
2232.3924 3252.4024 3278.0622

i63 – i35
Cartesian coordinates
C 1.025155 0.574689 0.195228
C -1.331316 -0.411052 0.117621
C 0.107613 -0.457760 0.113575
C 1.461126 -0.693936 -0.242432
H 1.352416 1.526546 0.580689
H -1.805577 -0.379045 1.102174
H -1.823033 -1.100654 -0.568295

Vibrational frequencies
-352.7609 212.3593 322.8665
510.8193 672.5183 867.0437
878.5341 916.0148 971.0382
1057.1831 1105.1477 1216.9925
1248.7211 1462.1734 1630.3238
3056.9797 3137.2128 3278.5525

i27 – i39
Cartesian coordinates
C -1.281632 -0.661651 -0.085030
C -0.071400 0.000001 0.280395
C 1.703518 -0.000001 -0.496692
C 1.264223 0.000001 0.732842
H -1.826455 1.576694 -0.254207
H -1.826454 -1.576695 -0.254202
H 1.654450 -0.000003 -1.570494

Vibrational frequencies

-739.3259	168.0598	295.2923
384.4742	486.4754	651.1651
731.9810	784.3608	906.0710
956.5996	981.9583	1110.3850
1477.0609	1611.3284	1693.2335
3257.4365	3297.6558	3319.2254

i39 – i37
Cartesian coordinates
C 1.354014 -0.564176 -0.273279
C 0.037292 -0.129400 0.147600
C -1.349969 -0.396778 0.318178
C -1.560806 0.613688 -0.514492
H 1.655857 1.596674 0.494828
H 1.999363 -1.289095 -0.740533
H -1.832670 -1.304347 0.669213

Vibrational frequencies
-255.1333 265.8553 292.4928
370.8510 635.0391 673.3145
766.9258 870.3204 932.7048
968.7467 1065.1296 1109.4399
1417.4194 1561.6806 1704.5324
3153.8343 3260.9004 3303.9657

i41 – i59
Cartesian coordinates
C -0.703208 -0.487338 0.354237
C 0.387927 0.575932 0.625421
C 0.654138 -0.705765 -0.193226
C -1.611753 0.318801 -0.422190
H -1.024579 -1.090239 1.197390
H 0.313424 1.654337 0.670760
H -1.282779 0.397325 -1.467451

Vibrational frequencies
-548.3950 244.6295 261.7750
327.4263 450.8717 570.7124
677.3157 845.6557 887.8015
983.3253 1028.3931 1108.0597
1168.0949 1279.1929 1720.9805
3065.9431 3181.1623 3242.0383

i27 – i29
Cartesian coordinates
C -1.317643 0.656011 0.034157
C -0.014375 0.000001 0.002020
C 1.920861 -0.000013 0.432360
C 1.249656 0.000021 -0.688710
H -1.883178 -1.572626 -0.001072
H -1.883189 1.572619 -0.001016
H 0.641224 -0.000032 1.118288

Vibrational frequencies
-901.7597 249.1379 405.2684
472.3699 646.0136 701.3656
721.7111 861.5112 922.9843
930.1475 1010.3997 1089.5140
1419.9539 1579.8188 1679.7429
1894.7827 3262.8738 3305.1929

i63 – i9
Cartesian coordinates
C 1.351810 0.163895 -0.000024
C -0.647898 -0.777227 0.000155
C 0.586143 -1.081964 -0.000074
C 0.479858 1.185472 0.000160
H -1.953730 0.617108 -0.928062
H -1.954977 0.616782 0.927421
H 2.424429 0.311989 -0.000128

Vibrational frequencies
-449.2008 202.1166 422.0357
437.9243 571.4783 649.8412
778.4692 886.6996 1008.1106
1040.8270 1128.0936 1236.9136
1470.9252 1515.6492 1757.9660
3132.9665 3221.9322 3224.5397

i4 – i10
Cartesian coordinates
C 1.304330 0.511313 0.000000
C -1.447770 -0.485793 -0.000004
C -0.229286 -0.844018 -0.000003
C 1.173944 -0.759818 0.000005
H -0.825417 1.421033 0.934893
H -0.825412 1.421042 -0.934881
H 1.858661 1.430740 -0.000022

Vibrational frequencies
-390.9845 352.4299 391.3705
395.6120 462.3572 514.5088
693.7003 765.5738 892.5540
1005.5608 1014.3683 1059.8983
1428.8161 1695.8715 1870.3558
3108.7808 3226.6187 3348.5653

i1 – i9
Cartesian coordinates
C -1.526084 0.803116 -0.078673
C 0.768784 -0.000581 0.096223
C -0.417400 -0.566827 0.115818
C -1.780766 -0.487749 -0.051059
H 2.639545 -0.819048 -0.429484
H 2.655794 0.942991 0.175025
H -0.162713 1.119216 0.109671

Vibrational frequencies
-1572.7939 168.4481 241.0125
307.3577 413.6104 479.2597
739.9800 779.1264 867.5087
924.1491 1014.4106 1288.2507
1432.6610 1510.0979 1728.3169
1758.7596 3160.3172 3263.0894

i3 – i24
Cartesian coordinates
C -1.700926 -0.285021 -0.031306
C 0.549747 0.828656 0.110068
C 1.502684 -0.168010 -0.455672
C 0.854339 -0.958874 0.317749
H -2.683905 -0.555017 -0.366601
H -0.649162 -1.094906 0.394185
H 0.881602 1.604050 0.792210

Vibrational frequencies
-2010.4212 245.0085 302.7921
402.4869 491.6688 592.9480
671.4065 760.1850 842.2322
1001.3198 1031.8058 1135.2268
1310.1425 1478.5649 1731.4873
1928.2857 3181.6967 3344.6086

i10 – i16
Cartesian coordinates
C 1.238900 -1.369899 -0.000015
C -0.615308 -0.113077 0.000008
C 0.844092 -0.138160 0.000031
C 0.648126 1.287079 -0.000009
H -2.895049 -0.279390 -0.000016
H 0.599903 1.816144 0.941327
H 0.599949 1.816098 -0.941372

Vibrational frequencies
-638.0125 98.1894 236.1987
308.2710 346.7927 402.1715
585.3189 652.7805 707.8628
904.3884 966.3720 1022.5816
1430.4166 1857.0994 1983.2393
3169.2509 3297.3182 3474.5348

i38 – p13+H
Cartesian coordinates
C -1.295477 0.536447 -0.074576
C 1.315147 -0.508066 -0.098589
C -0.012707 -0.032433 0.117140
C -1.406688 -0.781298 -0.116013
H -1.656364 1.548882 -0.139297

H 1.710454 -1.504543 -0.198803
H -0.008915 -0.158879 1.834544

Vibrational frequencies

-1089.8210 25.1070 249.3711
321.8950 360.5775 470.9636
550.2114 576.1496 752.4976
818.0203 857.4986 952.3559
1068.5986 1130.5544 1640.8038
1685.4499 3297.0527 3299.3021

i68 – i69

Cartesian coordinates

C 0.132003 -1.055232 -0.010096
C 0.205357 0.931415 -0.009694
C -0.894018 -0.000875 0.538264
C -0.797370 -0.064589 -0.861367
H 2.257067 -0.156074 0.087128
H 0.237714 2.005741 -0.104461
H -1.409132 -0.033871 1.479094

Vibrational frequencies

-329.6427 468.2670 614.8502
668.5390 784.8729 813.1008
831.8549 873.0518 936.1858
954.9972 1010.3932 1111.6674
1331.9518 1343.8207 1388.3951
3204.6813 3257.0975 3333.6416

i54 – i55

Cartesian coordinates

C -1.737946 -0.050523 0.176749
C 0.698176 -0.988703 -0.397879
C 1.290651 -0.016029 0.392498
C 0.564024 1.061970 -0.297202
H -2.341908 0.847177 0.136881
H -2.183228 -0.986039 0.488839
H 1.976689 0.006290 1.231330

Vibrational frequencies

-649.0663 329.2506 355.0732
405.1166 590.1996 697.2630
774.8577 855.9186 936.4345
1009.6773 1048.3965 1207.5232
1334.6464 1426.1144 1471.8012
3166.3116 3217.6030 3281.9073

i44 – i50

Cartesian coordinates

C 1.797142 -0.051736 0.107999
C -0.688933 0.933303 -0.190377
C -1.759729 -0.090619 0.373532
C -0.778952 -0.810901 -0.279859
H 2.217458 -0.764347 -0.605170
H 1.984268 -0.441211 1.113123
H 2.279753 0.920073 0.009985

Vibrational frequencies

-481.2294 121.6627 299.9757
344.6201 609.1079 662.1839
865.7768 921.1664 1031.8173
1100.2593 1322.7621 1399.5647
1470.0928 1471.5319 1658.9620
3055.1487 3126.3166 3166.4475

i65 – i55

Cartesian coordinates

C 1.461175 -0.348659 0.245712
C 0.212720 0.892671 -0.522443
C -0.948047 -0.501912 0.381097
C -1.229294 -0.771518 -0.151310
H 1.478666 -0.486489 1.332309
H 1.427633 1.054181 -0.223103
H -1.175743 0.882744 1.372768

Vibrational frequencies

-1348.7620 200.7455 437.4811
501.1094 684.8031 740.4459
783.9596 844.3624 898.6844

1003.5439 1021.9272 1064.7619
1226.0803 1276.8204 1393.4274
2198.1803 3094.8793 3191.1334

i8 – i66

Cartesian coordinates

C 1.505083 0.084910 -0.066783
C -0.953411 0.667217 -0.044156
C -0.807699 -0.728082 0.510660
C -0.461619 -0.505693 -0.862114
H 1.976303 0.942317 -0.537410
H 2.115069 -0.797801 0.099410
H -1.573259 1.534801 -0.177483

Vibrational frequencies

-375.6850 362.4614 572.0105
689.3643 739.4342 782.3914
820.2928 870.2050 967.8121
996.4292 1056.1375 1151.2343
1289.8320 1460.5263 1619.0733
3143.8583 3245.3009 3308.9544

i11 – p8+H

Cartesian coordinates

C 1.665647 -0.534074 -0.117239
C -0.127912 1.405148 0.237404
C -0.926970 0.251895 -0.058771
C -1.745345 -0.708489 -0.323983
H 1.595135 -1.586064 -0.355582
H 2.641596 -0.085128 0.027091
H -1.010433 -2.264202 1.870576

Vibrational frequencies

-273.5872 28.7245 87.9785
143.9312 248.7625 360.4051
384.7421 584.8559 594.7391
833.5701 917.3084 1035.6539
1046.3899 1438.1353 1676.8246
1830.6536 3171.1223 3280.0838

i54 – i60

Cartesian coordinates

C -1.556056 -0.157769 0.340519
C 0.665380 0.808043 0.114411
C 1.481788 -0.230999 0.230317
C 0.283023 -0.654865 -0.418245
H -1.658799 0.190292 1.363909
H -2.318496 -0.811889 -0.063092
H 2.428026 -0.606560 0.562837

Vibrational frequencies

-489.3468 216.3830 360.3481
522.6809 557.6109 658.2283
708.8082 780.4909 809.1778
1030.1179 1049.7000 1175.2175
1243.6052 1458.5483 1592.6117
3140.8510 3261.5562 3365.2202

i1 – i7

Cartesian coordinates

C -1.150991 0.717749 0.073491
C 0.302303 -0.775227 0.017084
C 1.551303 -0.306986 0.082106
C 1.052603 0.893905 -0.175273
H -1.739429 -1.446510 -0.335370
H -1.729075 1.274437 -0.657951
H -0.890647 1.241505 0.985864

Vibrational frequencies

-509.6966 268.7104 399.1935
444.4850 533.0976 639.4174
709.1580 853.9991 991.1753
1038.0333 1183.5029 1271.1443
1428.1614 1473.2285 1789.2815
3148.0945 3239.0156 3248.3992

i1 – i2

Cartesian coordinates

C 1.520403 -0.727762 0.013827

C 0.042052 0.333688 -0.053913
C -1.243003 0.081445 0.003915
C -2.487377 -0.204421 0.048336
H 1.860117 1.548092 0.275629
H 1.324873 -1.380856 -0.827121
H 1.971322 -1.176077 0.897783

Vibrational frequencies

-405.7085 149.5919 178.3856
361.1913 465.4233 671.9193
752.3029 867.8065 918.0709
995.5343 1152.6192 1257.3658
1479.5226 1716.7445 2097.6006
3122.0687 3235.4107 3243.6007

i50 – p22t+H

Cartesian coordinates

C 1.714259 0.000001 -0.146712
C -0.782815 0.884393 -0.200960
C -1.644843 -0.000002 0.412094
C -0.782815 -0.884392 -0.200966
H 2.262025 -0.933225 -0.151107
H 2.119671 -0.000014 2.273946
H 2.262024 0.933228 -0.151100

Vibrational frequencies

-373.2977 139.2043 152.1554
293.8987 359.1599 616.7277
631.8263 681.2872 738.4938
912.2010 956.1411 1034.7487
1163.3919 1314.5636 1440.1472
1734.5716 3176.4040 3278.6294

i50 – i55

Cartesian coordinates

C 1.488984 0.007398 0.074233
C -0.860349 0.964442 -0.217912
C -0.767919 -0.102526 0.819527
C -0.850999 -0.867205 -0.348341
H 2.090310 -0.899904 0.049755
H 0.464444 -0.085220 1.335541
H 2.038783 0.944974 0.131078

Vibrational frequencies

-1569.4789 305.4825 400.3356
442.9200 534.3512 682.6607
785.9855 941.7918 988.3011
1011.3109 1101.0531 1188.4581
1253.1417 1455.1811 1535.0929
1788.0014 3116.1210 3216.6031

i6 – i9

Cartesian coordinates

C -1.767250 -0.228838 -0.000002
C 0.958952 -0.907432 0.000003
C 1.818695 0.056187 -0.000002
C 0.552500 0.741194 -0.000003
H -2.316593 -0.407684 0.921960
H -0.541847 -1.067320 0.000004
H -2.316574 -0.407686 -0.921976

Vibrational frequencies

-2005.5127 63.3184 281.8817
325.7111 484.4882 518.3365
590.5223 887.3147 936.7151
1036.1005 1201.1497 1239.6121
1373.4262 1481.5244 1694.8931
1998.0828 3108.8226 3194.3705

i4 – i7

Cartesian coordinates

C 0.196071 1.013775 0.000002
C -0.826799 -1.000843 0.000001
C 0.581827 -0.931094 0.000002
C 1.459428 -0.037328 -0.000006
H -2.134406 0.767961 -0.000001
H 0.332128 1.617751 -0.898065
H 0.332122 1.617703 0.898102

Vibrational frequencies

-319.0601 248.9590 396.5047
676.2409 680.9812 807.6265
837.5218 911.8313 1085.9303
1107.9817 1152.7325 1223.7628
1388.3163 1580.4150 1879.9133
3097.1003 3175.0822 3248.2406

i65 – i7

Cartesian coordinates

C -0.760564 0.785982 -0.066624
C 0.336980 -1.178761 0.046344
C 1.236527 -0.227805 -0.059580
C 0.716538 0.998011 -0.043629
H -1.902435 -1.141242 0.054610
H -1.499936 1.562771 -0.210563
H -0.080104 1.142892 1.002512

Vibrational frequencies

-1373.5541 396.3697 565.5308
639.9739 773.3594 798.8265
863.0566 1021.7360 1039.6835
1154.9126 1189.1808 1310.4991
1380.3178 1384.0721 1402.6188
2096.2424 3229.0959 3251.4394

i4 – i7

Cartesian coordinates

C -0.698244 0.921452 0.000004
C 0.000871 -1.029969 -0.000015
C 0.700724 0.368205 -0.000034
C 1.901236 -0.075519 0.000025
H -2.226106 -0.928671 0.000026
H -0.924746 1.489987 -0.903419
H -0.924699 1.489991 0.903437

Vibrational frequencies

-302.9023 209.7681 426.6229
664.5251 666.3161 792.8047
884.7379 939.2573 961.0100
1123.8945 1152.0567 1210.6713
1453.4624 1613.7265 1908.6547
3082.3915 3154.9115 3274.4829

i67 – i26

Cartesian coordinates

C 1.276556 -0.615954 0.171630
C -0.386175 0.577419 -0.171247
C -1.569090 0.082079 0.195808
C -0.615232 -0.829883 -0.339973
H 1.709084 1.555839 -0.001027
H 2.137783 -1.215095 0.453183
H -2.501644 0.274119 0.708160

Vibrational frequencies

-681.7972 269.8911 444.5622
596.8791 688.4016 727.8654
815.5314 875.4290 920.9429
940.8750 1035.5021 1125.1401
1224.9860 1547.7233 1716.9319
3179.9876 3226.0453 3233.9224

i22 – i45

Cartesian coordinates

C -0.519992 0.889204 -0.037930
C 0.660025 0.089434 -0.041663
C -0.527835 -0.828441 -0.362301
C -1.587905 -0.406763 0.275806
H 2.766273 -0.665356 0.118098
H -1.708607 0.654470 0.793914
H -0.772535 1.521605 -0.886354

Vibrational frequencies

-1324.7512 234.7939 323.8770
492.5286 555.2076 609.2772
647.0374 690.7335 724.6072
943.5969 996.6485 1021.9640
1196.4253 1616.6127 1786.8593
2542.9684 3149.9721 3338.0678

i15 – i24

Cartesian coordinates

C 1.761706 0.616523 -0.148722
C -1.060593 -0.120264 -0.065014
C 0.208026 -0.661843 -0.233544
C 1.377160 -0.280313 0.622698
H -3.151997 0.728375 0.212065
H 2.124990 1.406143 -0.772411
H 0.359907 -1.442027 -0.968923

Vibrational frequencies

-566.8491 150.9264 231.4632
415.6055 563.3003 570.0879
607.4370 661.1368 715.2426
861.3199 954.9829 1142.0917
1314.2135 1837.0272 2108.3268
3203.8377 3417.2922 3478.4321

i9 – i10

Cartesian coordinates

C 0.921935 0.810878 0.121172
C -0.962216 -0.716348 0.198241
C 0.379462 -0.676153 0.188469
C 1.548775 -0.341289 -0.361577
H -2.570876 0.795958 -0.162368
H -0.422971 1.127409 -0.477317
H 1.219112 1.553464 0.856071

Vibrational frequencies

-1802.9762 305.8288 415.6762
468.1772 525.9805 649.5124
691.3607 872.3250 916.4132
998.3754 1080.2660 1172.1140
1263.4930 1533.8883 1638.3212
1750.9038 3189.0375 3295.1624

i63 – i7

Cartesian coordinates

C -0.161518 -1.105658 -0.084666
C 0.555262 1.081523 0.022977
C -0.717363 1.025527 0.020406
C -1.258478 -0.337105 -0.113164
H 1.740877 -0.549738 0.895193
H 1.791929 -0.497992 -0.871996
H -1.036218 -1.121154 0.896637

Vibrational frequencies

-1250.0191 272.6787 396.2749
487.2745 617.9234 779.4481
812.0003 861.2025 977.2345
1014.4997 1103.2085 1185.0788
1415.7004 1542.0407 1562.0259
2236.5408 3098.2607 3150.5025

i3 – p3+H

Cartesian coordinates

C -2.390978 -0.123385 0.000038
C 0.179993 0.061462 -0.000036
C 1.483518 -0.046847 -0.000009
C 2.754324 -0.184753 0.000047
H 0.244415 2.184230 -0.000123
H -2.949946 -0.172043 -0.930200
H -2.949787 -0.171626 0.930393

Vibrational frequencies

-728.6168 142.2492 144.7256
193.9214 275.7143 278.9026
350.6573 467.2368 574.2166
769.0258 973.9830 1033.1632
1368.6171 1521.4837 1993.4011
2200.3606 3137.7479 3227.4837

i3 – i63

Cartesian coordinates

C 0.165824 -0.844948 0.000005
C 0.215156 1.313610 0.000003
C -0.983333 0.790928 -0.000004
C -1.129421 -0.666668 -0.000001

H 1.958119 -0.204770 0.929365
H 1.958113 -0.204790 -0.929376
H -1.970437 -1.339973 0.000005

Vibrational frequencies

-497.1428 190.4639 311.5880
391.6341 568.7838 620.1536
837.1006 869.5807 975.4653
999.0551 1126.2260 1228.3601
1443.2552 1538.6479 1833.3398
3159.5776 3255.5610 3279.1598

i2 – p5

Cartesian coordinates

C -1.375342 -0.556100 -0.220842
C -0.106422 0.058763 -0.034414
C 1.224989 0.003123 -0.009598
C 2.485638 -0.051533 0.023039
H -1.842999 1.684448 0.217218
H -1.662115 -1.569678 1.458188
H -1.950699 -1.361105 -0.650122

Vibrational frequencies

-849.5849 139.6895 167.4599
236.0910 396.3724 498.5195
529.7919 740.7420 810.2101
937.1351 963.5016 982.3487
1139.8791 1436.6401 1665.2651
2108.4111 3266.7879 3301.7761

i13 – p2s+H

Cartesian coordinates

C -1.306636 0.070347 0.000000
C 0.000000 -0.034856 0.000000
C 1.306534 0.071659 0.000000
C 2.537096 0.146909 0.000000
H 3.598140 0.221728 0.000000
H -3.598383 0.218232 0.000000
H 0.001897 -2.830985 0.000000

Vibrational frequencies

-277.4583 113.9261 128.1618
159.0619 395.7694 397.1945
409.7048 414.9081 477.8446
480.5266 510.3429 513.4516
760.5762 1562.6603 1683.5356
1970.1234 3459.5081 3466.8901

i6 – p3+H

Cartesian coordinates

C 2.293591 -0.190141 0.000001
C -0.281910 -0.064713 -0.000001
C -1.579696 0.008055 0.000000
C -2.855312 0.099263 0.000001
H 2.852965 -0.241092 -0.929898
H 2.852958 -0.241096 0.929903
H 2.977772 2.160689 0.000002

Vibrational frequencies

-411.5942 113.7399 141.8822
180.8252 270.9438 283.0919
293.7347 477.8083 600.0033
768.3047 970.7787 1037.4182
1369.2013 1516.8039 1981.2996
2183.6293 3136.5680 3227.9675
180.8252 270.9438 283.0920

i22 – i10

Cartesian coordinates

C 0.684344 0.872739 -0.000004
C -0.728393 -0.205167 -0.000031
C 0.529177 -0.744235 -0.000010
C 1.762524 -0.368765 0.000025
H -2.881277 0.478588 0.000035
H 0.658794 1.421298 -0.934513
H 0.658759 1.421310 0.934497

Vibrational frequencies

-534.1622 212.9047 297.8384

478.1413 502.3090 552.8575
 633.6273 893.8069 927.3137
 973.9542 1041.1739 1044.0673
 1475.5051 1734.2862 1888.2421
 3134.4183 3260.1853 3388.4618

i63 – i67

Cartesian coordinates

C -1.024378 -0.579464 -0.047373
 C 1.317026 -0.071059 0.048036
 C 0.414890 0.949731 -0.071454
 C -0.894636 0.919936 -0.050453
 H -1.240833 0.229634 0.977649
 H -1.934081 -1.140183 -0.196918
 H 2.388842 -0.149302 0.041282

Vibrational frequencies

-1300.4387 343.0717 448.3802
 525.2031 581.2203 734.9679
 841.6617 973.5256 1040.1894
 1084.9993 1156.7327 1232.0029
 1252.2686 1416.1205 1619.0366
 2165.9684 3265.3748 3313.6267

i15 – p2+H

Cartesian coordinates

C -2.537181 -0.145721 0.000000
 C 0.000000 0.034903 0.000000
 C 1.306588 -0.070996 0.000000
 C 2.537181 -0.145721 0.000000
 H -3.598258 -0.220064 0.000000
 H 0.000000 2.831313 0.000000
 H 3.598258 -0.220064 0.000000

Vibrational frequencies

-277.8483 113.9184 128.0825
 158.9803 395.7701 397.1905
 409.7065 414.9126 477.8488
 480.5297 510.3879 513.4604
 760.5677 1562.6352 1683.5401
 1970.1230 3459.5065 3466.8881

i13 – i14

Cartesian coordinates

C -1.895066 -0.740646 0.011416
 C 0.080220 0.586354 -0.126994
 C 1.272125 0.015622 -0.026459
 C 2.526779 -0.420644 -0.034182
 H -1.939554 1.369738 0.021886
 H -2.873021 -1.196291 0.052208
 H 0.984213 0.453871 1.041517

Vibrational frequencies

-1198.0765 121.6529 165.7525
 267.8588 316.1718 405.6261
 441.3011 609.0701 724.0227
 860.4929 868.8491 1266.5042
 1329.7734 1595.0641 1665.7567
 2505.6160 3106.3907 3278.4532

i63 – i16

Cartesian coordinates

C -0.317103 -0.781327 0.000726
 C 0.874966 0.858066 -0.000400
 C -0.350104 1.294207 0.000374
 C -1.478004 -0.384194 -0.000464
 H 1.628808 -1.001832 0.894980
 H 1.627733 -1.002401 -0.895507
 H -2.539946 -0.295525 -0.000290

Vibrational frequencies

-465.2248 272.2756 316.4819
 326.9693 588.5650 684.3361
 740.8532 891.9099 955.8572
 1058.4204 1134.0914 1233.6614
 1472.1570 1595.3602 2063.5460
 3103.7209 3158.9178 3451.0491

i27 – i45

Cartesian coordinates

C 0.732217 0.905959 -0.009411
 C -0.796654 -0.216926 0.057800
 C 0.455165 -0.861933 0.246339
 C 1.548107 -0.142866 -0.213936
 H -2.963420 0.419572 -0.268073
 H 0.685315 1.717987 0.709435
 H 2.591960 -0.382678 -0.325668

Vibrational frequencies

-572.2650 221.1429 313.8344
 343.8422 466.5025 584.3883
 630.4085 710.2679 777.0224
 908.6396 959.5815 1097.1211
 1221.3310 1540.0784 1927.8309
 3178.4909 3285.6446 3470.9178

i11 – p2+H

Cartesian coordinates

C -2.433651 -0.245935 0.000000
 C 0.102754 -0.082714 0.000000
 C 1.408676 0.011309 0.000000
 C 2.638729 0.099147 0.000000
 H -3.310554 2.535624 0.000000
 H -3.490314 -0.367035 -0.000001
 H 3.699385 0.178987 0.000000

Vibrational frequencies

-257.7052 89.2996 120.4901
 137.3213 397.9535 399.9646
 457.4591 461.5692 462.8830
 483.4910 509.8760 516.0382
 762.6298 1573.7467 1655.0271
 1968.4450 3458.5106 3466.3728

i11 – i7

Cartesian coordinates

C 1.344071 -0.468467 0.000004
 C -0.914143 0.622708 -0.000021
 C -1.294680 -0.816883 0.000013
 C -0.024144 -0.869354 -0.000037
 H 0.687992 2.251484 -0.000098
 H 1.895270 -0.517773 -0.931958
 H 1.895354 -0.518205 0.931891

Vibrational frequencies

-844.3238 181.2041 276.7510
 292.3605 470.6749 518.0831
 522.0191 662.9957 854.4751
 884.2017 995.0376 1031.7543
 1432.0999 1717.2257 1855.1861
 3154.4286 3262.4395 3373.7991

i1 – i3

Cartesian coordinates

C -2.401033 -0.075472 -0.061131
 C 0.207447 0.056708 0.139008
 C 1.521055 -0.027902 -0.009727
 C 2.789868 -0.076234 -0.087184
 H -0.362410 1.141411 0.320717
 H -2.990146 0.773298 -0.381371
 H -2.900292 -1.004320 0.187189

Vibrational frequencies

-1067.9917 141.8227 145.8395
 311.6017 339.6890 457.4832
 557.0793 744.0851 754.2009
 877.6292 1016.5854 1307.8164
 1458.0050 1925.1734 2085.4025
 2304.5892 3171.3235 3271.5742

i11 – i10

Cartesian coordinates

C -1.955633 0.563145 0.000003
 C -0.126044 -0.403944 -0.000014
 C 1.195199 -0.062105 0.000018
 C 2.360929 0.241920 0.000022
 H -2.149611 1.064631 0.938562
 H -2.148921 1.065077 -0.938458

H 3.391561 0.506518 0.000016

Vibrational frequencies

-631.6152 173.3531 208.2197
 228.4748 449.3935 476.2374
 571.7440 622.4487 766.4174
 867.3538 968.4472 1111.8774
 1423.5537 1932.1901 2235.8460
 3164.9472 3290.0673 3480.5175

i13 – i15

Cartesian coordinates

C 2.567698 -0.179923 0.000061
 C -0.028304 -0.139195 -0.000105
 C -1.349958 -0.034614 -0.000026
 C -2.573271 0.021150 0.000050
 H 3.385831 0.525679 0.000132
 H 0.819745 1.134339 -0.000098
 H -3.635780 0.070591 0.000181

Vibrational frequencies

-1883.0661 103.4599 146.9556
 401.2906 418.2594 419.3263
 503.2050 515.8244 592.7090
 600.5851 652.2300 778.4715
 1448.2923 1702.0319 1948.8543
 2448.9260 3270.4733 3466.6545

i8 – i9

Cartesian coordinates

C -1.948892 0.078906 -0.095754
 C 0.981529 0.765753 -0.027205
 C 1.801549 -0.280520 -0.251521
 C 0.518936 -0.727709 0.259189
 H -2.331020 1.089493 -0.028413
 H -2.640411 -0.721876 -0.333554
 H 0.916710 1.731691 0.451076

Vibrational frequencies

-529.9745 227.5710 251.7260
 495.4477 525.2988 613.1828
 794.4166 833.6717 848.8773
 941.4547 1016.5034 1122.3806
 1422.1268 1487.3887 1860.6930
 3164.3730 3258.3803 3261.9751

i12 – i16

Cartesian coordinates

C -1.124806 0.099014 0.014589
 C 1.343057 0.013919 -0.032718
 C 2.447181 -0.609479 0.014478
 C -2.227823 -0.442857 -0.081638
 H 0.152556 1.797930 -0.169918
 H -0.638519 0.455104 1.106881
 H -3.183706 -0.897352 0.040217

Vibrational frequencies

-1305.0311 129.3978 220.0768
 295.6690 386.4415 464.7825
 578.3737 669.0702 752.1895
 918.6548 964.8216 1151.5322
 1342.9808 1948.5150 2057.6917
 2102.3653 3151.3266 3449.5943

i15 – i16

Cartesian coordinates

C 1.178522 0.093354 0.017670
 C -1.307698 0.009212 0.089549
 C -2.421316 -0.615962 0.012201
 C 2.265107 -0.424261 -0.005585
 H -0.115424 1.808191 0.104905
 H -0.898295 0.368032 -1.029661
 H 3.220868 -0.892033 -0.018788

Vibrational frequencies

-1391.3458 129.5875 283.0573
 294.3169 324.0557 569.9436
 599.3412 663.7658 740.3039
 847.8668 931.6191 1119.3312

1345.8389 1901.4681 2184.2512
2270.9854 3169.3609 3477.3452

i11 – i9

Cartesian coordinates

C	1.925667	0.572728	0.000000
C	-0.964120	-0.088268	0.000001
C	0.247429	-0.352655	0.000000
C	1.649138	-0.649858	-0.000001
H	-2.832058	0.263869	0.930409
H	-2.832054	0.263872	-0.930412
H	2.227978	1.599279	0.000000

Vibrational frequencies

-563.4239 173.2509 228.9294
286.5338 408.3658 424.2937
566.8070 747.0950 807.4941
864.6412 1028.8234 1328.1428
1483.6966 1759.2675 2018.4470
3150.9650 3244.7712 3411.1021

i27 – i29

Cartesian coordinates

C	-1.461183	0.659970	-0.032882
C	-0.188590	0.000020	0.019536
C	1.187847	0.000104	0.003662
C	2.478566	-0.000106	-0.119977
H	-2.021148	-1.579082	-0.093823
H	-2.021224	1.578980	-0.093997
H	0.709420	0.000418	1.162599

Vibrational frequencies

-906.8042 140.3268 258.2965
424.0176 535.0377 537.2591
703.6590 713.8436 907.2326
936.4136 966.7391 1093.0338
1410.7222 1658.6430 1874.4866
2123.1069 3266.7818 3309.3400

i21 – p6+H

Cartesian coordinates

C	-1.314368	0.536820	-0.063144
C	1.314368	0.536820	-0.063145
C	0.000001	0.014029	0.114563
C	-1.399226	-0.780069	-0.126012
H	-1.727975	1.529511	-0.121927
H	1.727977	1.529510	-0.121927
H	0.000000	-0.224205	1.826356

Vibrational frequencies

-1091.8486 169.3256 215.3211
265.0254 368.7508 470.9133
556.0804 594.1711 760.4915
807.1496 946.8044 961.7091
1013.7399 1070.7141 1632.1605
1659.4880 3289.2238 3293.1340

i65 – i63

Cartesian coordinates

C	1.123404	-0.411616	-0.033048
C	-1.305437	-0.106862	-0.031365
C	-0.451954	0.959177	0.035888
C	0.847144	0.966655	-0.016122
H	2.035431	-0.973775	-0.169215
H	0.505666	-1.008660	0.984874
H	-2.363866	-0.258811	0.061377

Vibrational frequencies

-1282.3331 393.5783 496.0484
555.1558 706.7135 719.6228
882.5715 909.8760 1136.8511
1173.0889 1176.9427 1254.0668
1311.7633 1351.1288 1609.2611
2083.1414 3256.8288 3327.7460

i13 – i26

Cartesian coordinates

C	1.754864	-0.716107	-0.110424
C	-0.127461	0.764173	-0.117391

C	-1.120500	-0.226429	0.193801
C	-2.371740	-0.165638	-0.190501
H	1.912688	1.358357	0.267331
H	2.707064	-1.184935	-0.315456
H	-0.938170	-1.136861	0.793916

Vibrational frequencies

-290.9120 77.1775 170.2029
328.5757 363.2724 610.7013
705.9111 771.3409 836.2743
920.2079 983.1785 1245.9252
1283.8908 1410.7806 1689.1242
2979.2543 3088.0944 3250.1243

i1 – i12

Cartesian coordinates

C	-1.989454	-0.435286	0.044783
C	0.043480	-0.099667	-0.138668
C	1.348497	-0.023224	-0.004108
C	2.623049	-0.059652	0.086196
H	-1.343712	1.695095	0.082242
H	-3.032227	-0.598257	0.311594
H	-0.735301	-1.176970	-0.174336

Vibrational frequencies

-2233.3468 63.1393 169.4514
199.8980 490.6507 617.1045
731.9570 866.2403 951.4613
1037.8007 1070.2584 1193.0012
1486.1935 1553.0471 1950.2921
2035.4230 3172.7055 3236.7043

i65 – i46

Cartesian coordinates

C	0.093966	0.970675	-0.000001
C	-0.811202	-0.901439	0.000000
C	0.604546	-0.564851	0.000004
C	1.798282	-0.112126	-0.000002
H	-2.160944	0.930324	0.000000
H	0.545009	1.947823	0.000002
H	-1.303333	-1.859696	-0.000007

Vibrational frequencies

-148.6824 205.9163 468.2128
529.8955 631.4862 696.9283
786.9085 849.5272 935.2610
964.8846 1129.8806 1182.9366
1304.3658 1424.6507 1928.1485
3252.3843 3294.5752 3313.0335

i13 – i15

Cartesian coordinates

C	2.340218	-0.403312	-0.131942
C	-0.026121	0.723833	-0.149770
C	-1.246987	0.090551	-0.024629
C	-2.374119	-0.353381	0.020247
H	3.291008	-0.694119	0.262502
H	0.852646	0.532664	1.107392
H	-3.353614	-0.765610	0.062323

Vibrational frequencies

-818.2309 135.0331 228.4380
326.6792 414.2077 443.1696
496.3677 544.1551 583.7025
778.3421 792.7234 880.6236
1291.3569 1845.1225 2116.6623
2400.3274 3386.7949 3477.7448
326.6793 414.2077 443.1696

i13 – i11

Cartesian coordinates

C	-2.569720	-0.191288	-0.063448
C	0.043277	-0.161210	-0.047325
C	1.363045	-0.030803	-0.005520
C	2.584745	0.032417	0.036001
H	-1.611307	1.136041	-0.312593
H	-3.173141	0.311872	0.705180
H	3.645417	0.096662	0.074763

Vibrational frequencies

-933.6353 90.2402 136.5201
377.5319 398.2343 467.3661
529.0747 543.9380 582.7111
751.8180 833.6202 998.7916
1345.5275 1814.7760 1982.7117
2621.3614 3071.3865 3471.8399

i14 – p4+H

Cartesian coordinates

C	1.987866	-0.695950	0.000178
C	-0.180240	0.752482	0.000224
C	-1.305848	0.040357	-0.000091
C	-2.401666	-0.619091	-0.000410
H	2.122349	1.764717	-0.000764
H	2.844869	-1.328807	0.000218
H	-0.220931	1.839683	0.000616

Vibrational frequencies

-872.9137 31.5922 146.7957
225.9922 351.8437 357.5442
528.4128 603.2576 661.5095
768.1420 903.2083 971.4745
1175.0681 1399.8799 2056.5846
2117.9406 3165.5027 3460.8952

i29 – p5+H

Cartesian coordinates

C	1.414267	-0.662882	-0.080701
C	0.173335	-0.000011	0.059267
C	-1.175561	-0.000010	-0.002326
C	-2.428263	0.000024	-0.172526
H	1.961456	1.588551	-0.155196
H	1.961514	-1.588490	-0.155370
H	-0.311125	-0.000263	1.972047

Vibrational frequencies

-886.1822 161.9227 200.6681
255.3032 419.4123 496.6425
511.3292 741.0018 784.3865
960.8119 971.5944 976.1915
1148.8809 1460.0874 1687.8213
2085.7576 3274.6084 3313.8326

i16 – p4+H

Cartesian coordinates

C	-1.135966	0.044018	-0.061913
C	1.294947	-0.029760	-0.055438
C	2.406686	-0.634650	0.113908
C	-2.229960	-0.433979	0.072669
H	0.154932	1.627157	-0.687533
H	0.181141	1.804169	1.593250
H	-3.192347	-0.871357	0.198182

Vibrational frequencies

-641.5171 136.8374 184.3103
242.9434 308.8298 318.2366
397.7196 597.0248 726.1885
774.5263 909.3919 965.2347
1152.6927 1390.2259 2033.3431
2227.3454 3143.9982 3476.2660

i65 – i45

Cartesian coordinates

C	0.217390	0.726562	0.303465
C	-0.621393	-0.590967	0.084138
C	0.712730	-0.937131	0.210616
C	1.306344	0.249638	-0.424418
H	-2.352789	0.351753	-0.915632
H	0.101444	1.295804	1.215648
H	2.325364	0.582807	-0.536107

Vibrational frequencies

-616.7132 319.4713 377.2850
512.3491 580.3899 656.5454
747.0351 781.8907 838.1218
983.6705 1075.3340 1131.1742
1146.2374 1295.8165 1805.1103
3230.3898 3257.3773 3283.5509

i26 – p13a+C2H2

Cartesian coordinates

C	2.228731	0.446967	-0.084597
C	-0.610868	-0.088506	0.157161
C	-1.677544	0.683549	0.043408
C	-1.811047	-0.719181	-0.184844
H	1.331334	-1.597316	0.165155
H	2.679903	1.403673	-0.205735
H	-2.203604	1.626051	0.064966

Vibrational frequencies

-416.7759 38.8720 94.0537
106.5046 261.7135 614.6623
691.3215 787.7109 806.7843
880.7526 900.2816 1056.0383
1203.0636 1665.5821 1952.1791
3268.7775 3395.9200 3489.7734

i9 – i26

Cartesian coordinates

C	2.172225	-0.085288	-0.284762
C	-0.380132	-0.025796	0.039521
C	-1.597170	0.545410	-0.067378
C	-1.597693	-0.834487	-0.009204
H	1.619040	1.046745	0.272107
H	3.119052	-0.067461	0.258607
H	-2.140282	1.473640	-0.148721

Vibrational frequencies

-1083.0073 181.9023 195.3621
378.1402 488.0584 662.9017
721.3986 844.3928 882.4616
981.7866 1076.7843 1223.6956
1287.5081 1615.7849 1824.8850
2328.5259 3124.7281 3274.3617

i1 – i6

Cartesian coordinates

C	-2.343890	-0.191593	0.012724
C	0.242661	0.047857	0.047440
C	1.537716	-0.005692	0.012351
C	2.814555	-0.094263	-0.038252
H	-1.621044	0.775526	-0.802276
H	-3.150313	0.499920	0.229169
H	-2.597729	-1.208537	-0.278920

Vibrational frequencies

-1500.0858 121.7204 146.1978
238.4622 359.7769 518.1179
584.5146 771.5112 831.5782
1000.7763 1070.9249 1319.4826
1485.5714 1850.1517 2090.7341
2323.8703 3120.7146 3239.4204

i12 – i13

Cartesian coordinates

C	-2.188921	0.555429	-0.048867
C	0.087178	-0.294424	-0.016589
C	1.376067	-0.015914	0.017561
C	2.682706	0.188031	-0.057720
H	-1.628550	-1.475190	0.104370
H	-3.267779	0.604381	-0.028901
H	0.801168	0.926870	0.451878

Vibrational frequencies

-1159.5300 108.9279 153.8069
274.6684 348.3293 370.1224
482.8824 522.3880 734.6532
786.2518 915.6587 1200.2364
1337.7126 1460.1568 1752.8845
2530.3617 3074.7215 3265.5087
1337.7126 1460.1569 1752.8845

i8 – i26

Cartesian coordinates

C	-1.875296	0.043542	-0.375675
C	0.677836	0.781349	-0.046295
C	1.582733	-0.296291	-0.425275

C	0.634465	-0.805557	0.379889
H	-1.177501	0.375645	1.184183
H	-2.317565	-0.950657	-0.188468
H	1.004126	1.730503	0.375851

Vibrational frequencies

-475.3617 325.4147 385.5999
564.2712 619.1353 708.1832
783.3075 832.7744 919.7780
965.6032 1008.0143 1054.4095
1135.5757 1428.6628 1456.7859
2690.3194 3020.3067 3144.0635

i3 – i5

Cartesian coordinates

C	-1.750348	-0.538732	-0.010520
C	0.270682	1.176619	0.023987
C	1.094400	0.067931	0.050025
C	1.753960	-1.036842	0.002570
H	-1.700187	-1.546811	-0.398548
H	-2.681301	-0.174409	0.410138
H	0.398175	2.186921	-0.335822

Vibrational frequencies

-479.5213 174.6586 305.3782
350.2413 398.0268 570.6345
663.2309 809.2777 956.9834
984.3294 1102.3856 1203.2627
1417.4229 1757.9903 1912.0882
3164.0380 3247.4461 3269.2038

i27 – i10

Cartesian coordinates

C	-1.457510	0.788546	-0.115952
C	-0.357729	-0.046851	-0.067728
C	1.045562	-0.009015	-0.012861
C	2.243414	0.044261	0.021662
H	-2.348382	-0.373130	-0.054177
H	-1.809061	1.522705	0.609377
H	3.305846	0.085198	0.056686

Vibrational frequencies

-780.5904 199.9243 224.2049
489.7384 550.5423 619.8761
696.2616 720.0100 811.3053
866.0996 895.9797 937.6513
1248.3319 1677.3037 2263.2989
2558.1790 3123.2570 3482.8389

i26 – p1+H

Cartesian coordinates

C	1.561337	-0.582577	-0.037404
C	0.390070	0.041123	0.008833
C	-1.011894	0.003318	0.095806
C	-2.185827	-0.050140	-0.205475
H	2.107356	-1.512969	-0.016822
H	-3.236144	-0.084243	-0.374332
H	-0.880137	0.189583	1.986475

Vibrational frequencies

-894.9946 66.0720 220.5427
243.7182 449.1738 535.4039
543.0894 664.7768 683.7282
736.1289 915.6181 949.5371
1138.0832 1299.5955 1748.0372
2144.3664 3269.2274 3470.7715

i65 – i26

Cartesian coordinates

C	-1.241746	0.623122	0.195380
C	0.375870	-0.609720	-0.138428
C	0.781030	0.748107	-0.146645
C	1.651960	-0.332967	0.276747
H	-1.741517	-1.514612	-0.173323
H	-2.126178	1.248818	0.315097
H	0.904992	1.695927	-0.645331

Vibrational frequencies

-1132.6393 259.9498 436.6956

618.8091 651.3711 670.0444
791.0578 839.1081 922.8529
930.1282 983.8857 1098.5794
1199.4706 1578.9512 1591.1029
3148.6714 3236.0236 3259.8694

i4 – p23+H

Cartesian coordinates

C	-0.388206	0.722418	0.341626
C	-0.501712	-1.094998	0.076407
C	0.732652	-0.189713	0.093443
C	1.990364	-0.052725	-0.184678
H	-2.415912	0.034565	-0.487834
H	0.049679	2.580504	-1.032397
H	-0.450076	1.391584	1.195615

Vibrational frequencies

-465.6091 152.9991 182.1841
209.1992 255.3536 559.4265
665.6496 681.0987 822.4075
881.7617 989.9707 1051.9530
1185.5291 1290.0089 1450.5664
1820.9016 3174.5805 3288.3149

i9 – p12+H

Cartesian coordinates

C	1.686331	0.406203	-0.315523
C	-0.933987	0.015708	-0.010563
C	0.353580	-0.078097	-0.056293
C	1.584966	-0.845466	0.156603
H	-2.830078	-0.732515	0.413033
H	-2.751988	0.994356	-0.281144
H	2.829199	2.169663	0.965756

Vibrational frequencies

-365.9722 40.5348 78.1710
102.5395 208.1383 359.0390
454.1938 566.0424 613.2920
723.4053 961.0155 1002.2647
1288.5774 1431.6646 1582.7650
2041.6181 3127.5310 3214.1706

i9 – p1+H

Cartesian coordinates

C	1.613896	0.585543	-0.024692
C	-0.939868	-0.034006	-0.137433
C	0.445291	-0.050802	-0.035036
C	1.650322	-0.812578	0.133986
H	-2.676148	0.461017	1.766163
H	-3.194774	-0.046057	-0.354416
H	2.146478	1.521553	-0.091713

Vibrational frequencies

-727.6259 42.1091 176.9738
202.2633 373.1819 536.5802
543.1823 630.4235 712.8024
836.2263 906.9951 950.8651
1132.9599 1293.2923 1743.1275
2169.0575 3268.6419 3461.6678

i10 – p1+H

Cartesian coordinates

C	-1.496402	0.489219	-0.200648
C	1.089474	-0.001934	-0.006103
C	-0.298260	-0.093896	-0.032730
C	-1.465117	-0.909104	0.071365
H	3.351133	0.131718	0.047645
H	-2.021833	1.218610	1.446485
H	-2.042362	1.321572	-0.619481

Vibrational frequencies

-911.3815 175.8348 201.2862
254.4656 429.1295 536.1812
579.5480 662.0041 704.6768
772.9135 907.2106 976.1400
1121.0444 1274.0095 1695.6780
2226.4503 3247.7236 3480.4789

i1 – i65

Cartesian coordinates
C -1.229598 0.757352 0.068133
C 0.236337 -0.822675 -0.138871
C 1.491616 -0.434268 0.127731
C 1.235097 0.821775 -0.079596
H -1.883812 -1.367985 -0.030184
H -2.143363 1.293563 -0.183622
H 0.469983 1.630665 0.058603

Vibrational frequencies
-895.4838 233.7656 298.4022
337.2665 400.6932 484.7563
539.1936 622.0246 793.6584
875.8422 1003.3169 1211.0083
1364.3863 1475.1637 1588.1365
2869.7362 3156.6556 3187.0847

i63 – i60
Cartesian coordinates
C -0.644394 0.932610 -0.193718
C 0.659836 0.897826 0.107846
C 0.110893 -0.755468 -0.456782
C -1.237654 -0.372412 0.211801
H 2.276754 -0.754135 0.284228
H -2.141412 -0.681970 -0.304045
H -1.221016 -0.651164 1.268591

Vibrational frequencies
-525.2119 427.4145 461.6248
572.9678 653.0200 761.7693
909.7903 969.9081 1007.0870
1081.9022 1115.9495 1165.5647
1355.0749 1428.0883 1483.0313
3074.0637 3197.9845 3313.1649

i13 – i11
Cartesian coordinates
C 1.630223 -0.730265 -0.000364
C -0.863813 -0.052347 -0.030363
C 0.087774 1.035470 -0.045982
C 1.323069 0.527748 0.068027
H -2.934922 -0.930193 0.074516
H 0.105005 -1.061383 -0.014953
H 2.523627 -1.334587 -0.100053

Vibrational frequencies
-2039.6990 36.8900 217.5430
289.4390 440.8243 547.5658
675.6017 718.8409 796.9826
830.4344 937.3679 1014.6590
1320.1075 1497.1321 1648.3388
1724.9428 3245.2336 3349.6053

i2 – i27
Cartesian coordinates
C -0.862351 0.793358 0.162547
C -0.128088 -0.442700 0.297969
C 1.252171 -0.606236 0.291743
C 1.604109 0.410522 -0.394968
H -2.110022 -1.016525 -0.807024
H 0.356425 1.245525 -0.544615
H -1.245335 1.629450 0.736179

Vibrational frequencies
-1729.8445 250.1822 409.2366
445.4730 538.9543 674.2684
795.2029 856.3429 966.3976
1021.6765 1064.0395 1115.1494
1246.1874 1419.6400 1658.3737
1699.0687 3204.0712 3272.5657

i67 – i45
Cartesian coordinates
C -0.897055 0.844523 0.049516
C 0.504007 0.357164 0.291889
C 0.099005 -1.045606 0.272709
C -1.234952 -0.433127 -0.209846
H 2.596873 0.241783 -0.716817
H -1.377306 1.814858 -0.005366

H -2.121092 -0.897597 -0.626652

Vibrational frequencies
-588.0515 274.5015 332.0391
395.4213 649.3225 712.8664
762.3124 828.5818 881.4335
941.1292 1016.0405 1124.7350
1250.3043 1549.2001 1723.4773
3198.9213 3232.5211 3324.7108

i30 – i53
Cartesian coordinates
C 1.751351 -0.355219 0.063585
C -0.826186 0.186565 0.822452
C -1.801873 -0.344014 -0.092268
C -0.607965 -0.004355 -0.639680
H 0.793167 1.550981 -0.273194
H 2.709129 0.084158 0.303774
H 1.643712 -1.431683 0.069306

Vibrational frequencies
-470.2380 247.0620 331.5457
356.8287 564.6390 681.2044
847.2377 864.1310 989.4742
1062.9373 1171.5775 1221.7808
1411.8949 1484.7939 1622.3375
3182.6918 3190.3892 3300.5723
356.8288 564.6390 681.2044

i26 – i39
Cartesian coordinates
C 1.457677 -0.553921 0.253373
C -0.144513 0.087266 -0.120034
C -1.428852 0.370725 0.343126
C -1.345669 -0.761621 -0.399368
H 1.600770 1.590959 -0.431861
H 2.141031 -1.205009 0.774621
H -2.037185 1.126338 0.815700

Vibrational frequencies
-831.5839 274.1939 293.9713
372.6885 550.5855 669.0466
713.8196 780.6484 881.1616
890.4179 994.2026 1080.9686
1180.7972 1583.7001 1670.6894
3178.4693 3266.0133 3291.1374

i6 – i11
Cartesian coordinates
C 1.483132 -0.480688 0.000000
C -0.360377 1.020892 0.000000
C -1.427000 0.212250 0.000000
C -1.242413 -1.046244 0.000000
H 0.185232 -1.198687 0.000000
H 1.972519 -0.815190 0.913999
H 1.972517 -0.815190 -0.914001

Vibrational frequencies
-1734.3633 147.5943 203.1892
394.6161 436.8803 486.5980
571.4292 1011.3441 1017.0377
1131.6603 1152.8542 1366.6688
1443.2794 1475.3369 1713.1502
2001.8632 3112.8125 3191.9215

i3 – i6
Cartesian coordinates
C 2.031683 -0.341551 -0.096222
C -0.088952 0.188268 0.205100
C -1.380775 0.018502 0.013421
C -2.624291 -0.215473 -0.127968
H 2.288789 -0.911276 0.794164
H 2.743567 -0.417113 -0.917743
H 0.665946 -0.981511 0.215972

Vibrational frequencies
-2160.4698 136.5731 188.0199
290.9011 463.3713 544.5824
572.8175 885.2844 957.6505

1036.4570 1078.6516 1244.6823
1457.5424 1556.9410 1653.5721
2092.6272 3108.4866 3202.1738

i53 – p22+H
Cartesian coordinates
C 1.839374 -0.000124 0.192560
C -0.694662 0.745190 0.011545
C -1.890465 -0.000107 0.138208
C -0.694605 -0.745197 0.010985
H 0.680407 0.001381 -2.013438
H 2.375927 0.936015 0.262017
H 2.375665 -0.936468 0.261291

Vibrational frequencies
-1023.6926 233.4641 301.5636
358.2306 534.4103 588.9501
612.8724 641.6749 821.8103
869.7248 990.4032 1064.5694
1109.4667 1433.3767 1490.1737
1739.1922 3188.2737 3298.1094

i65 – i13
Cartesian coordinates
C -0.883890 1.037347 0.000050
C -0.152845 -1.186664 0.000013
C 1.057763 -0.623588 -0.000061
C 1.473345 0.568011 -0.000100
H -2.283703 -0.556767 0.000153
H -1.435753 1.969757 0.000090
H 2.182801 1.367630 -0.000150

Vibrational frequencies
-501.6218 328.5268 386.7230
510.2030 517.7338 592.8657
650.0800 692.4358 824.5510
879.0616 1030.3121 1215.8181
1305.8365 1440.5272 1641.0392
3164.7457 3230.4879 3403.4741

i13 – i27
Cartesian coordinates
C -1.857280 -0.722192 0.000000
C -0.061588 0.407223 0.000010
C 1.189323 0.065642 0.000002
C 2.403010 -0.210528 -0.000005
H -2.016494 1.468539 -0.000016
H -2.665681 -1.431850 -0.000001
H 3.439617 -0.447176 -0.000002

Vibrational frequencies
-462.9151 110.0733 125.7730
306.0661 388.0861 392.5998
437.4683 462.7761 608.8691
818.6931 874.4517 1231.9330
1535.8519 1610.3849 1755.7479
3124.3986 3318.8267 3462.7147

i39 – p18at+H
Cartesian coordinates
C 1.085310 -0.900547 0.088608
C -0.106936 0.012371 -0.103510
C -1.465521 0.255385 0.520303
C -1.410710 0.116738 -0.777631
H 4.102399 2.318074 -0.003422
H 1.335271 -1.943085 0.193117
H -1.930855 0.426408 1.476570

Vibrational frequencies
-91.5277 27.2032 29.2609
304.7425 379.5330 385.4150
628.1909 653.2686 709.6408
716.8856 726.5614 928.6668
946.1606 1297.5896 1634.1174
1680.0552 3292.7501 3298.6405
628.1909 653.2686 709.6409
1680.0552 3292.7500 3298.6405

i39 – p18bt+H

Cartesian coordinates
C -1.312876 0.383754 -0.006740
C 0.107217 0.012489 -0.103646
C 1.465733 0.255568 0.520301
C 1.411309 0.114945 -0.777437
H -1.336482 -1.941494 0.195450
H -4.108186 2.308873 -0.003453
H 1.930825 0.427842 1.476461

Vibrational frequencies
-88.9540 26.8402 28.8802
304.7511 379.4974 385.4382
628.1923 653.2489 709.7812
716.8592 726.5169 928.5641
946.0901 1297.6002 1634.1006
1680.0435 3292.8612 3298.6925
628.1922 653.2489 709.7812

i38 – i24
Cartesian coordinates
C 1.526593 -0.389006 -0.211859
C -1.435704 0.347458 -0.257786
C -0.079857 0.112622 0.542111
C 1.152804 0.798107 -0.126579
H 1.869059 -1.396011 -0.329499
H -1.874004 1.256833 -0.620985
H -0.058512 0.183160 1.624029

Vibrational frequencies
-331.6151 197.0704 267.4658
418.7160 475.9457 636.4494
685.2635 740.1558 838.1993
899.2133 924.8978 969.9733
1301.7828 1777.7906 1862.8921
3168.3945 3352.4207 3408.4097

i65 – i58
Cartesian coordinates
C 0.682110 0.755198 -0.259922
C -0.724337 0.665885 0.279392
C -0.123272 -0.732117 0.051344
C 1.270166 -0.409008 0.260867
H 0.905048 1.175014 -1.244187
H -0.968730 1.079449 1.257414
H 2.161083 -0.929458 -0.066721

Vibrational frequencies
-740.8835 307.7079 446.7835
561.6459 710.7839 753.6914
844.2794 920.8976 1024.2332
1077.8411 1126.6320 1155.5718
1239.3841 1269.0840 1393.9415
3093.4480 3118.3891 3222.4009

i4 – i10
Cartesian coordinates
C -0.111948 1.192117 -0.000002
C 0.635329 -0.931767 -0.000004
C -0.629891 -0.246708 -0.000007
C -1.917026 -0.453139 0.000006
H 2.663297 0.132638 0.000025
H -0.159836 1.738805 0.935136
H -0.159815 1.738829 -0.935127

Vibrational frequencies
-824.2948 119.4953 158.3880
377.4404 528.0081 569.5104
632.2810 736.6414 845.6645
920.2795 1010.8398 1032.8031
1403.4805 1734.1741 1813.8396
3143.4337 3274.3022 3381.8856

i15 – i67
Cartesian coordinates
C 0.017950 1.297109 -0.115506
C -0.403226 -0.792749 0.116189
C 1.003739 -0.811588 0.034450
C 1.112521 0.547320 -0.026947
H -2.554968 -0.059250 0.000107

H -0.408859 1.917336 0.666277
H 1.671512 -1.628500 -0.171246

Vibrational frequencies
-674.4765 286.1878 387.8796
437.9246 465.9940 529.6961
586.1462 707.2572 734.5783
915.4343 1009.2156 1172.2977
1287.1247 1475.4104 1928.0605
3214.2206 3298.5679 3438.3356

i7 – i18
Cartesian coordinates
C 0.436194 1.039173 0.000128
C 1.192252 -0.256770 0.000018
C -0.946248 0.504396 -0.000504
C -1.723338 -0.423167 0.000299
H 0.629907 1.649576 0.885494
H 0.630574 1.650223 -0.884646
H 2.274748 -0.351802 0.000024

Vibrational frequencies
-547.9907 206.4944 251.4868
303.7349 596.2932 693.3515
935.3773 947.1647 993.3245
1087.8419 1173.5695 1268.4696
1461.2957 1660.4104 2194.1879
3075.5843 3119.3695 3185.4013

i8 – i5
Cartesian coordinates
C -1.712310 -0.057412 -0.077821
C 0.661685 1.014341 0.104154
C 1.325541 -0.183550 -0.349024
C 0.718801 -1.182799 0.239613
H -2.144760 -1.045667 -0.130013
H -2.361762 0.810187 -0.079493
H 0.913124 2.047284 0.261770

Vibrational frequencies
-783.9473 291.6355 348.1754
426.8237 487.6277 570.6145
654.9633 842.5645 888.8178
1037.9654 1104.3094 1159.8671
1439.0273 1469.0599 1635.8334
3171.0075 3286.0921 3311.6947

i16 – i24
Cartesian coordinates
C -1.638534 0.053520 -0.577139
C 0.992533 0.131302 0.060001
C -0.341054 0.563952 0.280156
C -1.444609 -0.824538 0.346912
H 3.121676 -0.566306 -0.283918
H -0.498455 1.278201 1.083560
H -0.777927 1.136115 -0.714970

Vibrational frequencies
-1349.5780 119.5528 200.2721
292.4610 402.9349 513.2876
698.3598 724.4681 817.8316
856.6909 1033.6740 1092.0534
1329.9985 1686.0018 2191.0009
2200.4539 3162.4147 3478.4903

i45 – i20
Cartesian coordinates
C 0.472402 0.843726 -0.077619
C -0.739772 0.141827 -0.025828
C 0.708048 -1.010902 -0.329686
C 1.478484 -0.097304 0.293552
H -2.865601 -0.622632 0.136341
H 0.618653 1.681836 -0.758231
H 2.511644 -0.014205 0.587009

Vibrational frequencies
-450.7602 243.7477 321.5233
461.7646 493.5417 645.0684
657.2183 777.8845 861.9527

991.8264 1051.3165 1214.8527
1297.1044 1528.3309 1863.2210
3141.5717 3291.1817 3408.1422

i1 – i13
Cartesian coordinates
C 1.175215 0.870421 0.012610
C -0.150490 -1.050870 -0.185107
C -1.214147 -0.441584 0.199918
C -1.535071 0.792561 -0.110164
H 2.030611 -1.079869 0.144060
H 2.019732 1.532641 -0.141500
H -0.505411 1.362356 0.232447

Vibrational frequencies
-1628.8756 204.9426 329.4337
378.7126 479.6149 591.4355
687.6069 763.5864 827.7440
888.8391 1074.1898 1194.8258
1408.8197 1464.6224 1652.8448
1844.1983 3156.0776 3220.1934

Products

trans-p9t
Cartesian coordinates
C -2.198829 -0.468309 -0.000002
C 0.103032 0.230243 0.000001
C 1.343205 -0.002225 0.000000
C 2.627623 -0.241043 -0.000001
H -1.530098 1.537031 0.000006
H -2.237995 -1.547890 -0.000006

Vibrational frequencies
131.6336 167.9340 262.7471
371.8316 580.3378 618.6853
783.2610 797.8975 906.1526
1214.1931 1378.9601 1524.1874
1938.5192 3117.8957 3267.5085

p10t
Cartesian coordinates
C 1.223644 -0.006492 0.000026
C -1.223242 -0.007112 -0.000039
C -2.247751 -0.636772 -0.000110
C 2.247374 -0.637190 -0.000029
H -0.000196 1.453959 0.879747
H -0.000143 1.454177 -0.879399

Vibrational frequencies
130.7640 197.7485 214.6477
221.6367 478.9107 871.5658
881.9989 1007.0027 1227.5823
1335.9638 1452.0977 2276.4283
2277.4537 3058.9920 3098.7789

trans-p7
Cartesian coordinates
C 2.404502 -0.014191 0.000036
C -0.005965 0.536606 -0.000031
C -1.264655 0.103426 -0.000025
C -2.475185 -0.304175 -0.000022
H 1.001181 -1.436731 0.000108
H 0.201434 1.604609 -0.000094

Vibrational frequencies
110.9267 130.4356 206.3386
244.6875 524.7356 690.3991
904.1854 910.2227 1094.2350
1201.2617 1414.4084 1737.1199
2064.4678 3105.3372 3167.1884

cis-p7
Cartesian coordinates
C 1.806104 -0.977174 0.000016
C -0.033954 0.788233 -0.000005
C -1.159445 0.075993 -0.000007
C -2.259993 -0.572515 -0.000009

H 2.186577 0.881078 0.000008
H -0.091919 1.875155 -0.000014

Vibrational frequencies
126.7126 136.0478 227.5765
240.7849 552.1813 609.9853
916.6245 926.3179 1000.1230
1192.7330 1429.2689 1766.6478
2064.5256 3036.2927 3160.1466

p14t
Cartesian coordinates
C 1.938534 -0.421910 0.000377
C -0.423341 0.096188 -0.000095
C -1.437150 -0.825482 -0.000423
C -1.751679 0.498492 0.000592
H 1.187726 1.538361 -0.001151
H 3.019019 -0.423608 0.000406

Vibrational frequencies
51.9247 187.9732 382.2590
513.9513 561.4350 716.9916
726.5785 883.4848 925.1506
1243.6209 1358.9858 1644.5127
1733.0483 3090.3956 3265.1031

p16t
Cartesian coordinates
C 2.064469 0.529819 0.000009
C -0.272423 -0.141353 -0.000002
C -1.305117 0.692225 -0.000007
C -1.590854 -0.689630 0.000003
H 1.454863 -1.474604 -0.000005
H -1.686020 1.702161 -0.000014

Vibrational frequencies
103.1793 229.3862 391.6487
525.8692 722.9789 808.7845
893.1060 963.1783 1129.6079
1234.2266 1326.7859 1529.1080
1766.4086 3105.3081 3267.6013

p21t
Cartesian coordinates
C 0.265613 0.466082 -0.000245
C -0.996182 -0.259305 0.000027
C 1.562359 -0.156233 -0.644354
C 1.562310 -0.155769 0.644556
H 0.175432 1.549599 -0.000460
H -1.000284 -1.362655 0.000143

Vibrational frequencies
142.4424 157.9144 311.1777
412.9237 629.1736 664.2003
777.7162 889.4000 967.3941
1060.9675 1359.1776 1712.4785
1740.7198 3042.7990 3148.5338

p12
Cartesian coordinates
C 1.732421 -0.670299 0.000000
C -0.850072 -0.000149 0.000000
C 0.441333 -0.000244 0.000000
C 1.732258 0.670535 0.000000
H -2.711898 0.931819 0.000000
H -2.712245 -0.931428 -0.000001

Vibrational frequencies
5.0557 204.5968 354.5283
458.2320 561.3795 616.6536
717.5640 960.6093 1004.6904
1293.3171 1434.8567 1585.9572
2044.4587 3132.0606 3219.5298

p15t
Cartesian coordinates
C 1.538612 -0.325588 0.643711
C -0.949873 0.131211 0.000006
C 0.400700 0.566123 -0.001506

C 1.538095 -0.329941 -0.642171
H -3.114107 -0.546427 0.001258
H 0.549693 1.644069 -0.004444

Vibrational frequencies
201.9679 202.1583 455.3712
536.7613 639.0110 673.2006
695.6444 837.3197 859.8228
1025.9779 1346.8586 1750.7577
2179.1613 3140.4951 3479.6306

p26
Cartesian coordinates
C 0.430687 0.986312 0.000009
C 0.524470 -1.103216 -0.000024
C -0.621912 -0.146379 0.000007
C -1.920804 -0.061097 0.000026
H 0.450455 1.583147 0.908726
H 0.450429 1.583175 -0.908690

Vibrational frequencies
127.7760 170.8177 395.0025
483.0334 759.6694 884.8201
912.8286 974.4753 1075.2207
1156.3002 1451.9801 1597.3842
1769.0469 3117.3992 3203.7466

p34
Cartesian coordinates
C -1.161640 -0.449947 0.069141
C 1.513737 -0.339993 0.043730
C 0.583074 0.792929 0.079505
C -0.656766 1.013075 -0.104666
H -1.450460 -0.667365 1.094434
H -1.891712 -0.790045 -0.660330

Vibrational frequencies
193.0558 278.1727 463.7738
627.0699 777.4469 876.8554
915.4334 1028.0907 1065.1801
1170.6308 1450.3151 1543.8802
1747.3913 3137.2971 3216.5919

p1
Cartesian coordinates
C -1.539536 0.577570 0.000000
C 1.030014 0.003462 0.000000
C -0.363404 -0.041306 0.000000
C -1.559540 -0.831107 0.000000
H 3.294818 0.053226 0.000000
H -2.085914 1.508075 0.000000

Vibrational frequencies
200.0049 215.1777 535.0161
536.4312 660.0839 710.3699
781.4863 911.5610 948.6497
1137.5856 1296.8550 1753.7295
2239.1604 3268.0559 3481.3614

p35
Cartesian coordinates
C 1.182172 -0.000106 0.000008
C -1.050546 0.716157 -0.000008
C -1.050739 -0.715991 -0.000005
C 0.157256 -1.137896 0.000003
H 1.813091 -0.000186 -0.889958
H 1.813078 -0.000182 0.889983

Vibrational frequencies
203.0034 399.2772 559.8209
689.3780 800.9963 827.8103
966.4804 1034.8032 1099.9168
1180.4953 1416.5333 1435.8419
1522.1233 3102.5000 3159.1835

p31t
Cartesian coordinates
C 0.883698 0.685011 0.000007
C -0.536943 -1.096581 -0.000006

C -1.275101 0.000143 0.000012
C -0.536622 1.096712 -0.000009
H 1.744180 -1.338904 0.000035
H 1.744528 1.338486 -0.000002

Vibrational frequencies
459.2949 551.3730 663.4726
710.8917 721.3149 899.3564
973.5463 1047.6369 1069.9176
1089.3011 1282.6641 1366.2290
1498.5383 3234.6903 3256.3556

p8
Cartesian coordinates
C 1.669051 -0.502278 0.000000
C -0.241749 1.354743 -0.000001
C -0.971702 0.120996 0.000000
C -1.722347 -0.925617 0.000000
H 1.666822 -1.583385 0.000001
H 2.614587 0.027735 0.000000

Vibrational frequencies
136.8997 234.7175 356.7330
382.6219 581.9036 608.4186
838.3658 914.8257 1036.6122
1048.5724 1437.2946 1719.0786
1875.3350 3178.5280 3286.0149

p17
Cartesian coordinates
C 0.215709 0.944954 0.000012
C -0.740089 -0.248969 -0.000009
C 0.604723 -0.606051 0.000000
C 1.855168 -0.349719 0.000014
H 0.299696 1.485115 -0.933970
H 0.299679 1.485096 0.934006

Vibrational frequencies
64.7728 139.8495 184.8067
393.7028 669.4055 807.8675
943.0630 1005.7872 1030.3968
1067.0273 1476.1063 1772.4271
2009.2991 3163.2236 3288.1516

p20t
Cartesian coordinates
C -1.217637 0.644134 -0.000125
C 0.134890 0.000000 0.000301
C 1.434527 0.000000 0.686542
C 1.434647 0.000000 -0.686654
H -1.706375 -1.603632 0.000180
H -1.706374 1.603632 0.000181

Vibrational frequencies
273.2505 321.9201 365.7947
467.4389 592.8751 648.2327
679.0347 840.1991 952.7869
985.5945 1111.3857 1421.6682
1743.4011 3277.8223 3331.4883

p19t
Cartesian coordinates
C -1.515956 0.605147 0.000003
C 1.164879 -0.058887 -0.000040
C -0.141828 -0.271811 -0.000013
C -1.345264 -0.845448 0.000019
H -1.751608 1.130604 0.924087
H -1.751644 1.130592 -0.924080

Vibrational frequencies
141.9283 170.4110 376.0736
426.7586 571.3554 865.6069
906.0730 928.9622 986.9108
1083.5486 1442.3802 1577.9286
2014.8878 3095.5018 3190.8288

p13a/p13b
Cartesian coordinates
C 0.693468 -0.000558 0.000000

C -0.496123 -0.681980 0.000000
H 1.774839 -0.003609 0.000000

Vibrational frequencies
314.1109 865.7790 918.2186
1260.0795 1634.8466 3256.0728

p23

Cartesian coordinates

C -0.388182 0.844544 0.099177
C -0.503175 -0.970402 0.314938
C 0.736202 -0.089388 0.086766
C 1.990925 -0.020910 -0.224144
H -2.412958 -0.018894 -0.532925
H -0.444560 1.736043 0.718375

Vibrational frequencies
179.4122 251.5333 551.8502
658.9354 678.2159 839.5462
878.4049 1002.9014 1045.5741
1184.8589 1294.5632 1464.8452
1825.5702 3175.3240 3289.8701

p13

Cartesian coordinates

C -1.302085 0.516262 0.000164
C 0.000174 0.000067 -0.000201
C 1.302030 -0.516375 0.000114
C 1.370910 0.803964 -0.000209
H -1.700022 1.517276 0.000994
H 1.700330 -1.517209 0.001145

Vibrational frequencies
184.6166 236.0749 400.1750
446.0969 552.9260 766.2270
836.2854 845.8898 972.1806
1072.9532 1157.1458 1636.0580
1726.5334 3300.5033 3302.9746

p18at

Cartesian coordinates

C 1.377228 -0.319299 0.410714
C 0.000111 -0.005240 -0.134999
C -1.376903 0.348833 0.386271
C -1.290554 -0.615749 -0.490648
H 1.871626 -0.953572 1.127301
H -1.869797 1.034938 1.054498

Vibrational frequencies
302.7547 376.0980 379.9005
625.2884 648.9002 705.3384
714.9856 723.4526 917.1403
926.0830 1296.2297 1633.7285
1680.4165 3299.5366 3300.2734

p18bt

Cartesian coordinates

C -1.289819 0.577917 -0.534947
C -0.000112 -0.005238 -0.134998
C 1.376900 0.348817 0.386287
C 1.290556 -0.615723 -0.490679
H -1.871615 -0.953621 1.127265
H 1.869794 1.034889 1.054550

Vibrational frequencies
302.7596 376.0998 379.9017
625.2942 648.9000 705.3440
714.9851 723.4517 917.1415
926.0869 1296.2299 1633.7260
1680.4142 3299.5305 3300.2737

p22

Cartesian coordinates

C -1.867293 0.000000 0.000015
C 0.673002 -0.746345 -0.000146
C 1.877250 0.000000 0.000327
C 0.673002 0.746345 -0.000146
H -2.410253 0.935142 0.000672
H -2.410251 -0.935142 0.000670

Vibrational frequencies

259.8676 338.0114 596.7873
597.8595 723.1485 820.6518
914.2878 983.4214 1060.6019
1118.0171 1433.2211 1490.8511
1873.3232 3191.4933 3295.1433

p22t

Cartesian coordinates

C -1.784010 -0.000008 -0.082957
C 0.701534 -0.881188 0.186965
C 1.629948 -0.000074 -0.304484
C 0.701665 0.881196 0.186993
H -2.327914 0.933285 -0.149524
H -2.327597 -0.933514 -0.149124

Vibrational frequencies

274.6768 356.1733 603.1168
638.4915 670.0711 750.3165
916.2659 948.8258 1044.9773
1183.7391 1414.0649 1447.7565
1794.2810 3179.9411 3280.1432

p27

Cartesian coordinates

C -0.909743 0.525668 0.000000
C 0.910071 0.525321 0.000000
C -0.000091 -0.000132 -1.044080
C -0.000091 -1.050671 0.000000
H -0.000164 -0.000160 2.118533
H -0.000164 -0.000160 -2.118533

Vibrational frequencies

549.2902 552.5373 707.5948
712.6970 851.5450 855.3299
872.1273 1016.8936 1017.4072
1130.3223 1131.9093 1295.2388
1330.8541 3335.5051 3338.4388
549.2280 552.5874 707.8668
712.4345 851.6098 855.2560
872.1265 1016.9607 1017.3390
1130.3954 1131.8286 1295.2428
1330.8551 3335.5052 3338.4387

p33

Cartesian coordinates

C 1.050748 -0.191825 -0.000259
C -1.252796 -0.161265 0.000060
C 0.009901 0.876701 -0.001225
C -0.081563 -0.403786 0.902890
H 2.126584 -0.223971 -0.001022
H 0.011188 1.950379 -0.004480

Vibrational frequencies

229.9357 330.8874 530.5899
723.8067 771.7269 814.6486
880.3476 918.0565 956.0284
1090.5242 1097.8675 1209.1531
1332.0310 3312.3544 3330.5262

p33t

Cartesian coordinates

C 0.727109 0.659067 -0.207193
C -0.722323 -0.806764 -0.271020
C -0.727096 0.659081 -0.207196
C -0.000001 -0.167327 0.959105
H 1.495938 1.388152 -0.008016
H -1.495910 1.388179 -0.008017

Vibrational frequencies

285.4232 462.0207 464.6338
710.0064 853.6365 919.9677
924.5629 1004.6177 1053.3947
1182.5000 1249.9485 1264.0722
1319.5286 3265.4286 3281.2851

p5

Cartesian coordinates

C -1.401606 -0.664547 0.000054
C -0.157059 -0.000004 -0.000126
C 1.176303 -0.000001 -0.000257
C 2.437541 0.000000 0.000221
H -1.960724 1.586522 0.000160
H -1.960739 -1.586513 0.000161

Vibrational frequencies

141.8708 172.7519 471.8867
503.2191 744.5514 788.9203
955.1777 972.7901 974.4631
1147.6297 1481.1414 1698.5523
2114.0693 3269.1766 3307.6434

p6

Cartesian coordinates

C -1.312454 0.528364 0.000000
C 1.312451 0.528367 0.000000
C -0.000001 0.030358 0.000001
C -1.366961 -0.795206 0.000000
H -1.756138 1.509948 0.000002
H 1.756106 1.509963 -0.000001

Vibrational frequencies

212.5847 259.7310 288.6458
440.0061 602.2141 774.7899
803.8139 986.1070 990.0498
1050.9060 1082.0352 1625.2173
1695.9225 3297.0680 3301.0818

p24

Cartesian coordinates

C -0.505914 0.806376 0.167391
C -0.506139 -0.806397 0.167295
C 0.721465 -0.000217 0.044820
C 1.999643 0.000052 -0.194293
H -0.636490 1.625951 0.866227
H -0.637017 -1.625966 0.866085

Vibrational frequencies

164.3534 250.7643 532.9204
677.6069 774.4555 868.9667
949.1051 981.8225 1082.2035
1130.6403 1159.8422 1371.6971
1803.8387 3205.8688 3213.5171

p24t

Cartesian coordinates

C -0.479405 1.044534 0.000003
C -0.479801 -1.044450 0.000004
C 0.602301 -0.000198 0.000006
C 1.910520 -0.000123 -0.000012
H -0.468406 2.120397 0.000001
H -0.469256 -2.120318 0.000013

Vibrational frequencies

61.7656 197.6307 457.0416
540.3896 567.9596 716.3879
826.2486 898.6251 1059.7961
1110.3661 1135.3239 1387.2631
1738.0902 3306.4717 3312.9459

p25

Cartesian coordinates

C 0.371244 -0.684897 -0.319486
C -0.854354 0.000831 0.048012
C 0.371835 0.685959 -0.317932
C 1.566792 -0.000664 0.260788
H 2.435672 -0.000372 -0.384179
H 1.767988 -0.002158 1.332988

Vibrational frequencies

140.6160 219.8685 413.6497
475.6679 775.3557 843.5533
979.6949 1077.3957 1119.3731
1235.5509 1394.8984 1531.1692
1842.8700 3101.1440 3238.6080

p32

Cartesian coordinates

C	0.680417	0.821460	-0.291205
C	-0.772295	0.665305	0.094098
C	-0.041160	-0.688342	0.141143
C	1.330157	-0.278047	0.137211
H	-1.187150	1.414761	0.761321
H	2.267400	-0.765616	-0.068963

Vibrational frequencies

352.4435	471.6537	562.9234
621.3631	721.5141	760.3086
868.9028	1037.5508	1120.1605
1143.1426	1155.0434	1436.2312
1571.4654	3176.7285	3297.5475

p36t

Cartesian coordinates

C	1.277924	0.000045	0.000000
C	-0.959825	0.747508	0.000024
C	-0.959907	-0.747346	-0.000024
C	0.010647	-0.000098	-0.829389
H	1.861415	0.917936	0.000030
H	1.861670	-0.917683	-0.000030

Vibrational frequencies

427.7804	595.5574	674.0886
875.3255	940.0950	962.9180
986.9965	1052.0052	1120.8916
1134.5535	1151.6788	1349.1600
1476.0784	3124.4641	3214.3206

p3

Cartesian coordinates

C	-2.385642	0.000008	-0.000087
C	0.189625	-0.000009	0.000131
C	1.486543	-0.000003	0.000153
C	2.765767	0.000010	-0.000199
H	-2.947648	0.930054	-0.000149
H	-2.947678	-0.930019	-0.000149

Vibrational frequencies

114.2822	141.0046	269.4069
272.2454	472.2036	606.1969
776.4773	990.1249	1035.8584
1378.7986	1528.1850	2009.2620
2251.8199	3135.4320	3224.7641

p4

Cartesian coordinates

C	-2.223089	-0.398850	-0.000020
C	0.146455	0.706200	-0.000002
C	1.295967	0.032395	0.000034
C	2.412182	-0.591084	-0.000024
H	-3.186841	-0.851410	0.000001
H	0.157668	1.796473	-0.000080

Vibrational frequencies

136.8667	216.7009	309.2008
314.4165	599.6205	716.4471
750.6861	896.7387	974.2880
1172.7331	1408.8933	2061.3401
2230.2870	3142.4242	3477.7637

p2s

Cartesian coordinates

C	0.000000	0.000000	2.538057
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.306605
C	0.000000	0.000000	-2.538057
H	0.000000	0.000000	3.601286
H	0.000000	0.000000	-3.601286

Vibrational frequencies

128.6196	128.6196	407.9750
407.9750	485.5065	485.5065
518.5526	518.5526	525.0785
525.0785	768.6906	1579.4769
1728.0330	2026.0283	3465.4915
3474.2926		

p2

Cartesian coordinates

C	0.000000	0.000000	2.542061
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	-1.307984
C	0.000000	0.000000	-2.542061
H	0.000000	0.000000	3.605756
H	0.000000	0.000000	-3.605756

Vibrational frequencies

122.2493	122.2493	399.0831
399.0831	463.6621	463.6621
479.9266	479.9266	485.5599
485.5599	761.3972	1572.4719
1661.1661	1971.0152	3458.1957
3465.9622		
122.2493	122.2493	399.0832
399.0832	463.6621	463.6621

cis-p9t

Cartesian coordinates

C	-2.189339	-0.519779	0.000001
C	0.135953	0.166862	0.000000
C	1.384393	-0.009657	-0.000001
C	2.676168	-0.207959	-0.000003
H	-1.482319	1.469818	0.000005
H	-3.268426	-0.491135	0.000002

Vibrational frequencies

134.3131	162.7676	276.3914
369.7515	531.0964	588.6254
747.6310	764.4707	934.1917
1207.5902	1382.7027	1546.6004
1942.3826	3069.5990	3275.1373
134.3131	162.7677	276.3914
747.6310	764.4708	934.1917

p30t

Cartesian coordinates

C	-0.963468	-0.680852	0.000223
C	1.533163	0.000555	0.000217
C	0.484254	0.837140	0.000046
C	-0.963391	0.681282	-0.000047
H	-1.724078	-1.444541	0.000404
H	-1.723479	1.445467	-0.000479

Vibrational frequencies

269.6663	450.6406	607.3852
663.7707	700.6202	777.0498
829.6684	1034.7119	1053.0245
1145.8364	1279.4094	1502.6325
1701.0972	3270.9575	3294.0590

p29

Cartesian coordinates

C	-0.000010	-0.756649	0.000123
C	0.660906	0.855747	0.193791
C	-0.660830	0.855693	-0.193790
C	-1.305233	-0.344697	0.123823
H	2.257509	-0.796000	0.089054
H	-2.257501	-0.795921	-0.089454

Vibrational frequencies

376.1253	468.8216	638.3081
659.9998	745.2328	750.0934
896.7765	1078.8310	1097.0266
1163.7624	1165.4109	1306.8059
1630.9372	3307.3220	3308.6962

p29t

Cartesian coordinates

C	0.000404	-0.819218	-0.000201
C	0.736430	0.893609	-0.000144
C	-0.737417	0.893644	0.000076
C	-1.295651	-0.350058	0.000114
H	2.268455	-0.804431	0.000258
H	-2.267361	-0.806510	-0.000116

Vibrational frequencies

346.3422	361.4386	534.3362
628.8961	676.9816	746.6732
919.5483	1026.4313	1088.9931
1143.1590	1190.5685	1447.1064
1622.3037	3323.7146	3326.3251

p28

Cartesian coordinates

C	-0.864784	0.712572	0.096824
C	0.492897	-0.938858	-0.236674
C	1.313382	0.000001	0.290759
C	0.492895	0.938859	-0.236675
H	-1.708822	-1.377723	-0.033177
H	-1.708823	1.377721	-0.033174

Vibrational frequencies

284.0222	365.1775	687.1481
786.3150	856.0236	889.0227
929.4955	1023.4523	1196.4362
1206.3881	1271.7287	1336.7083
1383.3169	3229.9520	3246.5116