

Binding the Power of Cycloaddition and Cross-  
Coupling in a Single Mechanism: An Unexpected  
Bending Journey to Radical Chemistry of  
Butadiynyl with Conjugated Dienes

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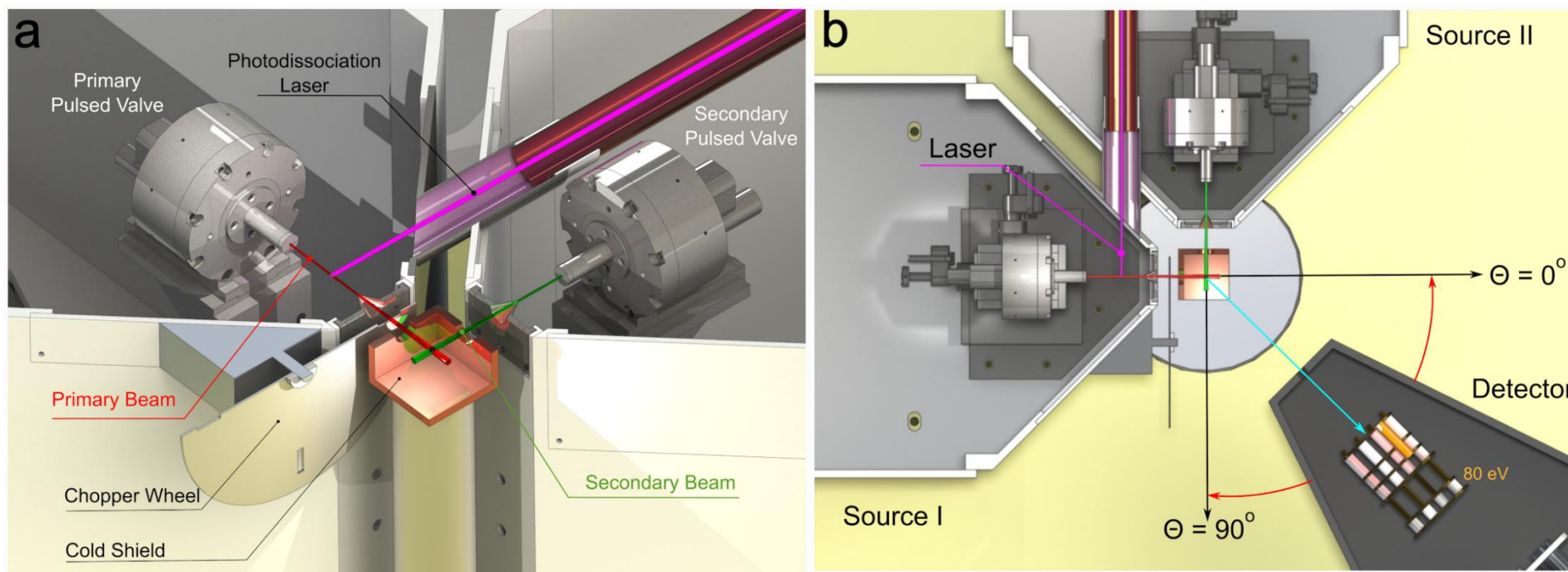
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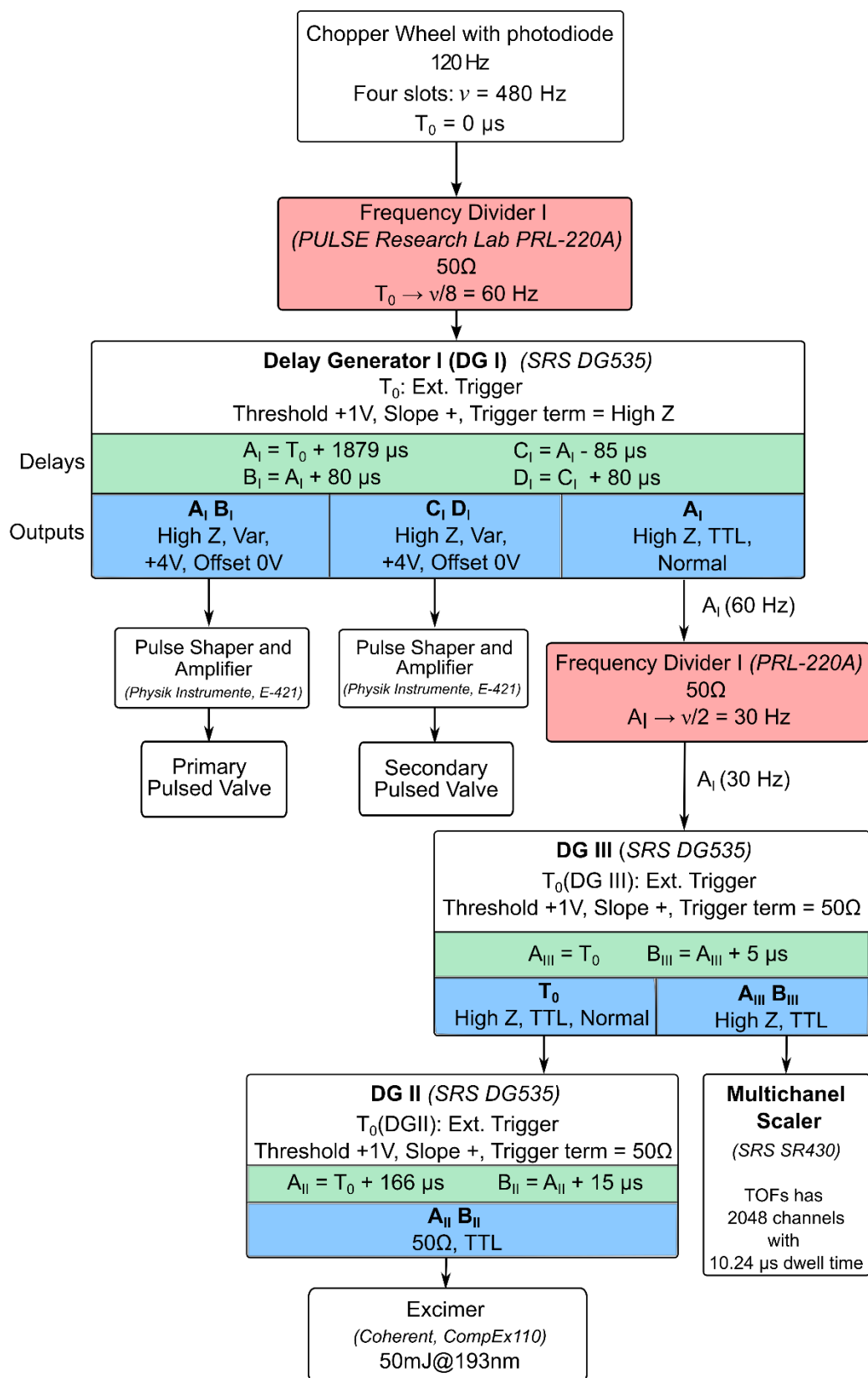
## 1. Details of the crossed molecular beams experiment



**Figure S1.** Experimental setup. (a) Side view on the cross point; (b) Top-view of the experiment.

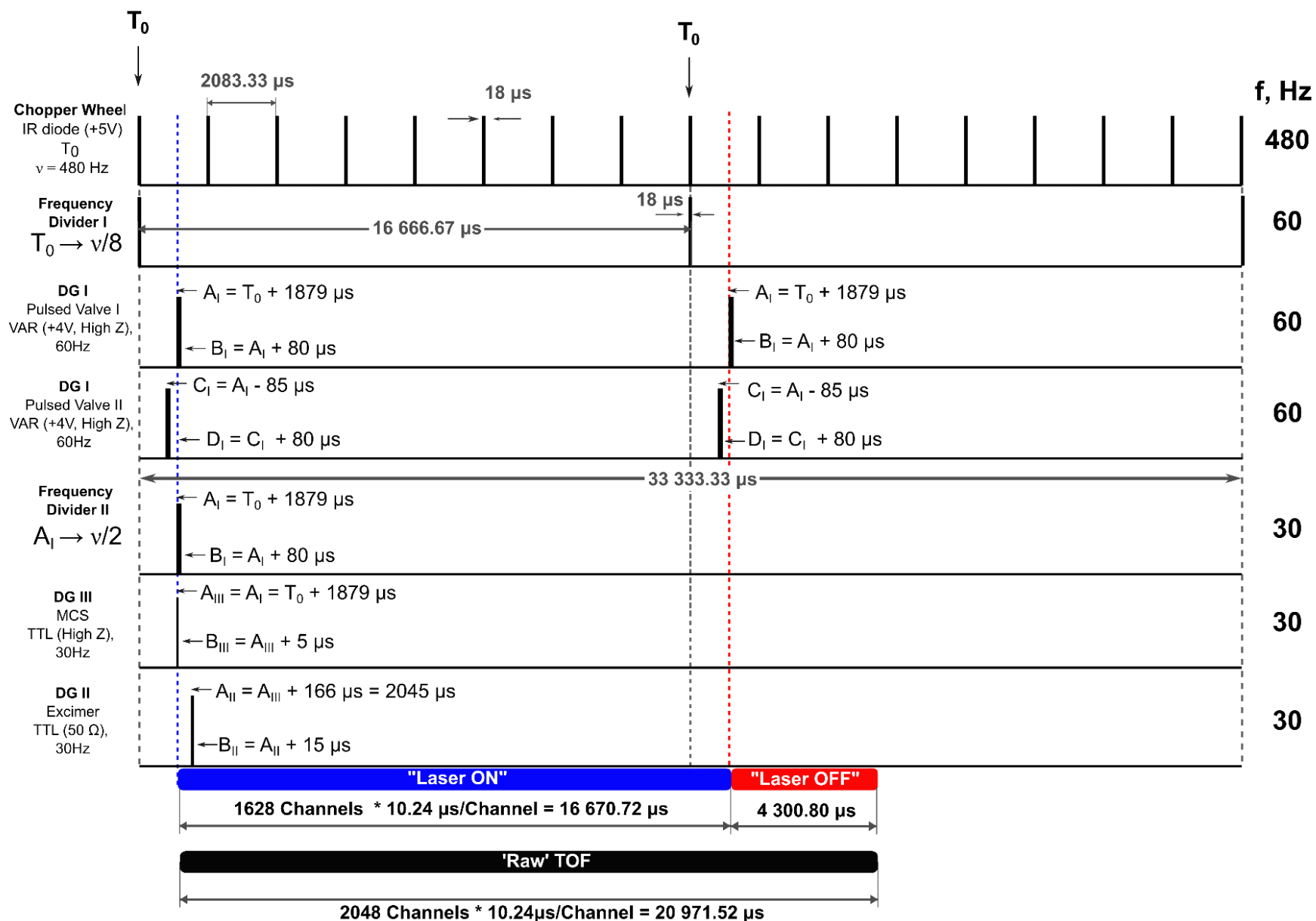
**Table S1.** Primary and secondary beam peak velocities ( $v_p$ ), speed ratios ( $S$ ), collision energy ( $E_c$ ), and center-of-mass angle ( $\Theta_{CM}$ ) for the reaction of 1,3-butadienyl radicals ( $C_4H$ ) with 1,3-butadiene ( $CH_2CHCHCH_2$ ) and 2-methyl-1,3-butadiene ( $CH_2C(CH_3)CHCH_2$ )

Beam	$v_p, m s^{-1}$	$S$	$E_c, kJ mol^{-1}$	$\Theta_{CM}, ^\circ$
1,3-butadienyl	$1071 \pm 28$	$16.3 \pm 1.1$	–	–
1,3-butadiene	$777 \pm 12$	$9.5 \pm 0.3$	$22.5 \pm 1.0$	$38.7 \pm 1.6$
2-methyl-1,3-butadiene (isoprene)	$701 \pm 19$	$5.1 \pm 0.5$	$23.3 \pm 1.2$	$42.3 \pm 2.2$



**Figure S2.** Pulse sequence for the crossed molecular beam experiment for the reaction of the 1,3-butadiynyl radical ( $C_4H$ ,  $X^2\Sigma^+$ ) with 1,3-butadiene ( $CH_2CHCHCH_2$ ,  $X^1A_g$ ) and 2-methyl-1,3-butadiene ( $CH_2C(CH_3)CHCH_2$ ,  $X^1A'$ ).





**Figure S3.** Timing chart for the crossed molecular beam experiment for the reaction of the 1,3-butadiynyl radical ( $\text{C}_4\text{H}$ ,  $X^2\Sigma^+$ ) with 1,3-butadiene ( $\text{CH}_2\text{CHCHCH}_2$ ,  $X^1A_g$ ) and 2-methyl-1,3-butadiene ( $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_2$ ,  $X^1A'$ )

## 2. Diacetylene Synthesis

### *Working with Hazardous Chemicals*

**Pure Diacetylene is unstable and explosive on air!!!**



*The procedures are intended for use only by persons with proper training in experimental organic chemistry.*

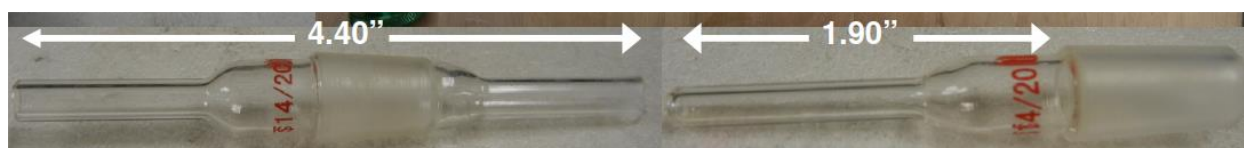
*All hazardous materials should be handled using the standard procedures for work with chemicals described in references such as "Prudent Practices in the Laboratory" (The National Academies Press, Washington, D.C., 2011; the full text can be accessed free of charge at [http://www.nap.edu/catalog.php?record\\_id=12654](http://www.nap.edu/catalog.php?record_id=12654)).*

*All chemical waste must be disposed of in accordance with local regulations.*

### 2.1 Required Chemicals, Glassware, and Other

Chemicals		
Chemical	Quantity	Supplier
1,4-Dichloro-2-Butyne	40 g	Aldrich, D59607-25G
Ethanol	15 mL	99.5%, Stock Room
Sodium Hydroxide Pellets	90 g and 2.6 g	Fisher Sci., S318-500
Glassware		
Item	Specification	Supplier
Flask, Three-Neck	500 mL, 14/20	Synthware, F431500
Water Condenser	250 mm, 14/20	ACE Glass, 9261-12
Funnel, Pressure-Equalizing (Additional funnel)	125 mL, 14/20	Synthware, F621125G
Bubbler	26 mm Body (OD), 0.25" Hose (OD)	Synthware, B257040
Custom Glass-metal LN <sub>2</sub> trap	40 mm body OD, 225 mm below joint, 16CF at the center and side tubes	Based on Synthware V103834, custom-made metal-glass connections
Gas inlet adapter	Inner 14/20, Straight, ¼ tube, 50 mm below joint	Custom-made, see Fig. S3
Vacuum/gas adapter (Gas outlet adapter)	Inner 14/20, Straight, to ¼ tube	Custom-made, see Fig. S3
Joint clips	45/50, 14/20	–
Other		
Item	Specification	Supplier
Scroll pump	Oil Free	Varian
Beverage cylinder	13 L	Matheson
Teflon tubing	¼ inch OD	McMaster
SS tubing	¼ inch OD	Swagelok
¼ Fittings	Union fittings	Swagelok
Valves, 5 ea.	SS-4H	Swagelok
Convectron gauge	10 <sup>-4</sup> Torr – 1 atm	275 MKS
Absolute Capacitance Manometer (Baratron)	1 – 1000 Torr	MKS

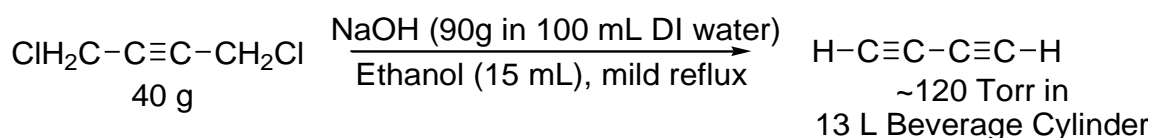
Heating plate	With magnetic stirrer Up to 200 °C	–
Two-steps regulator, 2 ea.	CGA 580	Matheson
Adaptor CF-tube, 2 ea.	16CF to ¼ SS tube	Swagelok
Ultra-Torr – Swagelok adapter union 5ea.	Straight, ¼ Ultra-Torr to ¼ Swagelok	Swagelok
Silicone hose	5/16	–
Dow Corning Vacuum Lubricant	–	Dow Corning
He 99.9999%	–	Matheson
Ar 99.9999%	–	Matheson
Mineral Oil	For up to 200 °C	Aldrich / Fisher
Glass Mineral Oil Bath	–	–

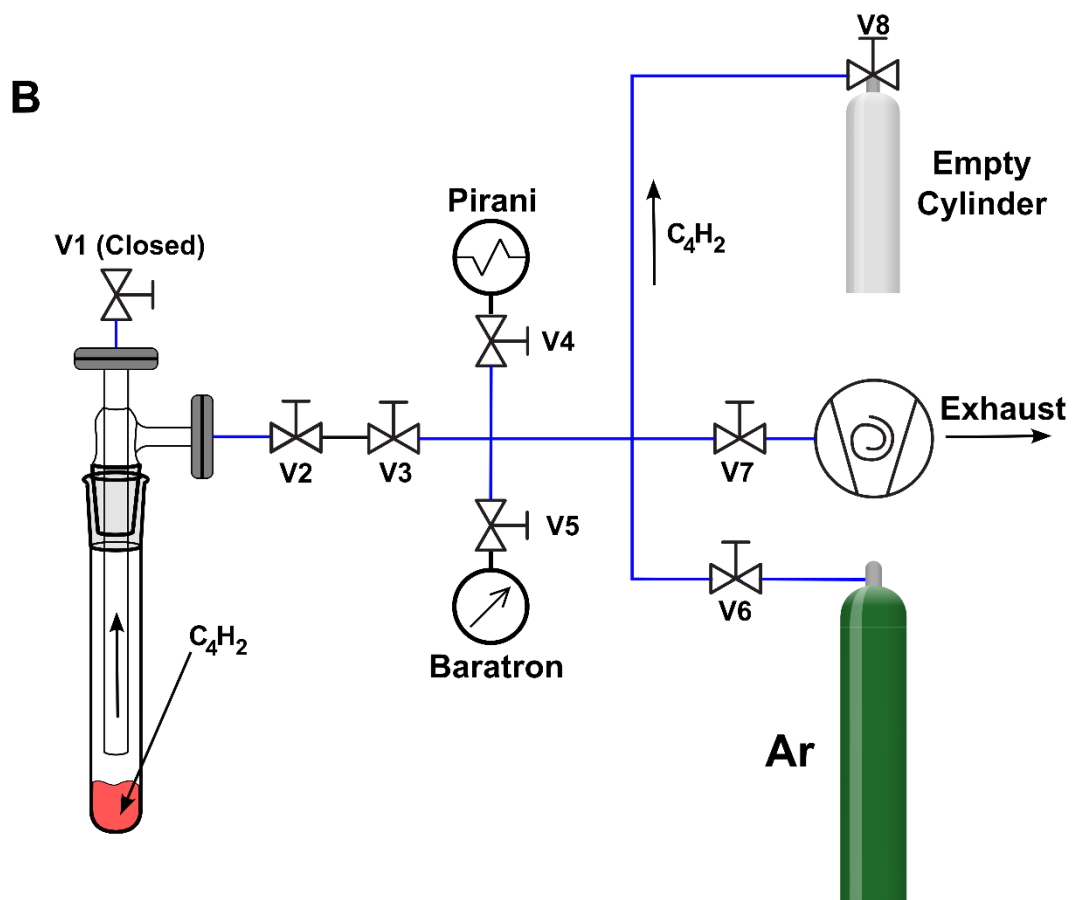
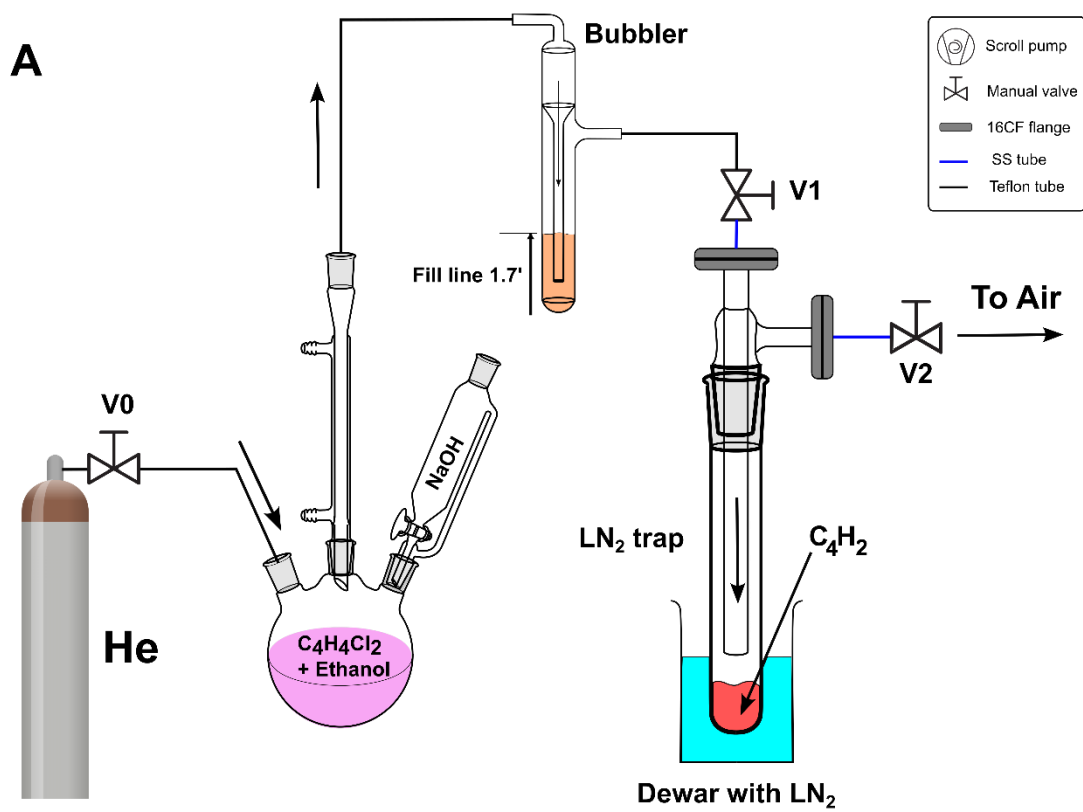


**Figure S4.** Gas inlet adapter (left) and Vacuum/gas adapter (right)

## 2.2 Outline

The synthesis procedure is based on previous works.<sup>1,2</sup> Diacetylene is prepared by one-step synthesis of treating 40 g 1,4-dichloro-2-butyne with concentrated sodium hydroxide (NaOH) solution under mild reflux. Gas transfers are facilitated by the combination of 1/4 inch (OD) Teflon tubing (McMaster), Swagelok fittings, and valves. Positive helium flows into the flask (Scheme S1), carrying away white vapors that evolve from the reaction mixture, through a water bubbler, to the liquid nitrogen (LN<sub>2</sub>)-cooled glass trap. Diacetylene is instantly solidified white inside the LN<sub>2</sub>-cooled glass trap, while helium gas continues to flow out to the air. After the reaction is complete, the glass trap is exposed to the active vacuum to remove the trapped helium gas. Subsequently into the pre-evacuated 13 L cylinder, about 120 Torr of diacetylene sublime within the period of 12 ± 1 minutes by simply warming up the glass trap in the air. Trap to trap distillation or cutting-down of warm-up period has not been attempted, as the crude diacetylene has a quality of ~99% - the mass spectrum.





**Scheme S1.** Experimental setup: (A) Synthesis, collecting diacetylene; (B) charging and diluting 13L cylinder.

### 2.3 Procedure (Scheme S1 A)

Into a 500 mL three-neck flask are placed a stirring bar and 40 g (0.33 mol) of 1,4-dichloro-2-butyne. About 15 mL of ethanol ( $C_2H_5OH$ ) follows into the flask. Concentrated NaOH solution needs to be prepared fresh by mortar and pestle grinding 90 g (2.25 mol) of NaOH pellets into fine powders and by dissolving in 100 mL water (use a clean 200 mL flask) – ensure a complete dissolution of NaOH powders free of any specks, which may clog the stopcock of the additional funnel.

Decant (transfer) the NaOH solution to the additional funnel, which will be fixed to the side neck of the reaction flask (Scheme S1 A). Afterward, ensure that helium flows into the flask and out to the top of the water condenser, bubbles through sodium hydroxide (NaOH) solution – concentration of 2.6 g (0.065 mol) in 20 mL deionized water, before it finally vents out of the top of T-shaped glass-metal trap. Please control the helium flow rate such that it bubbles through the NaOH solution once every second, the rate at which it should not over-pressurize the system but be sufficient to keep ambient air out. Clamp-tighten the inlet and outlet hoses of the water condenser to be leak-free, while running water.

At this point, ensure that the following components are functional/air-tight: custom-made glass-metal trap, scroll pump, and the whole glass apparatus (system). Perform in sequence 3 times helium charge-purge cycle to remove any air possibly trapped inside the system:

- (1) Close off the inlet Swagelok valve of the glass trap (V1) so that pressure starts to build up inside the system,
- (2) connect to your vacuum line the Teflon-tubing end coming out of the outlet Swagelok valve (Connect V2 and V3), glass trap – literally evacuate the body of glass trap down below 50 mTorr,
- (3) close off the outlet Swagelok valve to the vacuum side (V2) and gently open up the inlet Swagelok valve (V1) to the air side (system).

Once vigorous bubbling subsides, repeat (1) and open up simply the outlet Swagelok valve (V2) to the active vacuum for step (2). Proceed with the step (3) to complete the 2<sup>nd</sup> charge-purge cycle. Once vigorous bubbling subsides, the next step is gently to blow the positive helium pressure out to the ambient air, as you open up the outlet Swagelok valve (V2) and disconnect from the vacuum line the Teflon-tubing end coming out of the outlet Swagelok valve.

The reaction mixture (inside the silicone oil bath) can now be heated while stirring – power on the heating mantle and set at about 150 to 160 °C. Ensure water-running through the condenser leak-free. In a period of 20 minutes or so, ethanol starts to boil and condenses back to the flask as it refluxes. Pour liquid nitrogen ( $LN_2$ ) in the dewar, which surrounds the glass-metal trap (control its level during the reaction). Slightly open the additional funnel with caution and permit drops of the NaOH solution to flow into the reaction mixture. As a result, the solution turns red, permitting white vapors to emerge. Depending on NaOH dropping rates and how ethanol reflux goes, it can be a lapse up to ~20 minutes in between the color change of solution and a visible rise of white vapors. As NaOH flows in, the reaction mixture turns gradually redder and thicker. At the same time, it permits white vapors to stream out of the reaction flask, through the bubbler, to the  $LN_2$ -cooled glass trap. The addition of NaOH should last over 60 minutes, but no longer than 90 minutes - the stopcock of the additional funnel gets easily clogged as NaOH cools and precipitates. Near the completion of

addition, no further white vapors could be visible. Keep the reaction mixture stirred even after the addition is complete, at least additional one and a half hours to complete the reaction. Then, **isolate the LN<sub>2</sub>-cooled trap by closing off the outlet Swagelok valve (V2) to the air followed by the inlet Swagelok valve to the glass bubbler (V1)**. Now it is ready for charging the cylinder.

#### **2.4 Charging the pre-empted 13L beverage cylinder (Scheme S1 B)**

- (1) Connect to the vacuum line the Teflon-tubing end coming out of the outlet Swagelok valve of LN<sub>2</sub>-cooled glass trap (connect V2 and V3).
- (2) Open up the outlet Swagelok valve (V2) and evacuate the body of the glass trap down below 20 mTorr.
- (3) Open the manual valve of a pre-empted 13 L beverage cylinder (V8) – make sure no outgassing from the pre-evacuated cylinder.
- (4) Once an ultimate vacuum is established inside the system (glass trap and cylinder V2, V3, V4, V5, V7, V8 – open; V6 - closed) down below 20 mTorr regardless of scroll pump conditions, shut off the Swagelok valve to scroll pump (V7) and remove the dewar out of the glass trap.
- (5) Monitor the rise of pressure with the combination of a Convectron/Pirani gauge (below 1 Torr) and a membrane (Baratron) gauge (1 Torr to 800 Torr) - just let the glass trap warm up by itself or, if necessary, only rub with your hands the body of glass trap. The pressure may arise to 120 Torr within 12±1 minute period.
- (6) Close off the manual valve (V8) of the cylinder and place the LN<sub>2</sub>-containing dewar back to the glass trap in order to re-condense back diacetylene from the line – the condensed materials in the glass trap will be eventually discarded.

#### **2.5 Diluting (5%) in argon gas (Scheme S1 B):**

- (7) Evacuate the whole line down below 50 mTorr, which includes the regulator with diaphragm valve dialed in and outlet valve opened (V6 must be opened). Before continue, make sure that the cold trap is isolated so that no high pressure can go inside. Then, flush the regulator twice the charge-purge cycle as follows (8-10):
- (8) Close off the outlet valve of the argon regulator.
- (9) Twist-open the manual valve of the argon tank to release gas in; close off afterward.
- (10) Discharge the trapped gas to the active vacuum by opening up the outlet valve of the regulator and pumping down below 50 mTorr.
- (11) Repeat once the cycle (8-10).

You are ready to dilute (5%) diacetylene (for example, 156 Torr / ~3 psi) in argon gas.

- (12) Close off two Swagelok valves to the corresponding pressure gauges (V4 and V5) in order to prevent any damage. Check that V2 and V3 is closed. Permittable pressure range for Teflon tubes may be lower than you may need to build in 13L cylinder.
- (13) Dial-out all the way the diaphragm valve and close off the outlet valve of the argon regulator.
- (14) Twist-open the manual valve of the argon tank to release argon in.
- (15) Slowly dial inward the diaphragm valve to regulate the gas output at 60 psi.
- (16) Close off the Swagelok valve to the scroll pump (V7).
- (17) Open up the outlet valve of the regulator to fill the whole closed system at the regulated pressure.
- (18) Finally open up the manual valve (V8) of the diacetylene-containing cylinder and wait until the hissing stops - temporarily turn off the scroll pump for better hearing.
- (19) Close the manual valve of the diacetylene cylinder (V8).

(20) Close off the manual valve of the argon tank and evacuate the regulator and the vacuum line all the way to the scroll pump (open V7).

(20) after the high Ar pressure is gone (less than 1 atm) open V4 and V5 to monitor the pressure.

(21) Open V3 and evacuate the V2-V3 line.

5% diacetylene mixture in argon with a total pressure of about 60 psi is done. Label the diacetylene cylinder with the date, name of the mixture (diacetylene in Ar), formula, concentration, total pressure, and your name.

## 2.6 Finishing the experiment

After the experiment is done (typically at after lunch), the first thing is to assess “potential safety hazard” associated with after the experiment. Make sure to unplug/switch off heating elements, stop running water through the condenser, and stop helium flow.

The next thing would discard whatever materials still remain in the glass trap. Do this in the following sequence:

- (1) Remove the LN<sub>2</sub>-containing dewar out of the glass trap,
- (2) vent the glass trap to air,
- (3) take the orange clip off from the joint connection,
- (4) gently twist the glass trap off the inner male ground glass,
- (5) place the glass trap inside the cup sink of the fume hood.

After this, you may want to quench the reaction mixture in the round bottom flask with plenty of water. Please also soak and rinse in water all other glassware that include glass bubbler, additional funnel, etc. Next day, clean dirty glassware either chemically using liquid soap/ethanol/water/etc or mechanically brushing/sucking through an active vacuum/etc. Finally, dry out glassware inside the oven at about 100 °C.

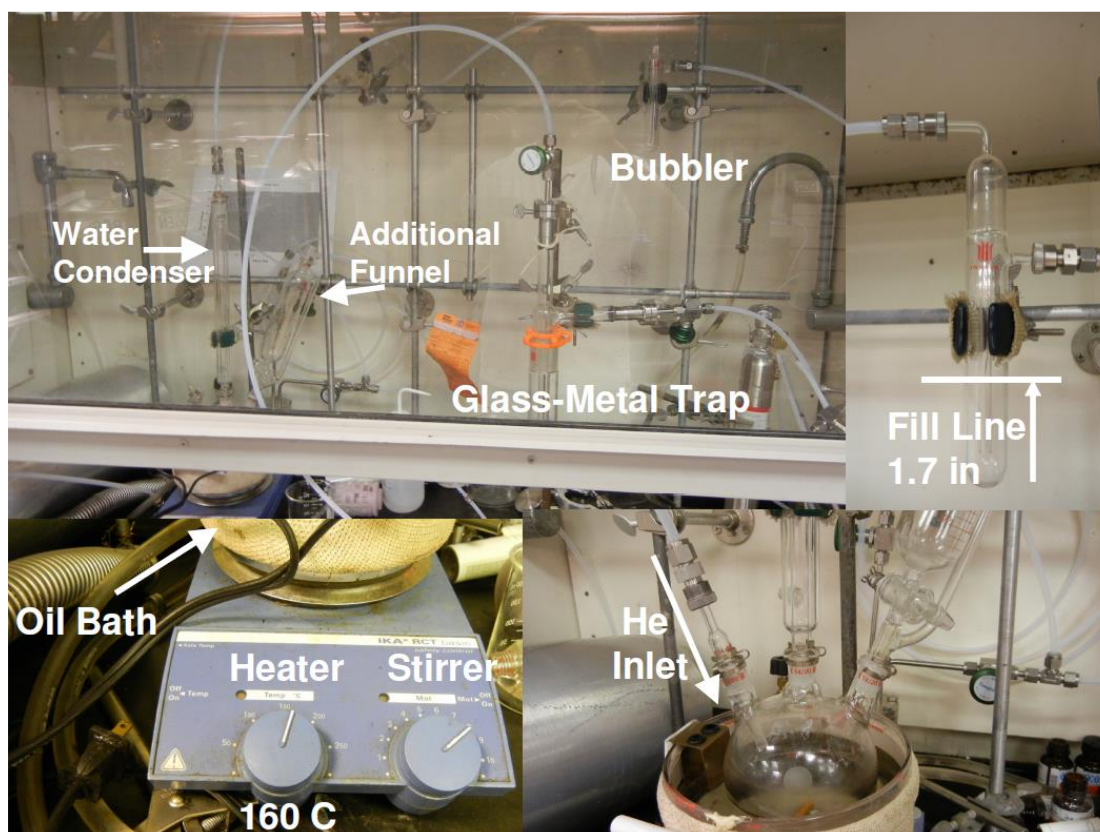


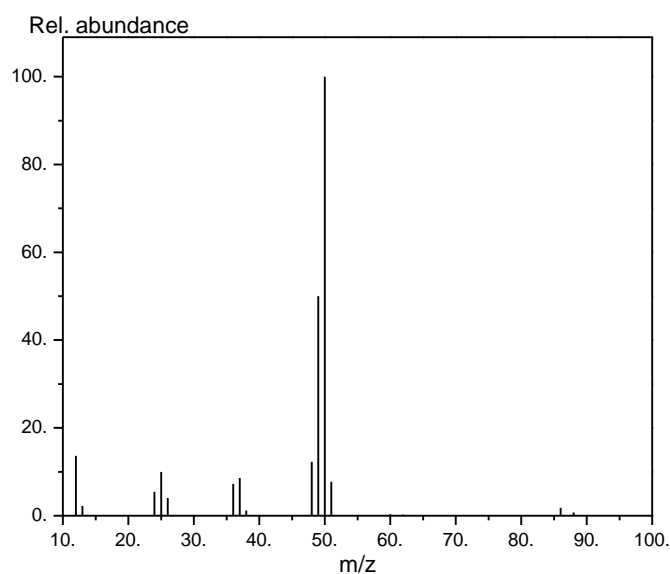
Figure S5. Photo of the experimental setup

## 2.7 Reference mass-spectrum

Mass spectrums (Figure S4) were recorded on the QMS QMI 422 (Pfeiffer Vacuum) at 100 eV.

**Table S1. Mass spectrum of crude diacetylene (C<sub>4</sub>H<sub>2</sub>) 5% in Ar – 100 eV EI**

m/z	assignment	relative intensity (%)
Main lines		
12	C <sup>+</sup>	14
13	CH <sup>+</sup>	2
24	C <sub>2</sub> <sup>+</sup>	5
25	C <sub>2</sub> H <sup>+</sup>	10
26	C <sub>2</sub> H <sub>2</sub> <sup>+</sup>	4
36	C <sub>3</sub> <sup>+</sup>	7
37	C <sub>3</sub> H <sup>+</sup>	9
38	C <sub>3</sub> H <sub>2</sub> <sup>+</sup>	1
48	C <sub>4</sub> <sup>+</sup>	12
49	C <sub>4</sub> H <sup>+</sup>	50
50	C <sub>4</sub> H <sub>2</sub> <sup>+</sup>	100
51	<sup>12</sup> C <sub>3</sub> <sup>13</sup> CH <sub>2</sub> <sup>+</sup>	8
Side product on the baseline		
m/z	assignment	relative intensity (%)
60	C <sub>2</sub> H <sup>35</sup> Cl <sup>+</sup>	0.4
62	C <sub>2</sub> H <sup>37</sup> Cl <sup>+</sup>	0.2
86	C <sub>4</sub> H <sub>3</sub> <sup>35</sup> Cl <sup>+</sup>	2
88	C <sub>4</sub> H <sub>3</sub> <sup>37</sup> Cl <sup>+</sup>	1



**Figure S6. Mass-spectrum of diacetylene recorded at 100 eV**



### 3. 1,3-butadiynyl + 2-methyl-1,3-butadiene PES, description of hydrogen loss channels.

The computational results of the 1,3-butadiynyl - 2-methyl-1,3-butadiene system correlate well with the reaction mechanisms derived in the 1,3-butadiynyl - 1,3-butadiene system. Our electronic structure calculations identified 28 reaction intermediates (**i14** – **i41**) connected via 36 transition states (Figures S11 and S12) on the pathways to atomic hydrogen elimination. Compared to the 1,3-butadiene – 1,3-butadiynyl system, the methyl substituent in the diene chain breaks the symmetry, which results in an increasing number of chemically non-equivalent carbon atoms in the diene chain. Therefore, the discussion of the reaction mechanisms is ‘split’ into two parts: (i) the addition of the 1,3-butadiene radical to the C1=C2 (Figures S12) and (ii) the addition of the 1,3-butadiene radical to the C3=C4 (Figures S11) double bonds in 2-methyl-1,3-butadiene. Both pathways reveal an improbability of the hydrogen loss channel from the initial collision complexes **i14** and **i29**; this finding is in analogy to the lack of the **i1**→**p6** + **H** pathway in the 1-butadiynyl – 1,3-butadiene system accounting for 2% at most. With respect to the radical addition to C1=C2, the major difference is the lack of pathways from **i32** and **i33** to **i34** in analogy of **i4** and **i5** isomerizing to **i6**. With respect to the C3=C4 addition pathways, the major distinguishing feature is the presence of an additional channel involving H losses from the methyl group of 2-methyl-1,3-butadiene after cyclization. These pathways access methyl-substituted derivatives of methylenecyclohexadiene **p7** and **p8**.

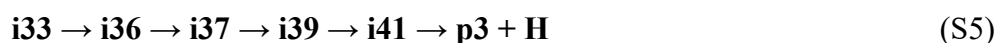
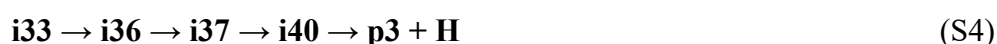
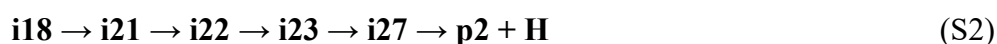
In detail, the 1-butadiynyl radical can be added without a barrier to any of the four carbon atoms of the C1=C2 and C3=C4 double bonds in 2-methyl-1,3-butadiene. Addition to C2 or C3 positions forms intermediates **i14** or **i29**. These structures can isomerize via two distinct cyclopropanyl ring closures. In the first type, closure occurs inside the diene moiety forming the C2–C4 sigma bond (**i14**→**i16**) or C1–C3 (**i29**→**i31**) followed by ring opening to **i19** and **i34**, respectively. During the second-type ring closure a sigma bond forms between C4 or C1 atoms and the nearest carbon atom of the 1-butadiynyl moiety accessing **i15** and **i30** with subsequent ring opening to **i17** and **i32**, respectively. Complexes **i17** and **i32** also can be accessed directly through the 1-butadiynyl radical addition to C4 and C1 of 2-methyl-1,3-butadiene. Intermediate **i32** further can undergo reaction steps to what for **i4** in the 1-butadiynyl + 1,3-butadiene reaction mechanism reaching **i33-i41**, which can be seen as methylated **i5-i13**. The only difference is the absence of possible steps from **i32** and **i33** to **i34**, analogues of **i4** and **i5** to **i6** with  $E_a$  of 165 and 160 kJ mol<sup>-1</sup>. Eventually, after addition to C1=C2 double bond five distinct products can be formed in unimolecular decomposition through hydrogen atom loss: *p*-tolylacetylene (**p3**; -391 kJ mol<sup>-1</sup>) from **i40** and **i41**; *E*-3-methylnona-1,3-dien-5,7-diyne (**p11**; -151 kJ mol<sup>-1</sup>) from **i32**, **i33**, **i36**, and **i38**; *Z*-3-methylnona-1,3-dien-5,7-diyne (**p12**; -149 kJ mol<sup>-1</sup>) from **i32**, **i33**, **i36**, **i37**, and **i38**; *Z*- and *E*-4-methylnona-1,3-dien-5,7-diyne (**p13** and **p14**; -148 and 142 kJ mol<sup>-1</sup>) from **i34**.

In the case of radical addition to C3=C4, intermediate **i17** also follows reaction steps to what for **i4** in the 1-butadiynyl + 1,3-butadiene reaction mechanism, but with two differences:

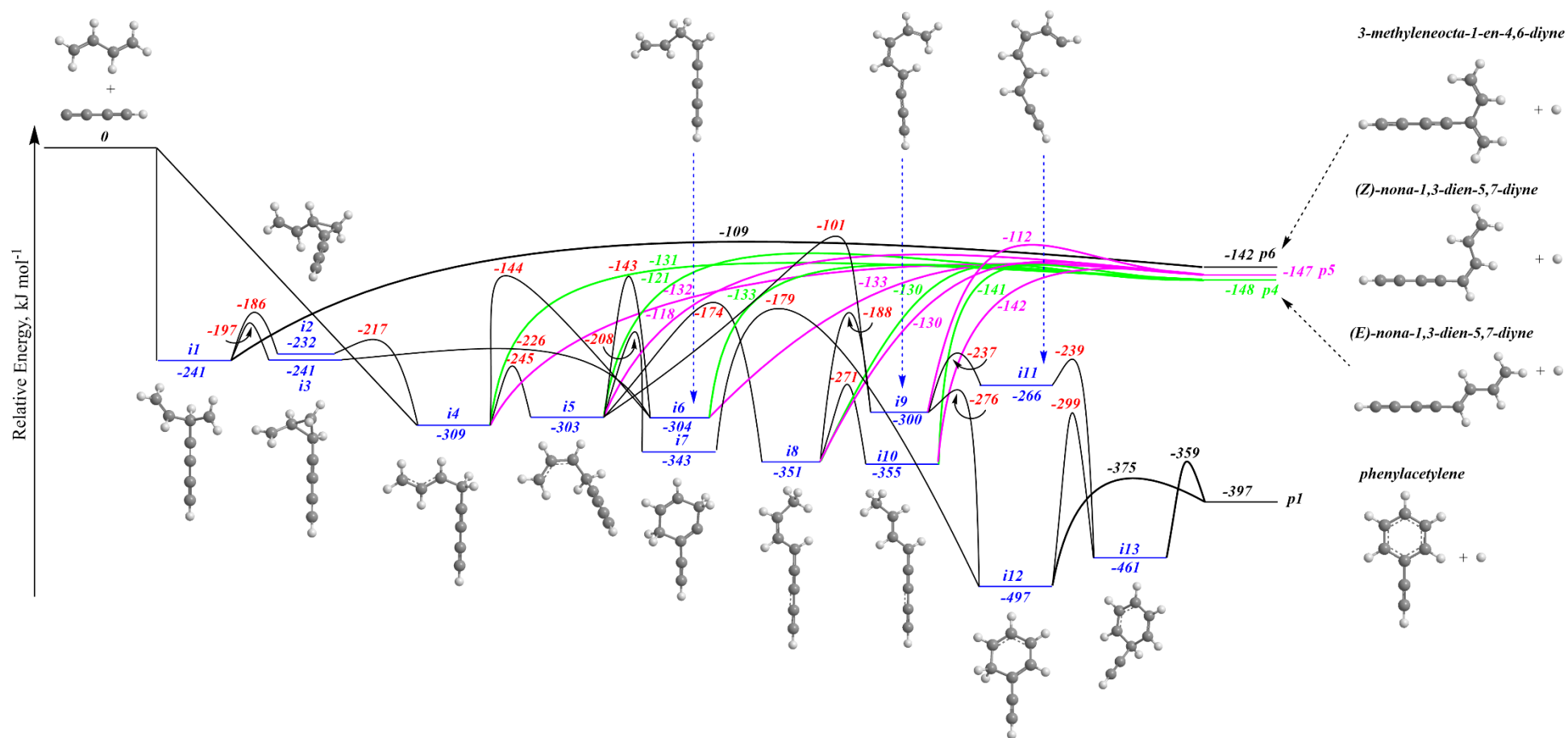
- (i) the major difference is the presence of an additional distinct channel that leads to methylenecyclohexadiene derivatives **p7** and **p8**, a chemical class of products that is not present even on full PES for 1-butadiynyl / 1,3-butadiene system and it cannot be formed in C1=C2 addition;
  - (ii) an absence of *cis/trans* isomerization step for **i21** (analog of **i8**→**i10/i35**→**i38**) around C3=C4 double bond, simply because there are not enough distinct substituent groups around this bond.
- This new pathway to **p7** and **p8** was opened by the specific structure of **i22** (homolog of **i9**, isomer of **i37**). Inter rotations in **i22** around single bonds allow low barrier ( $E_a = 64 \text{ kJ mol}^{-1}$ ) hydrogen atom migration from the methyl group of the 2-methyl-1,3-butadiene moiety and formation of resonantly stabilized radical **i24**, followed by six-membered ring closure to **i26** via a  $60 \text{ kJ mol}^{-1}$  barrier, which further one more time involves the CH<sub>3</sub> group of the 2-methyl-1,3-butadiene moiety in the hydrogen shift to access **i28** ( $E_a = 180 \text{ kJ mol}^{-1}$ ).

In summary, after addition of the 1,3-butadiynyl radical to the C1=C2 double bond in 2-methyl-1,3-butadiene, five distinct products can be accessed via unimolecular decomposition of distinct reaction intermediates through hydrogen atom loss: *p*-tolylacetylene (**p3**;  $-391 \text{ kJ mol}^{-1}$ ) from **i40** and **i41**; *E*-3-methylnona-1,3-dien-5,7-diyne (**p11**;  $-151 \text{ kJ mol}^{-1}$ ) from **i32**, **i33**, **i36**, and **i38**; *Z*-3-methylnona-1,3-dien-5,7-diyne (**p12**;  $-149 \text{ kJ mol}^{-1}$ ) from **i32**, **i33**, **i36**, **i37**, and **i38**; *Z*- and *E*-4-methylnona-1,3-dien-5,7-diyne (**p13** and **p14**;  $-148$  and  $142 \text{ kJ mol}^{-1}$ ) from **i34**. After addition of the 1-butadiynyl radical to the C3=C4 double bond, yet the additional five C<sub>9</sub>H<sub>8</sub> isomers can be prepared through atomic hydrogen losses: *m*-tolylacetylene (**p2**;  $-391 \text{ kJ mol}^{-1}$ ) from **i25** and **i27**; 1-ethynyl-3-methylenecyclohexa-1,4-diene (**p7**;  $-279 \text{ kJ mol}^{-1}$ ) from **i28**; 1-ethynyl-5-methylenecyclohexa-1,3-diene (**p8**;  $-265 \text{ kJ mol}^{-1}$ ) from **i25**, **i26**, and **i28**; (*E*)-2-methylnona-1,3-dien-5,7-diyne (**p9**;  $-147 \text{ kJ mol}^{-1}$ ) from **i17**, **i18**, **i19**, and **i21**; (*Z*)-2-methylnona-1,3-dien-5,7-diyne (**p10**;  $-139 \text{ kJ mol}^{-1}$ ) from **i17**, **i18**, **i19**, and **i22**.

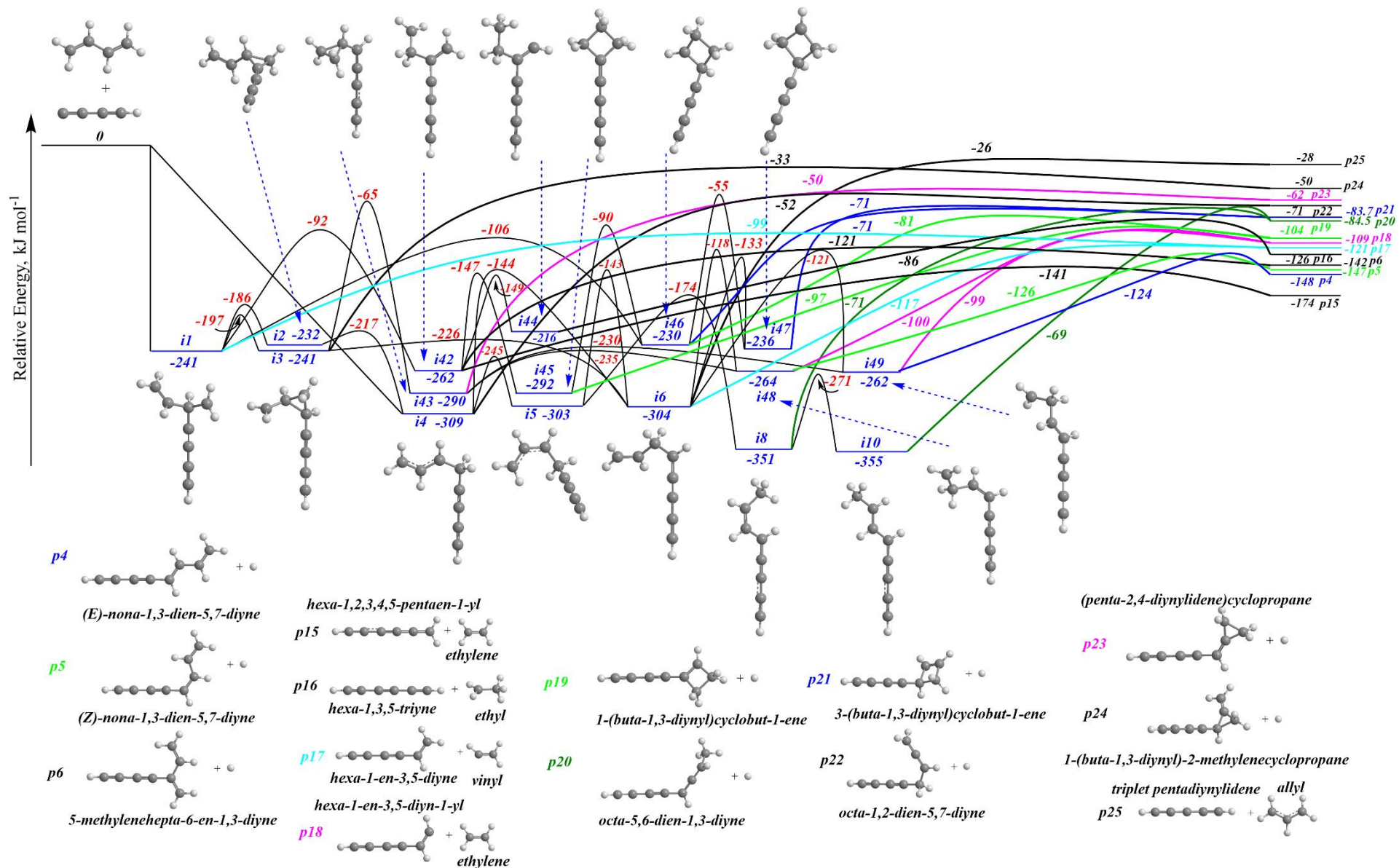
Overall, the barrierless addition of the 1,3-butadiynyl radical to the diene moiety in 2-methyl-1,3-butadiene followed by isomerization (hydrogen shifts, ring closure) accompanied by atomic hydrogen loss and aromatization leads to *m*-/*p*-tolylacetylene (**p2** and **p3**) via pathways (S1)-(S6):



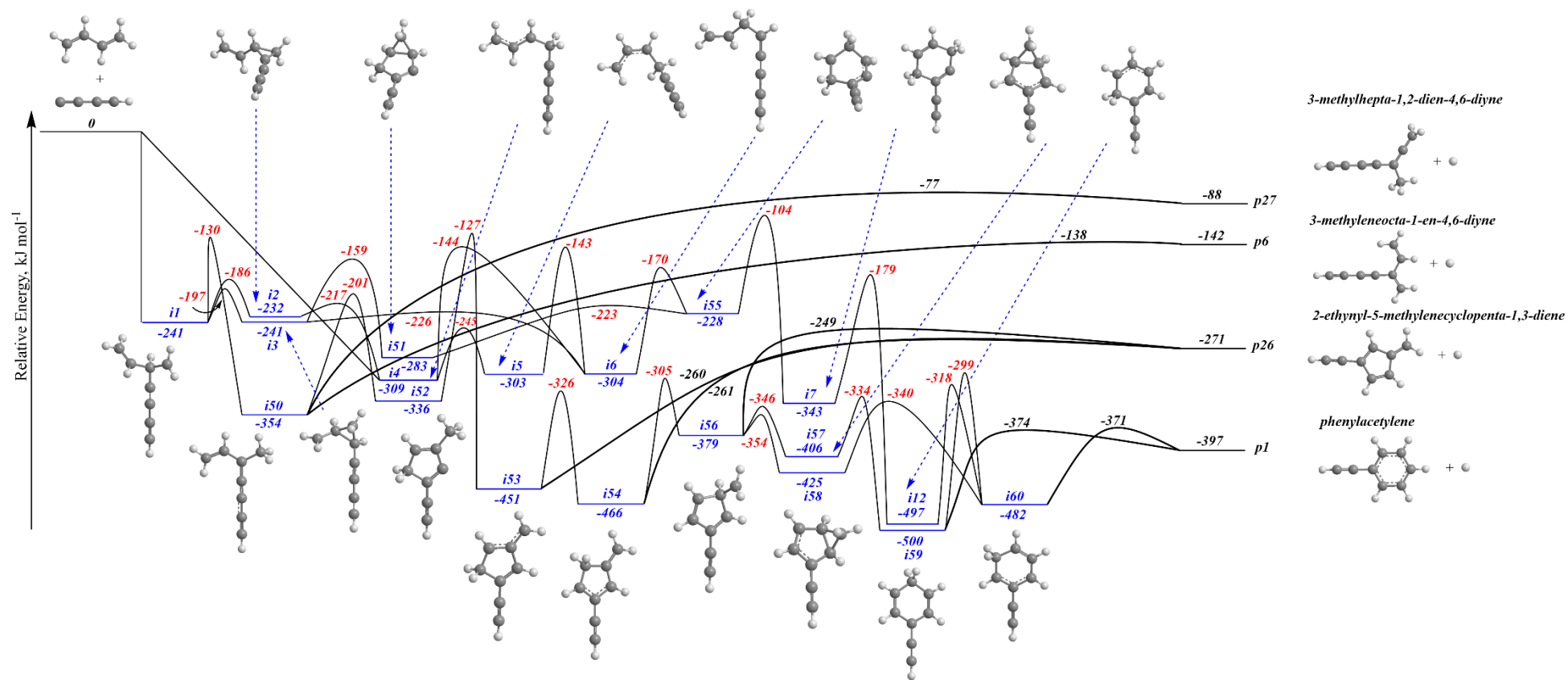
#### 4. Full PES for 1,3-butadiynyl + 1,3-butadiene



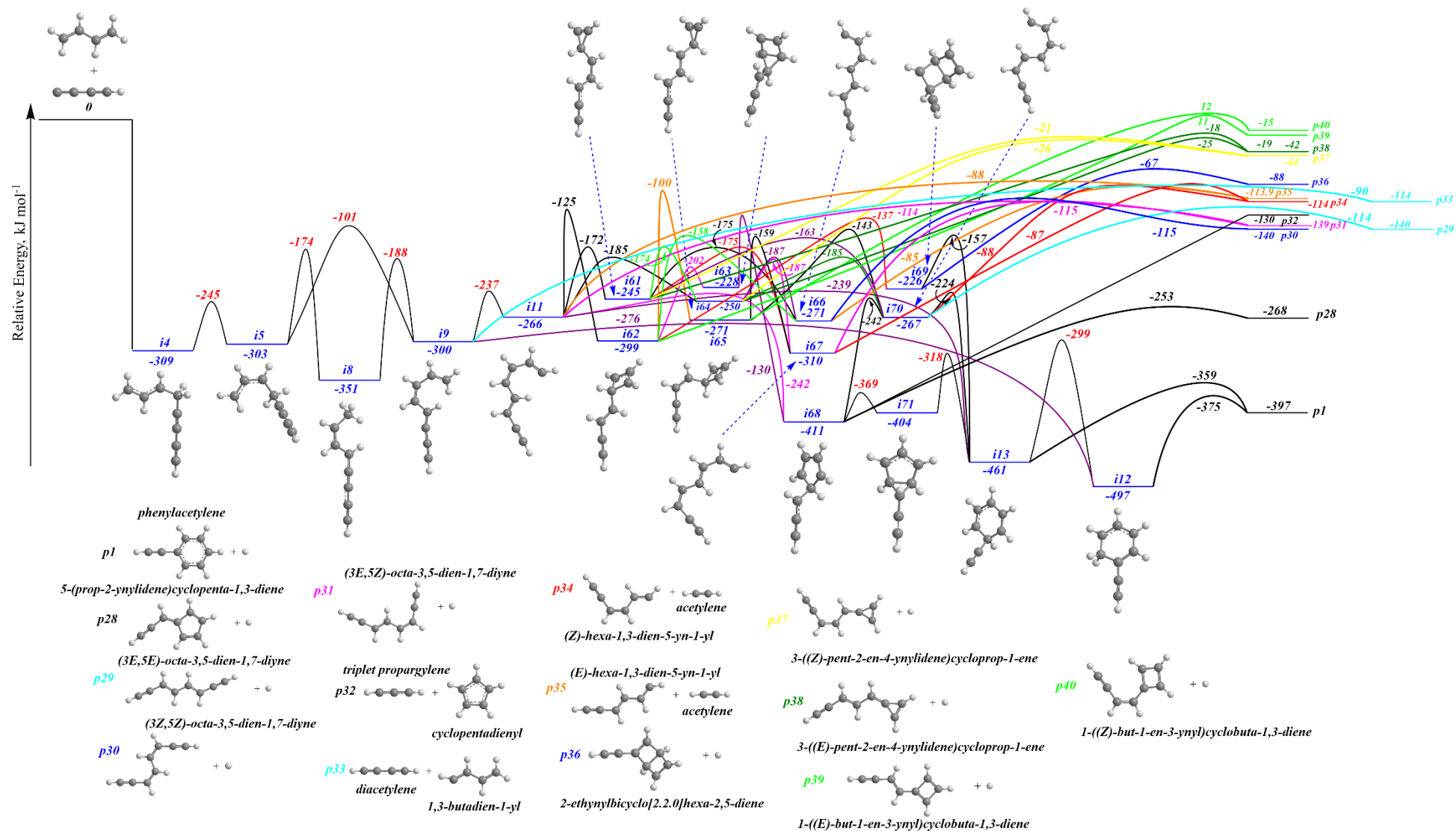
**Figure S7.** Potential energy surface for the bimolecular reaction of the 1,3-butadiynyl radical ( $\text{HCCCC}, X^2\Sigma^+$ ) with 1,3-butadiene ( $\text{CH}_2\text{CHCHCH}_2, X^1A_g$ ) leading to  $\text{C}_8\text{H}_6$  isomers plus the atomic hydrogen calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega\text{B97X-D}/6-311\text{G(d,p)}$  level of theory. Part I



**Figure S8.** Potential energy surface for the bimolecular reaction of the 1,3-butadiynyl radical ( $\text{HCCCC}, X^2\Sigma^+$ ) with 1,3-butadiene ( $\text{CH}_2\text{CHCHCH}_2, X^1A_g$ ) leading to  $\text{C}_8\text{H}_6$  isomers plus the atomic hydrogen as well as  $\text{C}_6\text{H}_4+\text{C}_2\text{H}_3$ ,  $\text{C}_6\text{H}_3+\text{C}_2\text{H}_4$ ,  $\text{C}_6\text{H}_2+\text{C}_2\text{H}_5$ ,  $\text{C}_5\text{H}_2+\text{C}_3\text{H}_5$  calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega\text{B97X-D/6-311G(d,p)}$  level of theory. Part II

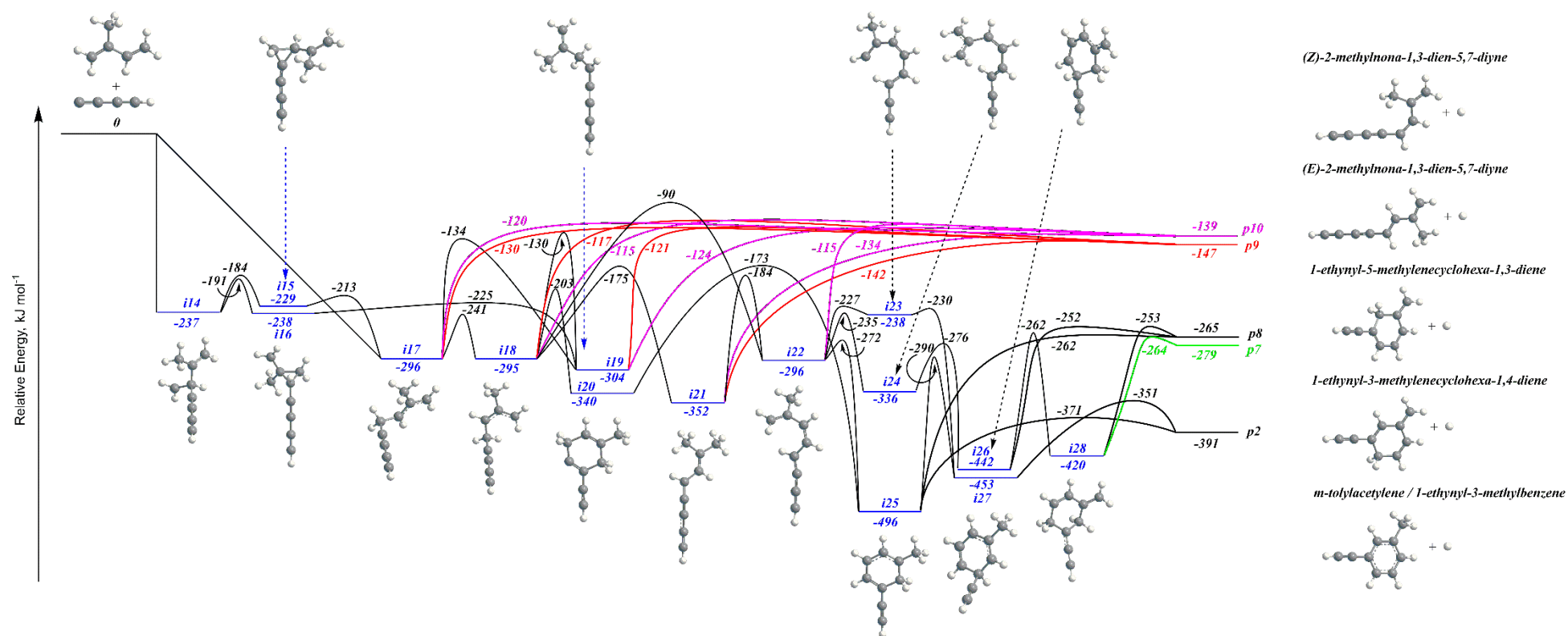


**Figure S9.** Potential energy surface for the bimolecular reaction of the 1,3-butadiynyl radical (HCCCC,  $X^2\Sigma^+$ ) with 1,3-butadiene ( $\text{CH}_2\text{CHCHCH}_2$ ,  $X^1A_g$ ) leading to  $\text{C}_8\text{H}_6$  isomers plus the atomic hydrogen calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega$ B97X-D/6-311G(d,p) level of theory. Part III



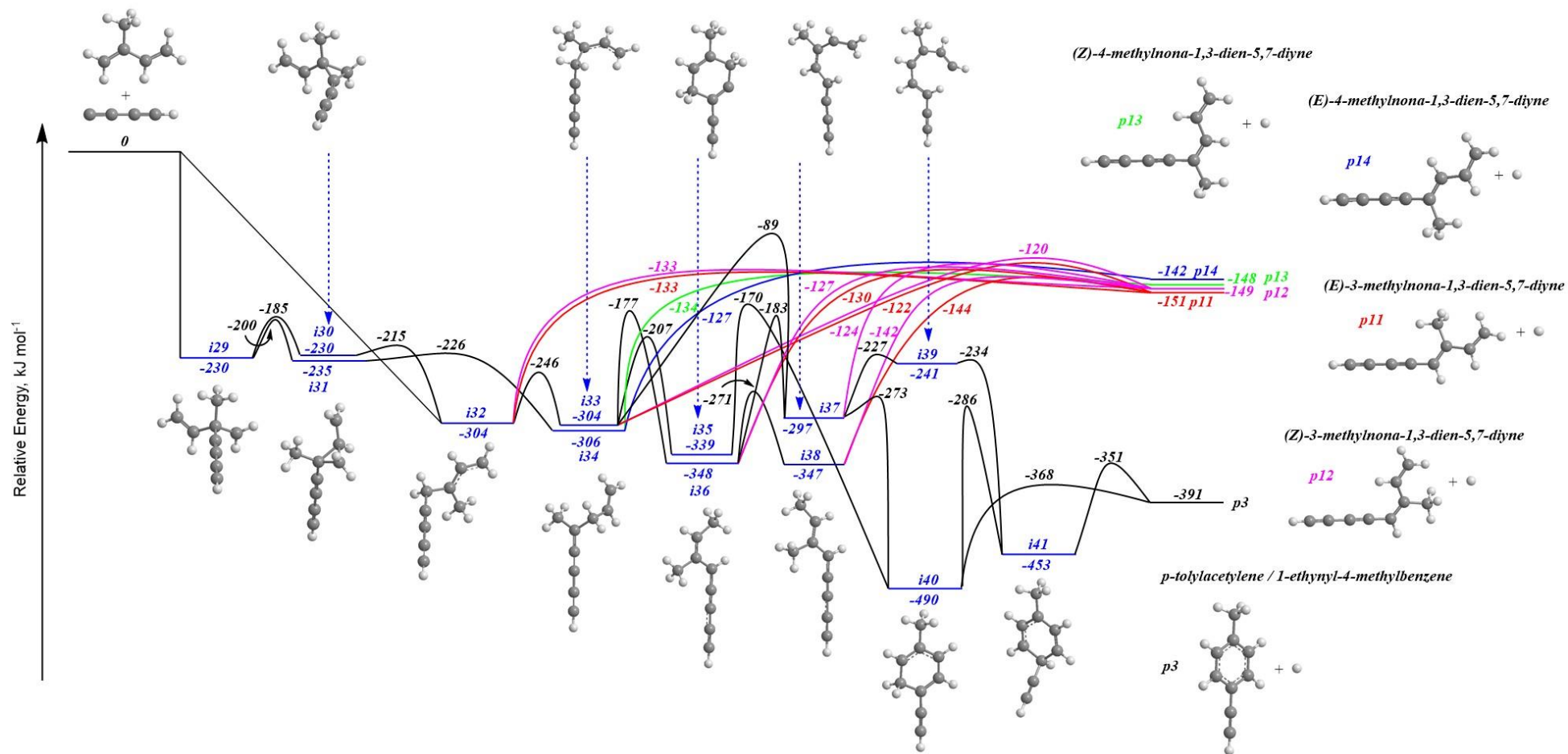
**Figure S10.** Potential energy surface for the bimolecular reaction of the 1,3-butadiynyl radical ( $\text{HCCCC}, X^2\Sigma^+$ ) with 1,3-butadiene ( $\text{CH}_2\text{CHCHCH}_2, X^1A_g$ ) leading to  $\text{C}_8\text{H}_6$  isomers plus the atomic hydrogen as well as  $\text{C}_6\text{H}_5+\text{C}_2\text{H}_2$ ,  $\text{C}_5\text{H}_5+\text{C}_3\text{H}_2$ ,  $\text{C}_4\text{H}_5+\text{C}_4\text{H}_2$  calculated at the CCSD(T)-F12/cc-pVTZ-F12// $\omega\text{B97X-D}/6\text{-311G(d,p)}$  level of theory. Part IV

## 5. Full PES for 1,3-butadiynyl + 2-methyl-1,3-butadiene



**Figure S11.** Potential energy surface for the bimolecular reaction of the 1,3-butadiynyl radical ( $\text{HCCCC}$ ,  $X^2\Sigma^+$ ) with 2-methyl-1,3-butadiene ( $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_2$ ;  $X^1A'$ ) leading to  $\text{C}_9\text{H}_8$  isomers plus the atomic hydrogen calculated at the G3(MP2,CC)// $\omega\text{B97X-D}/6\text{-}311\text{G}(\text{d,p})$  level of theory. Relative energies are given in  $\text{kJ mol}^{-1}$ . Part I

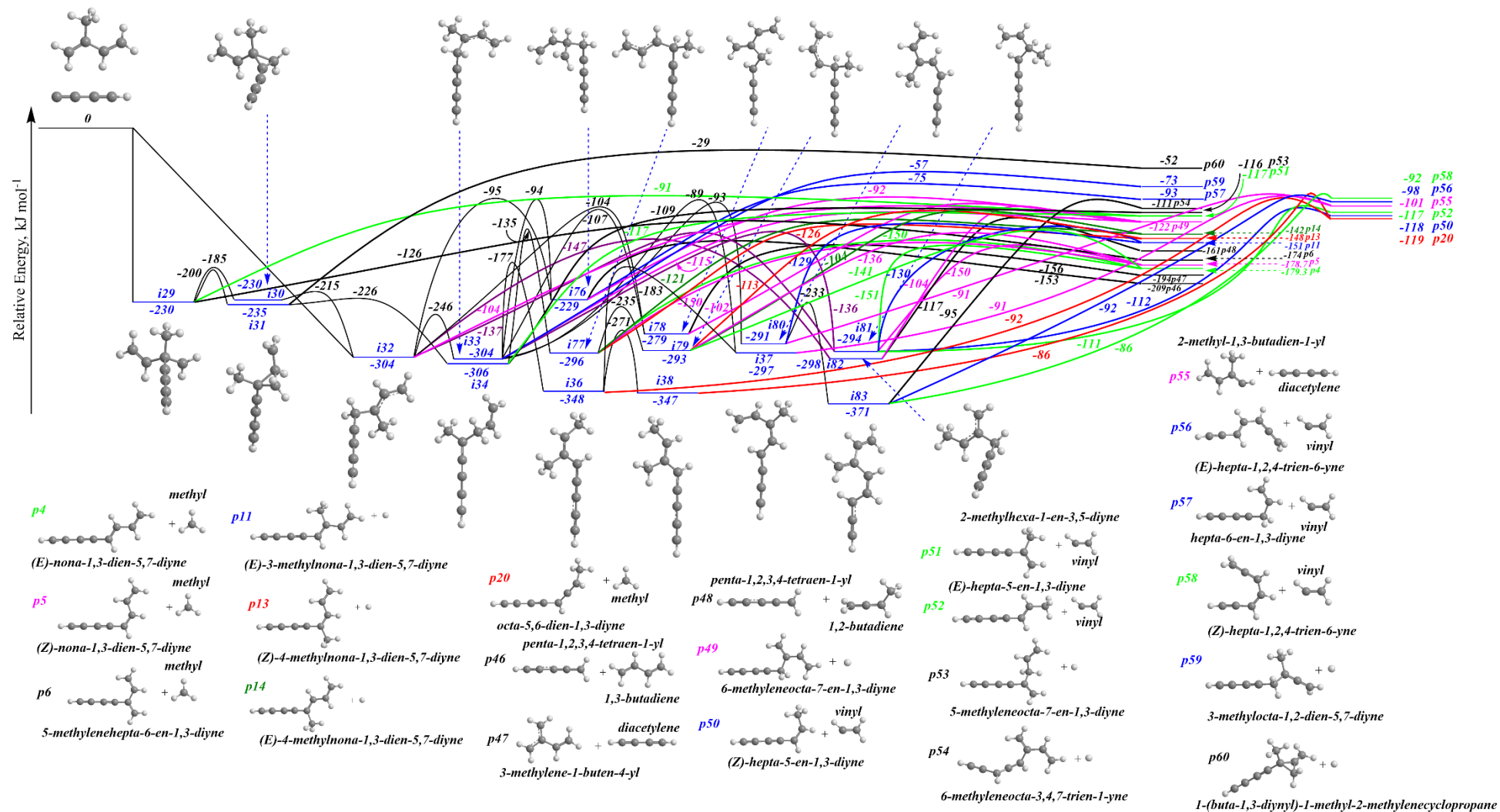




**Figure S12.** Potential energy surface for the bimolecular reaction of the 1,3-butadienyl radical ( $\text{HCCCC}, X^2\Sigma^+$ ) with 2-methyl-1,3-butadiene ( $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_2; X^1A'$ ) leading to  $\text{C}_9\text{H}_8$  isomers plus the atomic hydrogen calculated at the G3(MP2,CC)// $\omega$ B97X-D/6-311G(d,p) level of theory. Relative energies are given in  $\text{kJ mol}^{-1}$ . Part II





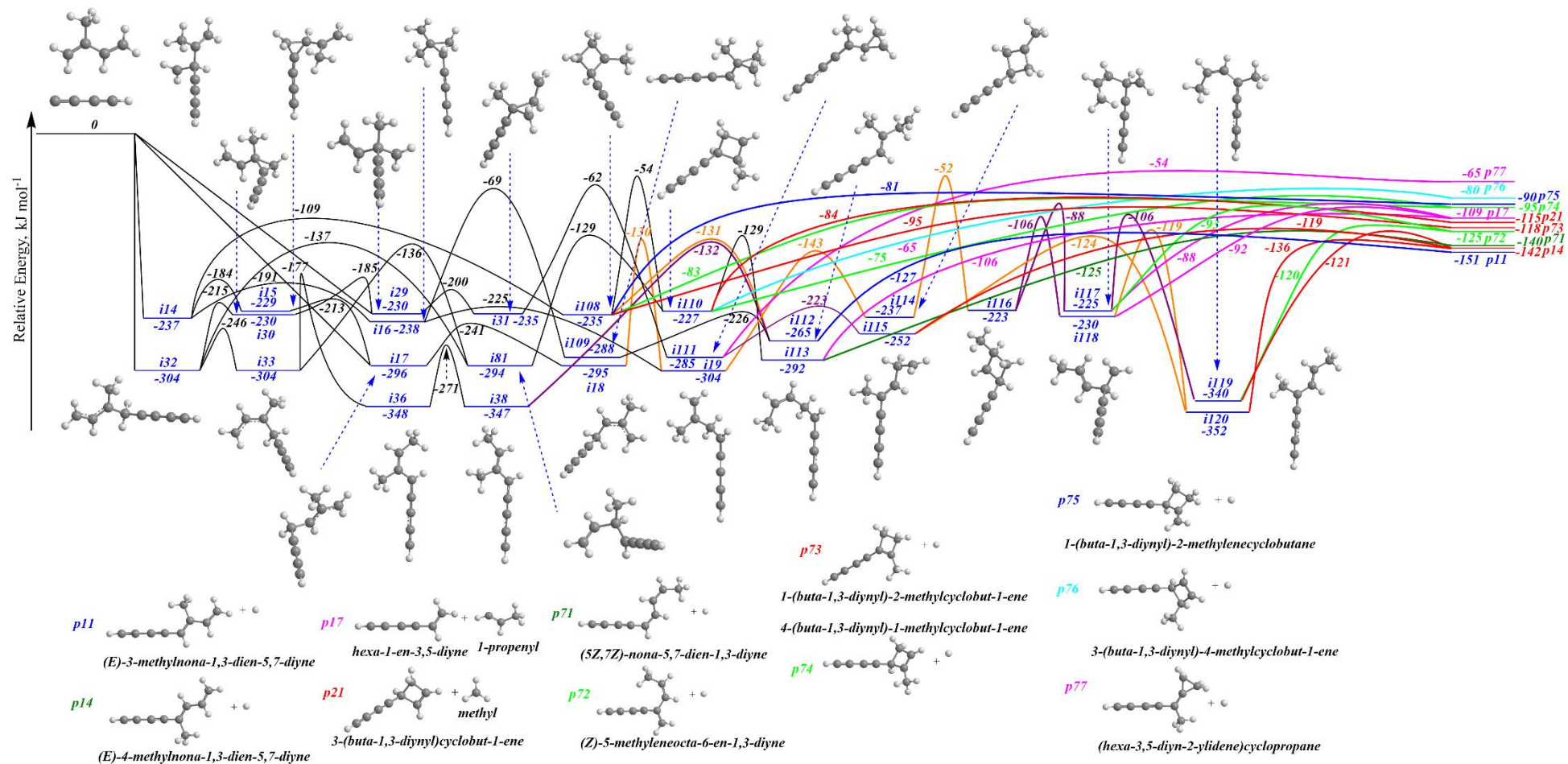


**Figure S14.** Potential energy surface for the bimolecular reaction of the 1,3-butadiynyl radical ( $\text{HCCCC}, X^2\Sigma^+$ ) with 2-methyl-1,3-butadiene ( $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_2; X^1\text{A}'$ ) leading to  $\text{C}_9\text{H}_8$  isomers plus the atomic hydrogen as well as  $\text{C}_8\text{H}_6+\text{CH}_3$ ,  $\text{C}_7\text{H}_6+\text{C}_2\text{H}_3$ ,  $\text{C}_5\text{H}_3+\text{C}_4\text{H}_6$ ,  $\text{C}_5\text{H}_7+\text{C}_4\text{H}_2$  calculated at the G3(MP2,CC)// $\omega\text{B97X-D}/6-311\text{G}(\text{d,p})$  level of theory. Relative energies are given in  $\text{kJ mol}^{-1}$ . Part IV

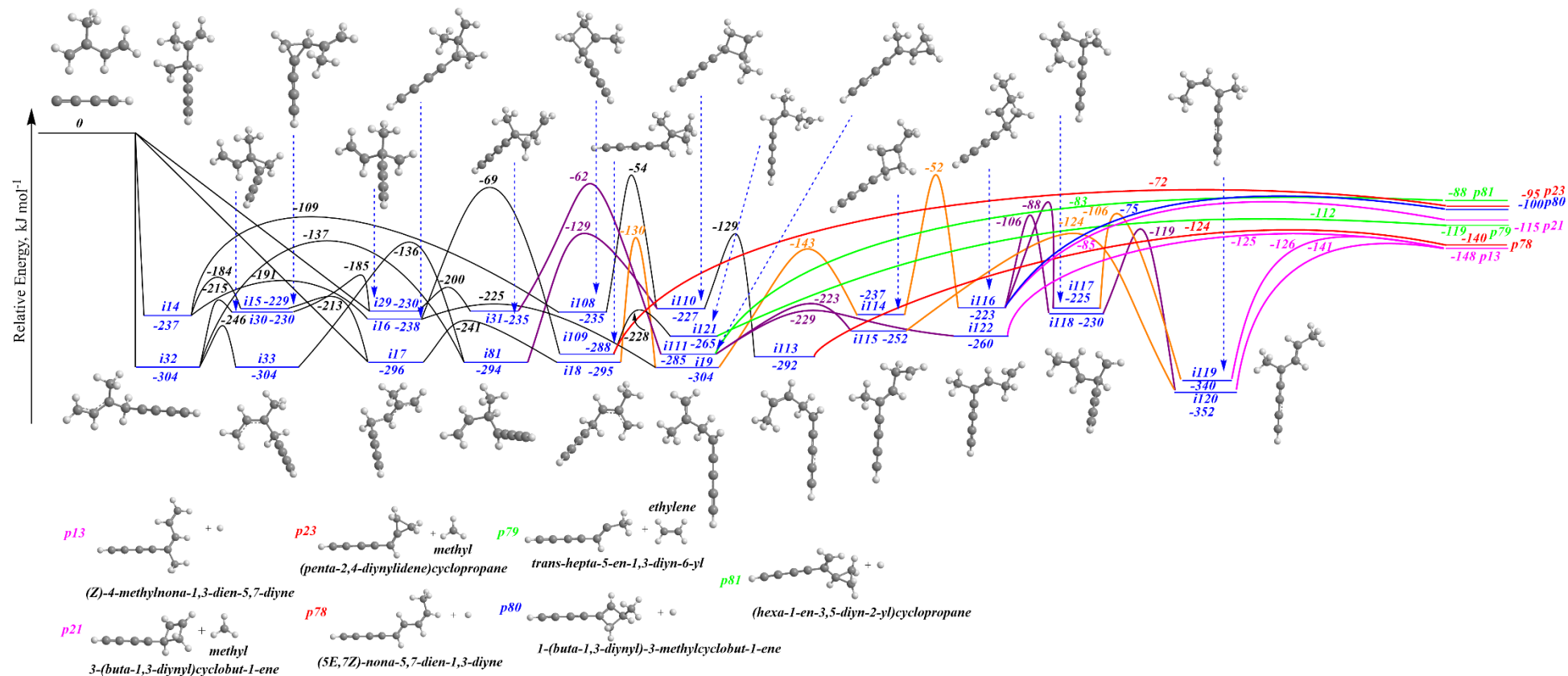








**Figure S17.** Potential energy surface for the bimolecular reaction of the 1,3-butadienyl radical ( $\text{HCCCC}, X^2\Sigma^+$ ) with 2-methyl-1,3-butadiene ( $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_2; X^1\text{A}'$ ) leading to  $\text{C}_9\text{H}_8$  isomers plus the atomic hydrogen as well as  $\text{C}_8\text{H}_6+\text{CH}_3$ ,  $\text{C}_6\text{H}_4+\text{C}_3\text{H}_5$  calculated at the G3(MP2,CC)// $\omega\text{B97X-D}/6-311\text{G(d,p)}$  level of theory. Relative energies are given in  $\text{kJ mol}^{-1}$ . Part VII



**Figure S18.** Potential energy surface for the bimolecular reaction of the 1,3-butadienyl radical ( $\text{HCCCC}$ ,  $X^2\Sigma^+$ ) with 2-methyl-1,3-butadiene ( $\text{CH}_2\text{C}(\text{CH}_3)\text{CHCH}_2$ ;  $X^1\text{A}'$ ) leading to  $\text{C}_9\text{H}_8$  isomers plus the atomic hydrogen as well as  $\text{C}_8\text{H}_6+\text{CH}_3$ ,  $\text{C}_7\text{H}_5+\text{C}_2\text{H}_4$  calculated at the G3(MP2,CC)// $\omega\text{B97X-D}/6-311\text{G(d,p)}$  level of theory. Relative energies are given in  $\text{kJ mol}^{-1}$ . Part VIII



## 6. Results of RRKM Calculations

**Table S2.** Statistical branching ratios (%) for the reaction of 1-butadiynyl+1,3-butadiene with *i1* and *i4* as initial intermediates at different collision energies ( $E_C$ , kJ mol<sup>-1</sup>)

$E_C$	0	23	0	23
Adduct	<i>i1</i>		<i>i4</i>	
<i>p1+H</i>	37.1	23.0	39.1	25.1
<i>p4+H</i>	29.9	36.1	28.9	35.1
<i>p5+H</i>	26.3	31.1	26.3	31.5
<i>p6+H</i>	1.6	2.0	1.4	1.7
<i>p15+C<sub>2</sub>H<sub>4</sub></i>	0.0	0.0	0.0	0.0
<i>p16+C<sub>2</sub>H<sub>5</sub></i>	0.0	0.0	0.0	0.0
<i>p17+C<sub>2</sub>H<sub>3</sub></i>	4.7	7.3	4.1	6.2
<i>p18+C<sub>2</sub>H<sub>4</sub></i>	0.1	0.3	0.1	0.2
<i>p19+H</i>	0.0	0.0	0.0	0.0
<i>p20+H</i>	0.0	0.0	0.0	0.0
<i>p21+H</i>	0.0	0.0	0.0	0.0
<i>p22+H</i>	0.0	0.0	0.0	0.0
<i>p23+H</i>	0.0	0.0	0.0	0.0
<i>p24+H</i>	0.0	0.0	0.0	0.0
<i>p25+C<sub>3</sub>H<sub>5</sub></i>	0.0	0.0	0.0	0.0
<i>p26+H</i>	0.0	0.0	0.0	0.0
<i>p27+H</i>	0.0	0.0	0.0	0.0
<i>p28+H</i>	0.2	0.2	0.2	0.2
<i>p29+H</i>	0.0	0.0	0.0	0.0
<i>p30+H</i>	0.0	0.0	0.0	0.0
<i>p31+H</i>	0.0	0.0	0.0	0.0
<i>p32+C<sub>3</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0
<i>p33+C<sub>4</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0
<i>p34+C<sub>2</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0
<i>p35+C<sub>2</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0
<i>p36+H</i>	0.0	0.0	0.0	0.0
<i>p37+H</i>	0.0	0.0	0.0	0.0
<i>p38+H</i>	0.0	0.0	0.0	0.0
<i>p39+H</i>	0.0	0.0	0.0	0.0
<i>p40+H</i>	0.0	0.0	0.0	0.0



**Table S3.** Statistical branching ratios (%) for the reaction of 1-butadiynyl + 2-methyl-1,3-butadiene with **i14**, **i17**, **i29**, and **i32** as initial intermediates at different collision energies ( $E_c$ ,  $\text{kJ mol}^{-1}$ )

<i>Adduct</i>	<i>i14</i>		<i>i17</i>		<i>i29</i>		<i>i32</i>	
	<i>0</i>	<i>24</i>	<i>0</i>	<i>24</i>	<i>0</i>	<i>24</i>	<i>0</i>	<i>24</i>
<i>p1+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p2+H</i>	79.0	69.0	79.5	70.0	0.0	0.0	0.0	0.0
<i>p3+H</i>	0.0	0.0	0.0	0.0	58.0	41.4	61.6	46.3
<i>p4+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	3.2	3.9	2.8	3.4
<i>p5+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	2.8	3.4	2.5	3.1
<i>p6+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.6	1.0	0.4	0.6
<i>p7+H</i>	2.0	1.9	2.0	1.9	0.0	0.0	0.0	0.0
<i>p8+H</i>	4.9	5.2	5.0	5.3	0.0	0.0	0.0	0.0
<i>p9+H</i>	9.9	16.2	9.8	16.0	0.0	0.0	0.0	0.0
<i>p10+H</i>	3.3	5.9	3.2	5.6	0.0	0.0	0.0	0.0
<i>p11+H</i>	0.0	0.0	0.0	0.0	13.2	16.8	14.0	18.8
<i>p12+H</i>	0.0	0.0	0.0	0.0	9.9	12.9	10.5	14.5
<i>p13+H</i>	0.0	0.0	0.0	0.0	4.6	6.7	2.9	3.9
<i>p14+H</i>	0.0	0.0	0.0	0.0	3.3	5.3	2.1	3.1
<i>p15+C<sub>3</sub>H<sub>6</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p17+C<sub>3</sub>H<sub>5</sub></i>	0.3	0.7	0.2	0.5	0.0	0.0	0.0	0.0
<i>p20+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p21+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p22+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p23+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p24+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p26+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p27+CH<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p35+C<sub>3</sub>H<sub>4</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p41+C<sub>3</sub>H<sub>4</sub></i>	0.4	0.7	0.2	0.5	0.0	0.0	0.0	0.0
<i>p42+H</i>	0.2	0.3	0.1	0.2	0.0	0.0	0.0	0.0
<i>p43+C<sub>4</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p44+C<sub>3</sub>H<sub>4</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p45+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p46+C<sub>4</sub>H<sub>6</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p47+C<sub>4</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p48+C<sub>4</sub>H<sub>6</sub></i>	0.0	0.0	0.0	0.0	0.3	0.6	0.4	0.6
<i>p49+H</i>	0.0	0.0	0.0	0.0	0.6	1.1	0.6	1.3
<i>p50+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p51+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	2.9	5.6	1.9	3.3
<i>p52+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p53+H</i>	0.0	0.0	0.0	0.0	0.4	0.9	0.3	0.5
<i>p54+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p55+C<sub>4</sub>H<sub>2</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p56+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p57+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p58+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p59+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p60+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p61+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p62+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p63+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p64+H</i>	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
<i>p65+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p66+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p67+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p68+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p69+C<sub>2</sub>H<sub>3</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p70+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

<i>p71+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p72+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p73+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p74+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p75+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p76+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p77+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p78+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p79+C<sub>2</sub>H<sub>4</sub></i>	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1
<i>p80+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p81+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p82+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p83+C<sub>2</sub>H<sub>4</sub></i>	0.0	0.0	0.0	0.0	0.1	0.2	0.1	0.2
<i>p84+C<sub>2</sub>H<sub>4</sub></i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p85+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
<i>p86+H</i>	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

**Table S4.** RRKM calculated rate constants ( $k(E)$ ,  $s^{-1}$ ) of the reaction of 1-butadiynyl+1,3-butadiene as functions of the internal energy ( $E$ ,  $\text{kJ mol}^{-1}$ ) of the intermediate states for unimolecular reaction steps at different collision energies ( $E_c$ ,  $\text{kJ}\cdot\text{mol}^{-1}$ )

$E_c$	0		23		$E_c$	0		23		
	Reaction step	$k(E)$	$E$	$k(E)$		$E$	Reaction step	$k(E)$	$E$	$k(E)$
	<i>i4 - i2</i>	1.98E+09	309	3.02E+09	332	<i>i13 - p1</i>	6.02E+10	461	7.76E+10	484
	<i>i2 - i4</i>	1.74E+12	232	1.91E+12	255	<i>i46 - i47</i>	6.80E+03	230	4.94E+04	253
	<i>i4 - p5</i>	1.43E+06	309	4.69E+06	332	<i>i47 - i46</i>	1.37E+04	236	1.02E+05	259
	<i>i4 - p22</i>	6.15E+00	309	1.13E+02	332	<i>i46 - i45</i>	9.41E+05	230	3.34E+06	253
	<i>i4 - i5</i>	5.38E+10	309	7.02E+10	332	<i>i45 - i46</i>	6.18E+04	292	2.90E+05	315
	<i>i5 - i4</i>	1.86E+11	303	2.39E+11	326	<i>i66 - p29</i>	7.45E+06	271	2.76E+07	294
	<i>i7 - i5</i>	1.55E+09	343	2.78E+09	366	<i>i46 - p21</i>	1.53E+05	230	9.76E+05	253
	<i>i5 - i7</i>	2.93E+08	303	4.52E+08	326	<i>i46 - p19</i>	2.97E+05	230	1.47E+06	253
	<i>i7 - i2</i>	4.93E+07	343	1.04E+08	366	<i>i70 - p30</i>	8.88E+06	267	3.16E+07	290
	<i>i2 - i7</i>	5.36E+03	232	1.56E+04	255	<i>i1 - i46</i>	5.28E+05	241	1.64E+06	264
	<i>i1 - p6</i>	4.43E+06	241	1.46E+07	264	<i>i46 - i1</i>	1.10E+07	230	3.35E+07	253
	<i>i1 - p17</i>	4.45E+06	241	1.79E+07	264	<i>i54 - i53</i>	6.56E+09	466	9.26E+09	489
	<i>i52 - i50</i>	1.58E+09	336	2.95E+09	359	<i>i53 - i54</i>	1.30E+10	451	1.79E+10	474
	<i>i50 - i52</i>	7.78E+06	354	1.49E+07	377	<i>i54 - i56</i>	2.26E+09	466	3.43E+09	489
	<i>i52 - i53</i>	3.00E+05	336	9.45E+05	359	<i>i56 - i54</i>	1.48E+10	379	1.86E+10	402
	<i>i53 - i52</i>	2.27E+02	451	9.35E+02	474	<i>i56 - i58</i>	1.39E+11	379	1.48E+11	402
	<i>i3 - p24</i>	8.98E+00	241	2.78E+02	264	<i>i58 - i56</i>	4.97E+11	425	5.97E+11	448
	<i>i5 - i8</i>	7.10E+07	303	1.39E+08	326	<i>i56 - i57</i>	7.56E+10	379	8.25E+10	402
	<i>i8 - i5</i>	3.23E+06	351	7.30E+06	374	<i>i57 - i56</i>	1.22E+12	406	1.44E+12	429
	<i>i5 - i9</i>	9.72E+04	303	4.27E+05	326	<i>i58 - i60</i>	1.05E+11	425	1.30E+11	448
	<i>i9 - i5</i>	3.93E+04	300	1.70E+05	323	<i>i60 - i58</i>	1.83E+09	482	2.52E+09	505
	<i>i8 - i9</i>	4.73E+06	351	9.67E+06	374	<i>i57 - i59</i>	1.68E+11	406	2.03E+11	429
	<i>i9 - i8</i>	8.41E+07	300	1.46E+08	323	<i>i59 - i57</i>	6.66E+08	500	9.63E+08	523
	<i>i9 - p33</i>	6.45E+04	300	4.00E+05	323	<i>i60 - i2</i>	1.69E+09	482	2.51E+09	505
	<i>i2 - i9</i>	8.07E+07	232	1.45E+08	255	<i>i2 - i60</i>	7.81E+08	232	1.19E+09	255
	<i>i9 - i2</i>	5.70E+10	300	6.20E+10	323	<i>i60 - p1</i>	1.05E+11	482	1.36E+11	505
	<i>i4 - p4</i>	1.87E+06	309	6.22E+06	332	<i>i60 - i59</i>	6.97E+08	482	1.09E+09	505
	<i>i5 - p4</i>	1.98E+06	303	7.44E+06	326	<i>i59 - i60</i>	7.17E+08	500	1.15E+09	523
	<i>i43 - i3</i>	4.37E+02	290	4.73E+03	313	<i>i59 - p1</i>	6.73E+10	500	8.93E+10	523
	<i>i3 - i43</i>	1.88E+04	241	1.63E+05	264	<i>i54 - p26</i>	3.49E+08	466	6.50E+08	489
	<i>i1 - i3</i>	2.11E+10	241	2.72E+10	264	<i>i56 - p26</i>	6.94E+08	379	1.13E+09	402
	<i>i3 - i1</i>	1.63E+11	241	2.13E+11	264	<i>i61 - i66</i>	9.28E+10	245	1.46E+11	268
	<i>i6 - i3</i>	4.53E+09	304	6.43E+09	327	<i>i66 - i61</i>	2.90E+09	271	5.12E+09	294
	<i>i3 - i6</i>	2.17E+12	241	2.37E+12	264	<i>i61 - i11</i>	2.69E+10	245	4.30E+10	268
	<i>i6 - p25</i>	1.37E-01	304	1.74E+01	327	<i>i11 - i61</i>	2.40E+09	266	4.23E+09	289
	<i>i42 - p15</i>	9.95E+08	262	2.42E+09	285	<i>i62 - i66</i>	1.10E+08	299	2.44E+08	322
	<i>i7 - i55</i>	9.74E+03	343	4.22E+04	366	<i>i66 - i62</i>	6.63E+07	271	1.31E+08	294
	<i>i55 - i7</i>	9.73E+06	228	2.68E+07	251	<i>i62 - i11</i>	1.57E+06	299	4.88E+06	322
	<i>i48 - i6</i>	3.97E+06	264	1.15E+07	287	<i>i11 - i62</i>	2.70E+06	266	7.34E+06	289
	<i>i6 - i48</i>	2.66E+05	304	9.09E+05	327	<i>i61 - p38</i>	1.29E-01	245	1.32E+01	268
	<i>i4 - i6</i>	3.67E+06	309	9.53E+06	332	<i>i64 - p38</i>	5.18E-01	250	2.97E+01	273
	<i>i6 - i4</i>	8.84E+06	304	2.26E+07	327	<i>i62 - i63</i>	1.66E+09	299	2.63E+09	322
	<i>i1 - i50</i>	6.28E+07	241	1.45E+08	264	<i>i63 - i62</i>	1.19E+12	228	1.40E+12	251
	<i>i50 - i1</i>	5.74E+04	354	2.03E+05	377	<i>i62 - p39</i>	0.00E+00	299	7.51E-05	322
	<i>i1 - i42</i>	2.48E+05	241	9.70E+05	264	<i>i71 - i68</i>	5.09E+12	404	5.59E+12	427
	<i>i42 - i1</i>	1.47E+05	262	6.34E+05	285	<i>i68 - i71</i>	2.20E+11	411	2.43E+11	434
	<i>i3 - i51</i>	3.26E+08	241	5.43E+08	264	<i>i11 - i68</i>	4.00E+11	266	4.49E+11	289
	<i>i51 - i3</i>	1.36E+09	283	2.85E+09	306	<i>i68 - i11</i>	3.43E+08	411	6.06E+08	434
	<i>i43 - i48</i>	3.08E+11	290	4.00E+11	313	<i>i70 - i68</i>	1.20E+11	267	1.35E+11	290
	<i>i48 - i43</i>	2.06E+11	264	2.37E+11	287	<i>i68 - i70</i>	3.08E+08	411	5.42E+08	434
	<i>i53 - p26</i>	6.41E+08	451	1.17E+09	474	<i>i62 - i69</i>	9.76E+05	299	2.55E+06	322
	<i>i1 - i2</i>	1.98E+10	241	2.76E+10	264	<i>i69 - i62</i>	2.32E+09	226	4.54E+09	249
	<i>i2 - i1</i>	1.17E+11	232	1.58E+11	255	<i>i68 - p28</i>	5.49E+08	411	9.43E+08	434
	<i>i2 - p1</i>	6.69E+10	232	8.80E+10	255	<i>i42 - i44</i>	6.44E+07	262	1.30E+08	285
	<i>i6 - i55</i>	2.85E+06	304	5.68E+06	327	<i>i44 - i42</i>	1.23E+10	216	2.00E+10	239
	<i>i55 - i6</i>	2.15E+10	228	3.18E+10	251	<i>i44 - p16</i>	2.42E+07	216	1.17E+08	239
	<i>i50 - p6</i>	5.95E+05	354	2.15E+06	377	<i>i63 - i68</i>	3.07E+09	228	6.93E+09	251
	<i>i51 - i55</i>	2.36E+11	283	3.18E+11	306	<i>i68 - i63</i>	6.36E+03	411	2.65E+04	434
	<i>i55 - i51</i>	8.94E+11	228	9.19E+11	251	<i>i71 - i13</i>	7.08E+10	404	8.96E+10	427
	<i>i42 - p6</i>	1.34E+07	262	4.21E+07	285	<i>i13 - i71</i>	1.47E+09	461	2.09E+09	484
	<i>i8 - i10</i>	7.30E+10	351	9.74E+10	374	<i>i13 - i69</i>	3.47E+03	461	1.14E+04	484
	<i>i10 - i8</i>	1.27E+11	355	1.71E+11	378	<i>i69 - i13</i>	2.32E+10	226	3.72E+10	249
	<i>i50 - p27</i>	3.99E+01	354	4.12E+02	377	<i>i66 - p35</i>	2.68E+05	271	1.70E+06	294
	<i>i8 - p4</i>	4.22E+05	351	1.67E+06	374	<i>i11 - p35</i>	4.47E+05	266	2.63E+06	289
	<i>i8 - p20</i>	1.71E+01	351	2.00E+02	374	<i>i69 - p36</i>	1.51E+05	226	9.52E+05	249
	<i>i8 - p5</i>	1.27E+06	351	5.02E+06	374	<i>i70 - p34</i>	3.63E+05	267	2.10E+06	290

<i>i9 - i11</i>	4.38E+09	300	5.74E+09	323	<i>i68 - p32</i>	6.99E+05	411	2.88E+06	434
<i>i11 - i9</i>	1.14E+11	266	1.32E+11	289	<i>i62 - i65</i>	1.40E+05	299	6.57E+05	322
<i>i5 - i6</i>	1.07E+07	303	2.76E+07	326	<i>i65 - i62</i>	1.26E+06	271	5.36E+06	294
<i>i6 - i5</i>	7.50E+06	304	1.92E+07	327	<i>i65 - p40</i>	0.00E+00	271	4.07E-04	294
<i>i42 - i45</i>	2.30E+07	262	4.82E+07	285	<i>i70 - i65</i>	6.82E+06	267	1.52E+07	290
<i>i45 - i42</i>	5.35E+07	292	1.30E+08	315	<i>i65 - i70</i>	1.07E+08	271	2.46E+08	294
<i>i48 - p5</i>	2.72E+07	264	7.95E+07	287	<i>i65 - i67</i>	1.04E+09	271	2.06E+09	294
<i>i6 - p17</i>	3.01E+06	304	1.21E+07	327	<i>i67 - i65</i>	4.97E+06	310	1.12E+07	333
<i>i6 - p5</i>	4.67E+06	304	1.50E+07	327	<i>i61 - p37</i>	1.39E-01	245	9.73E+00	268
<i>i48 - p18</i>	1.93E+06	264	8.47E+06	287	<i>i64 - p37</i>	6.42E-01	250	3.32E+01	273
<i>i9 - p5</i>	1.14E+05	300	4.65E+05	323	<i>i61 - i67</i>	4.34E+10	245	6.83E+10	268
<i>i10 - p4</i>	1.59E+06	355	5.53E+06	378	<i>i67 - i61</i>	9.65E+07	310	1.98E+08	333
<i>i10 - p20</i>	2.46E+01	355	3.14E+02	378	<i>i61 - i70</i>	7.77E+09	245	1.34E+10	268
<i>i43 - i49</i>	2.19E+11	290	2.92E+11	313	<i>i70 - i61</i>	2.31E+08	267	4.42E+08	290
<i>i49 - i43</i>	1.39E+11	262	1.62E+11	285	<i>i67 - p31</i>	1.02E+06	310	4.28E+06	333
<i>i6 - p4</i>	8.67E+06	304	2.81E+07	327	<i>i67 - p34</i>	2.76E+04	310	1.96E+05	333
<i>i6 - i47</i>	2.58E+05	304	7.41E+05	327	<i>i61 - i64</i>	2.34E+10	245	3.66E+10	268
<i>i47 - i6</i>	6.67E+08	236	1.46E+09	259	<i>i64 - i61</i>	1.55E+10	250	2.49E+10	273
<i>i47 - p21</i>	2.49E+05	236	1.64E+06	259	<i>i5 - p5</i>	1.27E+06	303	4.90E+06	326
<i>i2 - i13</i>	2.73E+08	232	4.39E+08	255	<i>i10 - p5</i>	1.44E+06	355	4.95E+06	378
<i>i13 - i2</i>	2.07E+09	461	3.13E+09	484	<i>i6 - i49</i>	7.37E+05	304	2.46E+06	327
<i>i11 - p31</i>	3.38E+07	266	1.22E+08	289	<i>i49 - i6</i>	1.04E+07	262	2.91E+07	285
<i>i43 - p23</i>	1.65E+01	290	2.93E+02	313	<i>i64 - i66</i>	1.06E+11	250	1.56E+11	273
<i>i49 - p18</i>	4.30E+06	262	1.91E+07	285	<i>i66 - i64</i>	2.49E+09	271	4.02E+09	294
<i>i49 - p4</i>	1.77E+07	262	5.29E+07	285	<i>i64 - i11</i>	6.10E+10	250	9.09E+10	273
<i>i13 - i11</i>	4.76E+07	461	9.44E+07	484	<i>i11 - i64</i>	4.08E+09	266	6.58E+09	289
<i>i11 - i13</i>	5.76E+10	266	6.50E+10	289	<i>i64 - i67</i>	7.86E+10	250	1.14E+11	273
<i>i45 - p19</i>	4.56E+05	292	2.29E+06	315	<i>i67 - i64</i>	1.31E+08	310	2.44E+08	333
<i>i13 - i70</i>	1.39E+07	461	2.97E+07	484	<i>i64 - i70</i>	7.27E+10	250	1.08E+11	273
<i>i70 - i13</i>	5.61E+09	267	6.86E+09	290	<i>i70 - i64</i>	1.63E+09	267	2.61E+09	290

**Table S5.** RRKM calculated rate constants ( $k(E)$ ,  $s^{-1}$ ) of the reaction of 1-butadiynyl+2-methyl-1,3-butadiene as functions of the internal energy ( $E$ ,  $\text{kJ mol}^{-1}$ ) of the intermediate states for unimolecular reaction steps at different collision energies ( $E_C$ ,  $\text{kJ}\cdot\text{mol}^{-1}$ )

$E_C$	0		24		$E_C$	0		24	
Reaction step	$k(E)$	$E$	$k(E)$	$E$	Reaction step	$k(E)$	$E$	$k(E)$	$E$
<i>i15 - i17</i>	5.32E+11	229	5.98E+11	253	<i>i75 - p44</i>	1.06E+02	297	1.54E+03	321
<i>i17 - i15</i>	2.60E+09	296	4.10E+09	320	<i>i82 - p48</i>	5.32E+04	298	2.45E+05	322
<i>i30 - i32</i>	1.51E+12	230	1.68E+12	254	<i>i82 - p49</i>	1.21E+04	298	7.31E+04	322
<i>i32 - i30</i>	1.13E+09	304	1.82E+09	328	<i>i109 - p23</i>	2.92E+02	288	3.62E+03	312
<i>i30 - i29</i>	7.33E+10	230	1.04E+11	254	<i>i21 - p45</i>	9.61E-01	352	1.61E+01	376
<i>i29 - i30</i>	3.20E+10	230	4.45E+10	254	<i>i78 - i101</i>	8.48E+09	279	9.99E+09	303
<i>i15 - i14</i>	5.07E+10	229	7.13E+10	253	<i>i101 - i78</i>	8.94E+06	429	1.77E+07	453
<i>i14 - i15</i>	9.22E+09	237	1.33E+10	261	<i>i78 - p47</i>	5.75E+07	279	1.43E+08	303
<i>i32 - i33</i>	1.28E+11	304	1.69E+11	328	<i>i78 - p49</i>	1.15E+04	279	6.18E+04	303
<i>i33 - i32</i>	1.22E+11	304	1.62E+11	328	<i>i31 - i111</i>	1.75E+03	235	2.29E+04	259
<i>i17 - i18</i>	1.55E+11	296	2.05E+11	320	<i>i111 - i31</i>	3.28E+01	285	5.60E+02	309
<i>i18 - i17</i>	3.30E+10	295	4.31E+10	319	<i>i116 - p85</i>	2.71E+03	223	1.99E+04	247
<i>i17 - p9</i>	1.15E+06	296	4.39E+06	320	<i>i37 - p12</i>	7.27E+04	297	3.00E+05	321
<i>i17 - p22</i>	2.05E+02	296	3.21E+03	320	<i>i76 - p46</i>	5.90E+09	229	1.15E+10	253
<i>i32 - p11</i>	6.66E+05	304	2.50E+06	328	<i>i114 - p85</i>	2.68E+04	237	1.79E+05	261
<i>i32 - p49</i>	3.34E+04	304	2.07E+05	328	<i>i76 - p57</i>	3.34E+04	229	2.69E+05	253
<i>i33 - p59</i>	1.76E+00	304	3.94E+01	328	<i>i76 - p49</i>	1.39E+05	229	6.87E+05	253
<i>i29 - p51</i>	4.86E+05	230	2.63E+06	254	<i>i114 - p86</i>	3.76E+04	237	2.47E+05	261
<i>i29 - p6</i>	7.64E+07	230	2.19E+08	254	<i>i81 - p4</i>	2.79E+07	294	8.16E+07	318
<i>i14 - p17</i>	7.72E+06	237	2.99E+07	261	<i>i81 - p52</i>	2.26E+05	294	1.17E+06	318
<i>i14 - p42</i>	3.89E+05	237	1.49E+06	261	<i>i81 - p11</i>	2.55E+05	294	9.52E+05	318
<i>i14 - i74</i>	4.50E+06	237	1.25E+07	261	<i>i19 - i114</i>	2.62E+05	304	7.76E+05	328
<i>i74 - i14</i>	1.68E+03	352	7.79E+03	376	<i>i114 - i19</i>	2.58E+08	237	5.63E+08	261
<i>i35 - i40</i>	4.24E+06	339	1.06E+07	363	<i>i116 - p21</i>	5.86E+04	223	3.36E+05	247
<i>i40 - i35</i>	8.60E+01	490	3.15E+02	514	<i>i115 - p84</i>	8.40E+04	252	4.93E+05	276
<i>i40 - p3</i>	2.71E+10	490	3.76E+10	514	<i>i115 - p14</i>	2.03E+06	252	7.22E+06	276
<i>i20 - i25</i>	1.78E+06	340	4.28E+06	364	<i>i92 - i87</i>	6.77E+01	447	2.86E+02	471
<i>i25 - i20</i>	4.95E+01	496	1.76E+02	520	<i>i87 - i92</i>	1.65E+06	323	4.96E+06	347
<i>i25 - p2</i>	1.09E+10	496	1.52E+10	520	<i>i101 - p64</i>	4.72E+07	429	9.51E+07	453
<i>i96 - p2</i>	1.98E+10	466	2.68E+10	490	<i>i111 - p77</i>	1.87E+00	285	4.19E+01	309
<i>i96 - p1</i>	2.08E+11	466	2.67E+11	490	<i>i111 - p81</i>	8.90E+03	285	7.65E+04	309
<i>i40 - i103</i>	6.70E+07	490	1.14E+08	514	<i>i111 - i115</i>	1.71E+11	285	2.44E+11	309
<i>i103 - i40</i>	1.78E+08	480	2.96E+08	504	<i>i115 - i111</i>	7.54E+10	252	8.94E+10	276
<i>i103 - i106</i>	3.34E+07	480	5.86E+07	504	<i>i21 - p10</i>	6.37E+04	352	2.85E+05	376

<i>i106 - i103</i>	4.70E+07	484	8.35E+07	508	<i>i108 - p75</i>	4.24E+04	235	2.86E+05	259
<i>i106 - p3</i>	9.39E+09	484	1.31E+10	508	<i>i108 - p74</i>	5.57E+04	235	3.56E+05	259
<i>i106 - p1</i>	8.58E+10	484	1.13E+11	508	<i>i108 - p73</i>	2.08E+05	235	9.96E+05	259
<i>i20 - i18</i>	9.24E+07	340	1.86E+08	364	<i>i110 - i108</i>	6.47E+02	227	5.99E+03	251
<i>i18 - i20</i>	3.90E+07	295	6.39E+07	319	<i>i108 - i110</i>	1.77E+02	235	1.73E+03	259
<i>i35 - i33</i>	2.99E+08	339	5.82E+08	363	<i>i110 - p74</i>	2.17E+04	227	1.55E+05	251
<i>i33 - i35</i>	8.92E+07	304	1.48E+08	328	<i>i110 - p76</i>	5.69E+03	227	5.44E+04	251
<i>i84 - i74</i>	7.97E+07	332	1.66E+08	356	<i>i110 - p21</i>	2.18E+05	227	1.30E+06	251
<i>i74 - i84</i>	2.97E+06	352	6.47E+06	376	<i>i116 - p80</i>	4.38E+03	223	2.97E+04	247
<i>i84 - i85</i>	7.75E+03	332	2.88E+04	356	<i>i116 - i118</i>	8.76E+05	223	3.00E+06	247
<i>i85 - i84</i>	1.09E+01	443	5.51E+01	467	<i>i118 - i116</i>	4.01E+05	230	1.39E+06	254
<i>i85 - p61</i>	1.28E+08	443	2.53E+08	467	<i>i110 - i113</i>	5.14E+07	227	1.24E+08	251
<i>i85 - p63</i>	2.08E+08	443	4.33E+08	467	<i>i113 - i110</i>	5.77E+03	292	1.90E+04	316
<i>i86 - p61</i>	2.10E+07	452	4.31E+07	476	<i>i110 - i81</i>	1.13E+08	227	2.77E+08	251
<i>i86 - p26</i>	4.42E+08	452	8.19E+08	476	<i>i81 - i110</i>	3.70E+04	294	1.25E+05	318
<i>i86 - i88</i>	2.98E+08	452	4.92E+08	476	<i>i108 - i112</i>	4.65E+07	235	1.19E+08	259
<i>i88 - i86</i>	1.23E+10	375	1.65E+10	399	<i>i112 - i108</i>	7.21E+05	265	2.08E+06	289
<i>i88 - i90</i>	4.83E+11	375	5.20E+11	399	<i>i102 - p67</i>	9.63E+06	425	2.28E+07	449
<i>i90 - i88</i>	2.12E+11	424	2.64E+11	448	<i>i102 - p65</i>	1.62E+07	425	3.46E+07	449
<i>i90 - i93</i>	3.26E+10	424	4.23E+10	448	<i>i102 - p70</i>	1.40E+04	425	5.25E+04	449
<i>i93 - i90</i>	2.73E+08	475	3.95E+08	499	<i>i102 - i104</i>	3.01E+05	425	7.68E+05	449
<i>i25 - i96</i>	4.97E+06	496	9.13E+06	520	<i>i104 - i102</i>	6.94E+07	329	1.33E+08	353
<i>i96 - i25</i>	5.47E+07	466	9.51E+07	490	<i>i104 - p67</i>	1.02E+08	329	2.11E+08	353
<i>i103 - p3</i>	5.43E+10	480	7.37E+10	504	<i>i104 - p69</i>	1.23E+08	329	2.81E+08	353
<i>i103 - p64</i>	4.44E+07	480	9.65E+07	504	<i>i104 - p68</i>	6.73E+07	329	1.43E+08	353
<i>i25 - p8</i>	1.61E+07	496	3.47E+07	520	<i>i83 - p56</i>	5.12E+01	371	5.16E+02	395
<i>i96 - i99</i>	1.29E+06	466	2.80E+06	490	<i>i83 - p54</i>	3.42E+01	371	3.13E+02	395
<i>i99 - i96</i>	8.07E+07	366	1.35E+08	390	<i>i81 - p50</i>	1.43E+05	294	7.14E+05	318
<i>i95 - p62</i>	1.75E+07	498	3.88E+07	522	<i>i109 - i112</i>	8.78E+10	288	1.24E+11	312
<i>i99 - p62</i>	8.17E+07	366	1.44E+08	390	<i>i112 - i109</i>	4.05E+10	265	5.04E+10	289
<i>i93 - i95</i>	4.32E+07	475	7.38E+07	499	<i>i37 - p55</i>	2.56E+03	297	1.95E+04	321
<i>i95 - i93</i>	1.42E+07	498	2.54E+07	522	<i>i118 - p82</i>	1.86E+06	230	7.15E+06	254
<i>i96 - i95</i>	8.64E+07	466	1.48E+08	490	<i>i118 - p17</i>	1.22E+06	230	6.53E+06	254
<i>i95 - i96</i>	7.49E+06	498	1.36E+07	522	<i>i81 - p5</i>	2.86E+07	294	8.46E+07	318
<i>i85 - i86</i>	3.21E+09	443	4.69E+09	467	<i>i83 - p58</i>	1.45E+01	371	1.66E+02	395
<i>i86 - i85</i>	1.64E+09	452	2.46E+09	476	<i>i122 - p13</i>	2.59E+06	260	8.77E+06	284
<i>i99 - i92</i>	3.11E+07	366	5.55E+07	390	<i>i112 - p11</i>	3.16E+06	265	1.06E+07	289
<i>i92 - i99</i>	1.75E+06	447	3.90E+06	471	<i>i112 - p83</i>	5.48E+06	265	2.41E+07	289
<i>i96 - i98</i>	1.31E+06	466	2.80E+06	490	<i>i83 - i105</i>	9.03E+08	371	1.24E+09	395
<i>i98 - i96</i>	1.29E+08	370	2.16E+08	394	<i>i105 - i83</i>	2.42E+09	415	3.81E+09	439
<i>i88 - i89</i>	1.12E+11	375	1.27E+11	399	<i>i118 - i120</i>	1.48E+07	230	4.18E+07	254
<i>i89 - i88</i>	3.17E+11	400	3.91E+11	424	<i>i120 - i118</i>	5.45E+02	352	2.65E+03	376
<i>i89 - i95</i>	7.09E+10	400	8.95E+10	424	<i>i38 - i112</i>	6.72E+03	347	2.66E+04	371
<i>i95 - i89</i>	3.03E+07	498	4.76E+07	522	<i>i112 - i38</i>	3.75E+06	265	1.05E+07	289
<i>i29 - i31</i>	6.01E+10	230	7.39E+10	254	<i>i115 - i120</i>	5.63E+06	252	1.66E+07	276
<i>i31 - i29</i>	1.62E+11	235	2.09E+11	259	<i>i120 - i115</i>	3.36E+03	352	1.51E+04	376
<i>i93 - p2</i>	1.75E+10	475	2.38E+10	499	<i>i113 - p17</i>	2.82E+04	292	1.56E+05	316
<i>i95 - p2</i>	5.96E+09	498	8.48E+09	522	<i>i113 - p78</i>	2.85E+05	292	1.15E+06	316
<i>i99 - i95</i>	5.09E+08	366	7.68E+08	390	<i>i113 - p71</i>	6.03E+05	292	2.43E+06	316
<i>i95 - i99</i>	7.03E+05	498	1.47E+06	522	<i>i34 - p14</i>	2.97E+05	306	1.24E+06	330
<i>i92 - p62</i>	8.02E+07	447	1.64E+08	471	<i>i105 - p66</i>	8.03E+07	415	1.65E+08	439
<i>i92 - p8</i>	3.42E+07	447	7.24E+07	471	<i>i105 - i107</i>	7.35E+06	415	1.59E+07	439
<i>i25 - i98</i>	7.38E+05	496	1.53E+06	520	<i>i107 - i105</i>	1.27E+08	362	2.38E+08	386
<i>i98 - i25</i>	1.60E+09	370	2.46E+09	394	<i>i111 - i122</i>	1.24E+11	285	1.69E+11	309
<i>i98 - p8</i>	3.95E+08	370	6.92E+08	394	<i>i122 - i111</i>	4.37E+10	260	5.19E+10	284
<i>i92 - i98</i>	1.25E+06	447	2.80E+06	471	<i>i116 - i117</i>	1.61E+04	223	7.58E+04	247
<i>i98 - i92</i>	6.99E+07	370	1.28E+08	394	<i>i117 - i116</i>	6.88E+03	225	3.16E+04	249
<i>i14 - i16</i>	8.69E+09	237	1.20E+10	261	<i>i122 - p84</i>	8.59E+04	260	4.84E+05	284
<i>i16 - i14</i>	8.86E+10	238	1.25E+11	262	<i>i120 - p82</i>	2.11E+04	352	9.33E+04	376
<i>i16 - i19</i>	2.24E+12	238	2.44E+12	262	<i>i120 - p14</i>	3.38E+04	352	1.50E+05	376
<i>i19 - i16</i>	1.14E+09	304	1.72E+09	328	<i>i120 - p13</i>	4.41E+04	352	1.81E+05	376
<i>i16 - p24</i>	3.25E+01	238	8.18E+02	262	<i>i107 - p64</i>	4.46E+08	362	8.15E+08	386
<i>i31 - p60</i>	1.24E-01	235	7.74E+00	259	<i>i107 - p66</i>	9.53E+08	362	1.75E+09	386
<i>i31 - i34</i>	4.25E+12	235	4.55E+12	259	<i>i117 - p17</i>	1.99E+05	225	1.10E+06	249
<i>i34 - i31</i>	1.04E+09	306	1.58E+09	330	<i>i117 - p72</i>	1.91E+05	225	8.99E+05	249
<i>i74 - p42</i>	4.01E+04	352	1.78E+05	376	<i>i119 - i117</i>	2.90E+02	340	1.64E+03	364
<i>i74 - p27</i>	2.94E+02	352	2.60E+03	376	<i>i117 - i119</i>	4.66E+06	225	1.54E+07	249
<i>i33 - p11</i>	2.99E+05	304	1.33E+06	328	<i>i119 - p72</i>	6.51E+03	340	3.46E+04	364
<i>i33 - p49</i>	1.34E+05	304	6.73E+05	328	<i>i119 - p14</i>	1.97E+03	340	1.03E+04	364
<i>i18 - p9</i>	6.46E+04	295	2.98E+05	319	<i>i119 - p13</i>	8.77E+03	340	4.26E+04	364
<i>i18 - p22</i>	2.31E+01	295	4.00E+02	319	<i>i88 - p61</i>	6.50E+08	375	1.14E+09	399
<i>i32 - p12</i>	6.70E+05	304	2.53E+06	328	<i>i19 - p10</i>	7.56E+04	304	3.22E+05	328
<i>i33 - p12</i>	1.48E+05	304	6.82E+05	328	<i>i121 - i109</i>	5.92E+10	265	7.27E+10	289

<i>i17 - p10</i>	1.37E+05	296	5.89E+05	320	<i>i109 - i121</i>	9.00E+10	288	1.25E+11	312
<i>i18 - p10</i>	3.76E+04	295	1.78E+05	319	<i>i121 - p79</i>	2.40E+06	265	1.04E+07	289
<i>i33 - i80</i>	1.92E+03	304	1.19E+04	328	<i>i121 - p12</i>	5.66E+06	265	1.90E+07	289
<i>i80 - i33</i>	3.19E+03	291	1.86E+04	315	<i>i36 - p12</i>	1.42E+04	348	6.95E+04	372
<i>i33 - i37</i>	7.09E+02	304	4.72E+03	328	<i>i38 - p12</i>	1.09E+05	347	4.38E+05	371
<i>i37 - i33</i>	2.37E+02	297	1.52E+03	321	<i>i34 - i77</i>	2.28E+05	306	7.45E+05	330
<i>i33 - i36</i>	4.76E+07	304	1.00E+08	328	<i>i77 - i34</i>	1.14E+06	296	3.60E+06	320
<i>i36 - i33</i>	9.75E+05	348	2.39E+06	372	<i>i22 - i23</i>	1.14E+09	296	1.63E+09	320
<i>i33 - i81</i>	4.41E+05	304	1.40E+06	328	<i>i23 - i22</i>	1.10E+12	238	1.20E+12	262
<i>i81 - i33</i>	4.40E+05	294	1.34E+06	318	<i>i77 - p13</i>	2.64E+05	296	1.06E+06	320
<i>i33 - i76</i>	1.34E+03	304	7.88E+03	328	<i>i77 - p5</i>	4.19E+07	296	1.26E+08	320
<i>i76 - i33</i>	3.08E+05	229	1.24E+06	253	<i>i77 - i79</i>	1.19E+11	296	1.63E+11	320
<i>i18 - i22</i>	6.91E+02	295	4.28E+03	319	<i>i79 - i77</i>	1.04E+11	293	1.40E+11	317
<i>i22 - i18</i>	5.13E+02	296	3.20E+03	320	<i>i79 - i91</i>	6.53E+07	293	1.12E+08	317
<i>i18 - i19</i>	2.09E+05	295	6.93E+05	319	<i>i91 - i79</i>	3.74E+08	328	7.61E+08	352
<i>i19 - i18</i>	1.91E+05	304	6.60E+05	328	<i>i91 - i97</i>	5.03E+06	328	1.21E+07	352
<i>i18 - i21</i>	2.57E+07	295	5.28E+07	319	<i>i97 - i91</i>	3.77E+01	490	1.37E+02	514
<i>i21 - i18</i>	7.55E+05	352	1.92E+06	376	<i>i91 - i94</i>	7.39E+06	328	1.82E+07	352
<i>i18 - i75</i>	2.69E+01	295	2.31E+02	319	<i>i94 - i91</i>	5.77E+04	365	1.57E+05	389
<i>i75 - i18</i>	1.95E+02	297	1.70E+03	321	<i>i21 - i22</i>	2.16E+06	352	5.07E+06	376
<i>i14 - i108</i>	1.67E+05	237	5.60E+05	261	<i>i22 - i21</i>	5.46E+07	296	1.04E+08	320
<i>i108 - i14</i>	1.20E+06	235	4.19E+06	259	<i>i37 - i36</i>	1.31E+07	297	2.52E+07	321
<i>i21 - p9</i>	2.03E+05	352	8.35E+05	376	<i>i36 - i37</i>	8.04E+05	348	1.87E+06	372
<i>i32 - i81</i>	8.54E+05	304	2.70E+06	328	<i>i79 - p4</i>	1.08E+07	293	3.56E+07	317
<i>i81 - i32</i>	8.17E+05	294	2.46E+06	318	<i>i26 - i24</i>	2.76E+08	442	4.83E+08	466
<i>i32 - i76</i>	1.78E+03	304	1.04E+04	328	<i>i24 - i26</i>	1.10E+10	336	1.39E+10	360
<i>i76 - i32</i>	3.94E+05	229	1.57E+06	253	<i>i22 - i24</i>	3.98E+09	296	5.34E+09	320
<i>i25 - i22</i>	2.88E+06	496	5.73E+06	520	<i>i24 - i22</i>	7.32E+08	336	1.15E+09	360
<i>i22 - i25</i>	3.25E+10	296	3.59E+10	320	<i>i77 - p14</i>	2.45E+05	296	1.05E+06	320
<i>i16 - i109</i>	3.28E+03	238	3.33E+04	262	<i>i77 - p4</i>	6.31E+07	296	1.91E+08	320
<i>i109 - i16</i>	7.81E+01	288	1.03E+03	312	<i>i97 - i94</i>	7.94E+05	490	1.71E+06	514
<i>i34 - p53</i>	3.77E+04	306	2.14E+05	330	<i>i94 - i97</i>	8.27E+08	365	1.31E+09	389
<i>i34 - p13</i>	4.10E+05	306	1.55E+06	330	<i>i94 - p7</i>	6.21E+08	365	1.05E+09	389
<i>i34 - p51</i>	2.65E+05	306	1.32E+06	330	<i>i94 - i28</i>	3.76E+07	365	7.03E+07	389
<i>i17 - i19</i>	8.53E+05	296	2.69E+06	320	<i>i28 - i94</i>	3.62E+06	420	7.92E+06	444
<i>i19 - i17</i>	1.65E+05	304	5.40E+05	328	<i>i94 - i100</i>	2.08E+07	365	4.02E+07	389
<i>i80 - i83</i>	2.43E+10	291	3.26E+10	315	<i>i100 - i94</i>	1.17E+07	388	2.43E+07	412
<i>i83 - i80</i>	5.20E+07	371	9.40E+07	395	<i>i97 - p2</i>	1.81E+10	490	2.52E+10	514
<i>i80 - p55</i>	1.11E+04	291	8.40E+04	315	<i>i93 - i97</i>	1.83E+08	475	2.95E+08	499
<i>i80 - p11</i>	4.52E+06	291	1.70E+07	315	<i>i97 - i93</i>	1.10E+08	490	1.84E+08	514
<i>i14 - i73</i>	8.00E+03	237	4.52E+04	261	<i>i97 - p7</i>	5.23E+07	490	1.04E+08	514
<i>i73 - i14</i>	9.93E+03	251	6.13E+04	275	<i>i79 - p5</i>	6.10E+06	293	2.12E+07	317
<i>i40 - i37</i>	7.54E+06	490	1.49E+07	514	<i>i79 - p14</i>	7.01E+03	293	3.82E+04	317
<i>i37 - i40</i>	3.71E+10	297	4.11E+10	321	<i>i79 - p13</i>	5.49E+04	293	2.67E+05	317
<i>i83 - i102</i>	2.90E+07	371	5.22E+07	395	<i>i28 - p7</i>	5.25E+08	420	9.48E+08	444
<i>i102 - i83</i>	1.02E+07	425	2.15E+07	449	<i>i28 - p8</i>	2.98E+08	420	5.70E+08	444
<i>i36 - p20</i>	1.60E+02	348	1.56E+03	372	<i>i100 - p7</i>	1.39E+09	388	2.36E+09	412
<i>i14 - i72</i>	3.23E+07	237	6.76E+07	261	<i>i100 - p62</i>	5.16E+08	388	9.47E+08	412
<i>i72 - i14</i>	8.61E+05	297	2.46E+06	321	<i>i26 - i28</i>	3.45E+07	442	6.31E+07	466
<i>i36 - p11</i>	2.07E+04	348	9.71E+04	372	<i>i28 - i26</i>	1.16E+08	420	2.01E+08	444
<i>i36 - i38</i>	2.29E+10	348	3.13E+10	372	<i>i26 - p8</i>	3.60E+07	442	7.28E+07	466
<i>i38 - i36</i>	2.58E+10	347	3.54E+10	371	<i>i24 - p35</i>	1.95E+01	336	2.41E+02	360
<i>i38 - p20</i>	1.82E+01	347	2.01E+02	371	<i>i37 - i39</i>	8.92E+08	297	1.27E+09	321
<i>i38 - p11</i>	1.50E+05	347	5.86E+05	371	<i>i39 - i37</i>	1.07E+12	241	1.18E+12	265
<i>i116 - i114</i>	8.52E+01	223	8.03E+02	247	<i>i39 - i41</i>	7.86E+11	241	8.23E+11	265
<i>i114 - i116</i>	1.05E+02	237	1.07E+03	261	<i>i41 - i39</i>	1.18E+06	453	2.65E+06	477
<i>i32 - i82</i>	1.44E+06	304	3.98E+06	328	<i>i23 - i27</i>	6.04E+11	238	6.37E+11	262
<i>i82 - i32</i>	5.69E+05	298	1.52E+06	322	<i>i27 - i23</i>	8.63E+05	453	1.98E+06	477
<i>i32 - i78</i>	4.49E+03	304	2.06E+04	328	<i>i41 - p3</i>	3.02E+10	453	4.07E+10	477
<i>i78 - i32</i>	7.98E+03	279	3.28E+04	303	<i>i40 - i41</i>	1.42E+07	490	2.55E+07	514
<i>i22 - p10</i>	2.99E+04	296	1.41E+05	320	<i>i41 - i40</i>	6.30E+07	453	1.05E+08	477
<i>i22 - p43</i>	3.77E+03	296	2.88E+04	320	<i>i41 - p66</i>	3.32E+07	453	7.07E+07	477
<i>i33 - i78</i>	6.14E+03	304	2.68E+04	328	<i>i27 - p2</i>	1.68E+10	453	2.27E+10	477
<i>i78 - i33</i>	1.14E+04	279	4.45E+04	303	<i>i25 - i27</i>	1.48E+07	496	2.67E+07	520
<i>i19 - p9</i>	9.43E+04	304	4.24E+05	328	<i>i27 - i25</i>	1.16E+08	453	1.91E+08	477
<i>i73 - p15but</i>	1.05E+08	251	2.89E+08	275	<i>i97 - i27</i>	1.98E+07	490	3.52E+07	514
<i>i73 - p42</i>	7.47E+05	251	2.87E+06	275	<i>i27 - i97</i>	8.83E+07	453	1.46E+08	477
<i>i73 - p6</i>	1.00E+08	251	2.89E+08	275	<i>i81 - p12</i>	1.38E+05	294	5.30E+05	318
<i>i72 - p41</i>	3.43E+05	297	1.65E+06	321	<i>i101 - i107</i>	2.40E+05	429	5.46E+05	453
<i>i75 - i87</i>	8.28E+08	297	1.23E+09	321	<i>i107 - i101</i>	4.06E+07	362	7.74E+07	386
<i>i87 - i75</i>	7.12E+09	323	1.22E+10	347					

**Table S6.** Statistical branching ratios (%) of three selected channels leading to phenylacetylene (*p1*) for the reaction of 1,3-butadiene+butadiynyl with *i1* and *i4* as initial intermediates at different collision energies when excluding all the other products

Collision energy, kJ mol <sup>-1</sup>	0		23	
	<i>Initial intermediate</i>			
Main exit channels	<i>i1</i>	<i>i4</i>	<i>i1</i>	<i>i4</i>
<i>i5</i> → <i>i8</i> → <i>i9</i> → <i>i12</i> → <i>p1</i>	45.6	45.6	46.0	46.0
<i>i5</i> → <i>i8</i> → <i>i9</i> → <i>i11</i> → <i>i13</i> → <i>p1</i>	44.6	44.6	44.5	44.5
<i>i5</i> → <i>i7</i> → <i>i12</i> → <i>p1</i>	9.8	9.8	9.5	9.5

**Table S7.** Statistical branching ratios (%) of three selected channels leading to m-tolylacetylene (*p2*) for the reaction of 2-methyl-1,3-butadiene+butadiynyl with *i14* and *i17* as initial intermediates at different collision energies when excluding all the other products

Collision energy, kJ mol <sup>-1</sup>	0		24	
	<i>Initial intermediate</i>			
Main exit channels	<i>i14</i>	<i>i17</i>	<i>i14</i>	<i>i17</i>
<i>i18</i> → <i>i21</i> → <i>i22</i> → <i>i25</i> → <i>p2</i>	49.9	49.9	50.2	50.2
<i>i18</i> → <i>i21</i> → <i>i22</i> → <i>i23</i> → <i>i27</i> → <i>p2</i>	48.2	48.2	47.9	47.9
<i>i18</i> → <i>i20</i> → <i>i25</i> → <i>p2</i>	1.9	1.9	1.9	1.9

**Table S8.** Statistical branching ratios (%) of three selected channels leading to p-tolylacetylene (*p3*) for the reaction of 2-methyl-1,3-butadiene+butadiynyl with *i29* and *i32* as initial intermediates at different collision energies when excluding all the other products

Collision energy, kJ mol <sup>-1</sup>	0		24	
	<i>Initial intermediate</i>			
Main exit channels	<i>i29</i>	<i>i32</i>	<i>i29</i>	<i>i32</i>
<i>i33</i> → <i>i36</i> → <i>i37</i> → <i>i40</i> → <i>p3</i>	49.0	49.0	49.1	49.1
<i>i33</i> → <i>i36</i> → <i>i37</i> → <i>i39</i> → <i>i41</i> → <i>p3</i>	48.1	48.1	47.9	47.9
<i>i33</i> → <i>i35</i> → <i>i40</i> → <i>p3</i>	2.9	2.9	3.0	3.0

## 7. References

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- (2) Zhou, L.; Kaiser, R. I.; Tokunaga, A. T. Infrared Spectroscopy of Crystalline and Amorphous Diacetylene ( $C_4H_2$ ) and Implications for Titan's Atmospheric Composition. *Planetary and Space Science* **2009**, 57 (7), 830–835.  
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## 8. Optimized Cartesian coordinates (Å) and vibrational frequencies (cm<sup>-1</sup>) for all intermediates, transition states, reactants, and products involved in the C<sub>4</sub>H<sub>6</sub> + C<sub>4</sub>H and C<sub>5</sub>H<sub>8</sub> + C<sub>4</sub>H reactions at the ωB97X-D/6-311G(d,p) level.

<b>Reactants</b>			H	0.878466	2.363866	-0.841104		3252.607	3281.444	3484.894
<b>1,3-butadiene</b>			H	2.504652	2.189523	0.069142				
<b>Cartesian coordinates</b>			H	-5.074402	-0.559317	-0.194174				
C	-1.838912	-0.110778								
C	-0.609780	0.401525								
C	0.609781	-0.401527								
C	1.838912	0.110779								
H	-2.718610	0.521982								
H	-2.003266	-1.184255								
H	-0.476875	1.481589								
H	0.476876	-1.481591								
H	2.718610	-0.521980								
H	2.003265	1.184257								
<b>Vibrational frequencies</b>										
154.5481	304.2800	524.5559								
530.7604	788.9380	902.6179								
947.1043	951.2222	1006.3630								
1009.6451	1053.4804	1235.2147								
1328.4726	1329.7492	1421.3049								
1475.6592	1685.3408	1752.8546								
3148.8774	3151.4242	3163.1706								
3168.1714	3242.8677	3243.1637								
<b>(trans-)-2-methyl-1,3-butadiene</b>										
<b>Cartesian coordinates</b>										
C	1.973854	0.006578	0.000167							
C	0.833035	-0.680452	-0.000194							
H	2.931617	-0.500421	0.000144							
H	1.996166	1.091273	0.000490							
H	0.874839	-1.767502	-0.000613							
C	-0.517629	-0.100332	-0.000109							
C	-1.583514	-0.904863	0.000160							
C	-0.653664	1.397459	-0.000078							
H	-2.593738	-0.510187	0.000344							
H	-1.474113	-1.984540	0.000162							
H	-1.702903	1.695636	-0.000034							
H	-0.172206	1.832714	-0.881248							
H	-0.172155	1.832679	0.881081							
<b>Vibrational frequencies</b>										
137.3939	225.5480	297.6232								
401.6022	437.5583	541.3986								
639.7032	785.0651	801.3264								
928.0969	943.5573	972.6251								
1015.7076	1028.9680	1076.1723								
1094.4048	1327.0370	1340.6146								
1418.9358	1443.5148	1464.2737								
1488.5355	1511.4583	1691.9826								
1743.8405	3047.6580	3110.6408								
3139.9049	3154.9701	3160.7078								
3172.2382	3243.8763	3253.1487								
<b>butadiynyl</b>										
<b>Cartesian coordinates</b>										
C	0.396625	0.196213	-0.351482							
C	-0.541020	-0.267558	0.479455							
C	-1.441418	-0.713043	1.277251							
C	1.252485	0.619517	-1.109854							
H	1.999970	0.989228	-1.772222							
<b>Vibrational frequencies</b>										
145.3264	359.1098	489.6033								
585.7224	745.8863	922.0621								
1886.4475	2148.6999	3461.0199								
<b>Intermediates</b>										
<b>PART1. 1,3-butadiene+ butadiynyl</b>										
<b>i1</b>										
<b>Cartesian coordinates</b>										
C	2.840123	-1.371535	0.091344							
C	1.898961	-0.607177	-0.443497							
C	1.127809	0.452803	0.331456							
C	1.511735	1.819427	-0.153141							
C	-1.497330	0.026130	0.119551							
C	-2.846745	-0.195291	0.002241							
C	-4.029163	-0.388569	-0.100823							
C	-0.313337	0.220006	0.225452							
H	3.385206	-2.094186	-0.504835							
H	3.096438	-1.303533	1.144523							
H	1.648666	-0.686345	-1.497920							
H	1.408650	0.355231	1.388873							
<b>Vibrational frequencies</b>										
77.1515	98.3484	177.7237								
197.8095	240.9032	334.3499								
374.0539	457.6167	492.4615								
527.9212	546.1282	585.5538								
685.8711	690.9118	708.5455								
747.8721	825.2777	879.0327								
924.7769	1003.865	1070.557								
1088.862	1115.09	1176.938								
1208.504	1241.418	1389.058								
1398.407	1478.529	1490.056								
2201.139	2393.866	3155.917								
3170.846	3177.021	3188.613								
<b>i2</b>										
<b>Cartesian coordinates</b>										
C	-2.845422	-1.411030	0.094416							
C	-1.973028	-0.537463	-0.393915							
C	-1.213650	0.427979	0.425834							
C	-0.781601	1.767574	-0.167382							
C	1.416153	0.270242	0.002457							
C	2.603844	-0.326427	-0.000415							
C	3.711308	-0.844723	-0.017020							
C	0.217075	0.712479	0.073367							
H	-3.375173	-2.099936	-0.552655							
H	-3.057171	-1.467930	1.157750							
H	-1.773648	-0.509941	-1.463472							
H	-1.439281	0.428151	1.489037							
H	-1.054651	1.973872	-1.198207							
H	-0.777071	2.630265	0.490719							
H	4.668924	-1.306268	-0.027220							
<b>Vibrational frequencies</b>										
34.3494	95.0406	107.3544								
210.2226	281.6922	344.4574								
370.2586	413.5747	447.0378								
464.4544	538.0365	558.1429								
663.6914	714.1764	820.1662								
851.2787	921.9248	948.5709								
992.7463	1024.376	1028.225								
1064.952	1093.831	1213.125								
1236.931	1314.572	1348.463								
1457.646	1470.444	1729.734								
1923.849	2045.43	3122.794								
3152.008	3157.428	3166.713								
3215.179	3250.121	3475.595								
<b>i3</b>										
<b>Cartesian coordinates</b>										
C	1.800983	1.650146	0.062292							
C	2.194393	0.290679	-0.257447							
C	1.132157	-0.832188	-0.444666							
C	2.049818	-0.829287	0.747528							
C	-1.425938	-0.268996	-0.144480							
C	-2.756167	0.023353	0.014684							
C	-3.923138	0.279965	0.155313							
C	-0.257291	-0.533534	-0.282714							
H	2.275968	2.488165	-0.428703							
H	0.975050	1.840791	0.736420							
H	3.026961	0.191333	-0.944887							
H	1.356412	-1.543350	-1.232103							
H	1.608020	-0.575064	1.703376							
H	2.823597	-1.586246	0.782379							
H	-4.954908	0.503535	0.280460							
<b>Vibrational frequencies</b>										
30.017	89.3317	137.2133								
200.5697	277.9433	317.2627								
337.2262	451.1476	535.7854								
546.3987	559.9294	601.6402								
654.044	689.7504	710.4366								
772.2082	822.7049	883.9853								
990.9101	1002.658	1051.531								
1160.496	1190.407	1224.43								
1243.976	1324.588	1426.19								
1469.293	1476.686	1532.951								
2202.756	2404.107	3044.85								
3095.891	3165.551	3173.431								
3206.99	3265.455	3485.928								
<b>i4</b>										
<b>Cartesian coordinates</b>										
C	-3.050098	-1.489993	-0.000087							
C	-1.919605	-0.697855	0.000286							
C	-1.938591	0.682270	-0.000286							
C	-0.729637	1.576993	0.000126							
C	1.618711	0.324365	0.000068							
C	2.831352	-0.318737	-0.000043							
C	3.893660	-0.882286	-0.000165							
C	0.555231	0.889451	0.000125							
H	-2.977650	-2.570029	0.000451							
H	-4.042257	-1.051053	-0.000963							
H	-0.948989	-1.188882	0.001089							
H	-2.895005	1.198246	-0.001025							
H	-0.767691	2.243290	-0.872389							
H	-0.767941	2.242850	0.872978							
H	4.833393	-1.379678	-0.000282							
<b>Vibrational frequencies</b>										
28.7906	63.6195	142.2734								
188.5396	200.7341	299.0805								
333.6668	409.6328	527.5857								
548.5483	550.0379	610.3434								
682.5891	712.1831	712.5502								
747.571	785.3873	914.4272								
916.5366	1004.327	1055.896								
1171.257	1205.672	1229.102								
1301.698	1325.267	1379.597								
1453.786	1510.62	1530.847								
2204.481	2408.155	3017.819								
3041.672	3160.517	3173.278								
3180.436	3263.449	3484.88								
<b>i5</b>										
<b>Cartesian coordinates</b>										
C	-2.190412	1.507692	0.466032							
C	-2.461447	0.562759	-0.497823							
C	-1.913298	-0.709274	-0.565051							
C	-0.943227	-1.257213	0.451875							
C	1.526970	-0.313501	0.105354							
C	2.793489	0.182808	-0.076674							
C	3.903621	0.617579	-0.234712							
C	0.414740	-0.746408	0.267609							
H	-2.669757	2.477988	0.442141							
H	-1.475494	1.328190	1.261101							
H	-3.162564	0.832036	-1.283651							
H	-2.166978	-1.350443	-1.401234							
H	-1.274830	-0.101694	1.467707							
H	-0.916579	-2.348840	0.389463							
H	4.883586	1.005097	-0.375191							
<b>Vibrational frequencies</b>										
30.017	89.3317	137.2133								
200.5697	277.9433	317.2627								
337.2262	451.1476	535.7854								
546.3987	559.9294	601.6402								
654.044	689.7504	710.4366								
772.2082	822.7049	883.9853								
990.9101	1002.658	1051.531								
1160.496	1190.407	1224.43								
1243.976	1324.588	1426.19								
1469.293	1476.686	1532.951								
2202.756	2404.107	3044.85								
3095.891	3165.551	3173.431								
3206.99	3265.455	3485.928								
<b>i6</b>										
<b>Cartesian coordinates</b>										
C	-2.378022	1.711542	-0.265336							
C	-1.946302	0.678354	0.443330							
C	-2.096750	-0.756866	0.032513							
C	-0.799368	-1.509118	-0.084433							
C	1.532614	-0.390513	-0.037511							
C	2.752151	0.196284	-0.014224							
C	3.841820	0.721445	0.006503							
C	0.422958	-0.926222	-							

H -0.851686 -2.586004 -0.216755  
H 4.799105 1.183727 0.024537

**Vibrational frequencies**

53.1821 78.0286 109.7131  
146.4231 201.1059 330.2786  
379.9532 417.2879 478.8238  
512.9069 557.1029 610.9961  
627.1211 689.754 696.219  
750.5336 907.1226 931.0359  
978.6398 1031.24 1052.374  
1126.181 1235.038 1251.51  
1323.874 1345.323 1438.746  
1465.002 1479.792 1744.928  
2045.803 2153.644 3019.989  
3051.241 3148.221 3167.321  
3175.974 3242.102 3481.266

**i7**

**Cartesian coordinates**

C -0.001526 1.271298 -0.000108  
C 1.498517 1.192858 0.000071  
C 2.199652 0.065570 0.000090  
C 1.568653 -1.311614 -0.000012  
C -0.661755 -0.104000 -0.000074  
C -2.090461 -0.148367 -0.000044  
C -3.291434 -0.123962 0.000123  
C 0.100624 -1.180179 -0.000064  
H -0.349331 1.834257 -0.874735  
H -0.349547 1.834423 0.874323  
H 2.026039 2.142366 0.000159  
H 3.285244 0.100596 0.000198  
H 1.904350 -1.879987 -0.876051  
H 1.904262 -1.880068 0.876009  
H -4.354632 -0.121203 0.000197

**Vibrational frequencies**

70.5452 146.9225 171.0821  
343.0468 392.0102 425.1022  
510.215 538.9895 573.6465  
654.8574 671.4567 698.2611  
724.3448 899.8353 922.8255  
954.0834 963.899 966.5041  
1012.639 1086.672 1158.554  
1203.579 1205.484 1213.51  
1336.06 1359.169 1408.489  
1471 1474.277 1738.738  
1766.636 2238.036 3032.195  
3036 3059.059 3064.893  
3172.369 3195.942 3483.397

**i8**

**Cartesian coordinates**

C -3.706998 0.555769 -0.007144  
C -2.849113 -0.666450 -0.000652  
C -1.488176 -0.716183 0.005244  
C -0.613917 0.395769 0.008650  
C 1.977140 0.151628 0.003925  
C 3.332259 0.023007 -0.001922  
C 4.533325 -0.093022 -0.007830  
C 0.761439 0.264745 0.007372  
H -4.431384 0.519181 0.812699  
H -4.286127 0.609979 -0.935698  
H -3.378135 -1.615374 -0.010065  
H -1.018658 -1.695532 0.004687  
H -3.139350 1.481996 0.087302  
H -1.013570 1.404746 0.008744  
H 5.591463 -0.196571 -0.013528

**Vibrational frequencies**

55.9113 66.665 73.9394  
173.592 206.8857 262.9624  
346.3886 407.658 467.8648  
526.8234 554.7904 560.7724  
635.4266 696.113 725.4462  
760.5107 811.1891 932.1872  
989.7487 1044.772 1063.59  
1173.559 1238.977 1268.995  
1370.97 1423.801 1477.5  
1483.199 1484.923 1573.062  
2129.284 2214.263 3041.882  
3096.031 3147.201 3175.532  
3192.051 3198.439 3481.497

**i9**

**Cartesian coordinates**

C -2.588044 1.377946 -0.231114  
C -2.782007 0.136758 0.213518  
C -1.945637 -1.027150 -0.092070  
C -0.604163 -1.086300 -0.123317  
C 1.611878 -0.059380 0.068619  
C 2.914697 0.165642 0.017891  
C 4.130120 0.314810 -0.059582  
C 0.307670 -0.006574 0.233749  
H -3.267676 2.179072 0.036066

H -1.768138 1.624148 -0.897610  
H -3.662254 -0.066385 0.820641  
H -2.486274 -1.949151 -0.291571  
H -0.127341 0.885993 0.686401  
H -0.137053 -2.027064 -0.397747  
H 5.181650 0.458873 -0.122355

**Vibrational frequencies**

39.5908 61.6865 152.5465  
166.7946 249.9477 310.2459  
357.9444 381.9657 430.8693  
440.4293 509.8526 603.0457  
648.2055 726.4591 801.6393  
871.1179 900.7204 964.2751  
973.8748 1016.107 1035.319  
1098.126 1116.529 1264.386  
1296.186 1335.656 1440.468  
1471.722 1691.416 1713.638  
1797.764 1996.117 3112.3  
3149.463 3161.661 3169.407  
3197.413 3252.406 3472.38

**i10**

**Cartesian coordinates**

C -3.971774 -0.694578 -0.000016  
C -2.832207 0.267959 0.000000  
C -1.521242 -0.087590 0.000029  
C -0.455350 0.842716 -0.000001  
C 2.054747 0.158093 0.000015  
C 3.368610 -0.196819 0.000003  
C 4.533442 -0.512225 -0.000019  
C 0.875557 0.476301 0.000016  
H -4.609320 -0.546435 0.878445  
H -3.624373 -1.729881 0.000017  
H -4.609246 -0.546464 -0.878536  
H -3.081326 1.327545 -0.000043  
H -1.260688 -1.143562 0.000073  
H -0.685570 1.904975 -0.000058  
H 5.559827 -0.789317 -0.000056

**Vibrational frequencies**

64.6076 87.1551 150.4536  
188.7388 196.5279 252.0364  
297.6678 408.1108 411.202  
509.3725 515.4799 569.9601  
652.8944 690.1008 746.8689  
789.706 818.7542 945.6355  
991.8369 1048.687 1114.108  
1178.168 1224.067 1294.166  
1318.499 1414.417 1448.356  
1479.653 1490.324 1579.421  
2124.73 2208.696 3029.751  
3085.601 3125.701 3153.389  
3161.623 3169.139 3484.103

**i11**

**Cartesian coordinates**

C 2.071059 1.676953 0.081546  
C 2.694277 0.525334 -0.044558  
C 2.132498 -0.828189 -0.008220  
C 0.837760 -1.191752 0.004166  
H 2.349981 2.720673 0.080773  
H 3.779713 0.565675 -0.185183  
H 2.871492 -1.623026 0.003878  
H 0.616616 -2.255902 0.038720  
C -1.570771 -0.748749 0.042810  
C -2.708178 0.102212 0.002478  
C -3.683228 0.804718 -0.028765  
C -0.304950 -0.305124 -0.032699  
H -1.765372 -1.813711 0.145722  
H -4.541259 1.432005 -0.056414  
H -0.121973 0.761863 -0.128046

**Vibrational frequencies**

54.5729 86.5775 120.4855  
161.4777 198.7545 326.5462  
381.8252 407.2764 497.4233  
547.141 640.4008 682.31  
697.0396 697.9693 766.0933  
860.8905 881.0098 900.3263  
978.7838 991.5146 1026.336  
1046.551 1144.647 1259.861  
1283.658 1305.498 1340.156  
1459.368 1639.45 1674.198  
1717.143 2234.082 3064.53  
3162.109 3167.213 3175.57  
3199.073 3256.489 3484.754

**i12**

**Cartesian coordinates**

C -0.096049 -1.270988 -0.000009  
C -1.588159 -1.157072 0.000004  
C -2.222575 0.036357 0.000006  
C -1.492111 1.260763 -0.000003  
C 0.613738 0.059579 -0.000004

C 2.027432 0.050639 0.000001  
C 3.232202 0.005028 0.000007  
C -0.096761 1.244579 -0.000005  
H 0.235177 -1.862109 -0.868054  
H 0.235191 -1.862126 0.868021  
H -2.156339 -2.081173 0.000013  
H -3.306772 0.070632 0.000019  
H 0.452185 2.179697 -0.000003  
H -2.020761 2.205768 0.000000  
H 4.295014 -0.023994 0.000010

**Vibrational frequencies**

91.592 152.531 201.4202  
361.6145 446.1651 511.5613  
531.6324 541.0983 595.6978  
610.2392 687.5592 696.0939  
741.4612 786.5331 930.5747  
937.6545 954.7963 982.1945  
986.3535 1015.653 1119.944  
1193.284 1203.48 1208.802  
1293.026 1335.678 1428.926  
1430.163 1445.088 1530.426  
1640.464 2181.473 2982.445  
2992.697 3186.364 3201.828  
3207.045 3226.993 3480.431

**i13**

**Cartesian coordinates**

C -0.158598 1.257304 0.322817  
C -1.428884 1.222860 -0.152762  
C -2.098468 0.000002 -0.395904  
C -1.428886 -1.222858 -0.152765  
C 0.613859 -0.000002 0.641576  
C 1.924559 -0.000001 -0.029764  
C 2.990218 0.000001 -0.579138  
C -0.158600 -1.257306 0.322815  
H 0.349894 2.199516 0.491186  
H -1.941567 2.156621 -0.358206  
H -3.110352 0.000004 -0.780829  
H -1.941571 -2.156619 -0.358211  
H 0.829912 -0.000005 1.725074  
H 3.932606 0.000002 -1.071451  
H 0.349892 -2.199518 0.491187

**Vibrational frequencies**

69.9232 149.9395 262.3606  
379.3011 432.1455 522.6219  
530.0088 591.8354 619.4879  
676.733 702.4578 708.959  
759.3104 793.2093 872.5332  
958.3741 991.8034 992.6932  
998.6671 1036.082 1050.732  
1113.231 1181.089 1212.599  
1280.165 1293.242 1345.466  
1403.488 1461.692 1561.831  
1630.178 2245.24 2942.527  
3188.654 3191.067 3211.144  
3212.265 3227.613 3484.629

**i14**

**Cartesian coordinates**

C 3.265592 -0.774998 0.125786  
C 1.803757 -0.912625 -0.095773  
C 1.009400 0.384419 -0.043535  
C 1.558973 1.601066 -0.039404  
C -1.604869 0.050033 -0.001335  
C -2.961874 -0.139358 0.019464  
C -4.153141 -0.306340 0.038006  
C -0.410935 0.229373 -0.018239  
H 3.972055 -1.339550 -0.468273  
H 3.638375 -0.228798 0.984669  
H 1.602639 -1.396226 -1.057666  
H 1.371221 -1.586743 0.661167  
H 0.944997 2.492597 -0.009430  
H 2.635252 1.723422 -0.075444  
H -5.205961 -0.454130 0.055152

**Vibrational frequencies**

73.3202 77.7926 124.3856  
171.8938 221.2781 291.8847  
297.3606 389.7719 496.0469  
500.8199 520.543 559.381  
595.8425 674.3053 693.9771  
710.2449 744.6447 832.1963  
900.2732 958.5811 1057.118  
1173.534 1114.209 1235.175  
1290.142 1376.933 1428.029  
1460.498 1472.621 1707.202  
2198.05 2383.018 2982.198  
3074.551 3163.944 3166.756  
3262.124 3274.597 3483.001

**i13**

**Cartesian coordinates**

C 2.093483 -0.908778 0.745288

C	2.111154	0.417603	0.000008
C	0.927363	1.289846	0.000001
C	2.093498	-0.908767	-0.745294
C	-1.495033	0.368065	0.000003
C	-2.759560	-0.122765	0.000000
C	-3.884959	-0.564127	-0.000003
C	-0.352523	0.821205	0.000002
H	2.999542	-1.192826	1.266391
H	1.169082	-1.162830	1.250578
H	3.056147	0.946888	0.000021
H	1.080395	2.363944	-0.000014
H	1.169106	-1.162809	-1.250606
H	2.999567	-1.192806	-1.266385
H	-4.874385	-0.953257	-0.000006

**Vibrational frequencies**

64.7725	68.8049	131.0939
190.0589	328.5058	354.7496
373.2728	488.8175	520.5699
581.6077	609.3199	637.1116
680.4083	743.1733	801.6522
820.9699	851.1615	892.3466
1011.611	1060.059	1089.339
1119.836	1121.575	1212.335
1217.489	1262.022	1407.796
1449.606	1471.957	1514.908
2072.894	2169.229	3148.237
3152.72	3187.156	3201.96
3237.069	3251.587	3479.48

**i44**

**Cartesian coordinates**

C	-3.328545	-0.579318	0.000020
C	-1.831156	-0.855755	-0.000022
C	-0.975504	0.396415	-0.000013
C	-1.459297	1.624483	-0.000006
C	1.640437	0.043824	0.000007
C	2.996869	-0.148009	0.000009
C	4.187914	-0.317895	0.000000
C	0.444937	0.215714	0.000002
H	-3.622602	-0.007113	0.883570
H	-3.887974	-1.517222	0.000024
H	-1.550628	-1.452668	0.874552
H	-1.550667	-1.452647	-0.874622
H	-1.059917	2.628539	0.000007
H	-3.622647	-0.007094	-0.883503
H	5.240505	-0.468548	-0.000012

**Vibrational frequencies**

48.3805	75.3156	120.8081
214.0321	242.845	271.9938
305.2438	374.8946	482.2437
493.6529	557.1154	578.1392
672.2366	701.5553	706.8732
713.0366	798.5693	807.445
964.0154	1049.143	1107.527
1108.512	1249.256	1297.351
1377.256	1424.728	1476.28
1504.284	1504.852	1659.558
2194.958	2374.503	3047.591
3050.646	3081.292	3125.101
3134.698	3265.962	3482.411

**i45**

**Cartesian coordinates**

C	3.028705	0.000024	0.112296
C	1.937792	-1.098251	-0.038971
C	0.900054	-0.000015	-0.050813
C	1.937753	1.098260	-0.038975
C	-1.682876	-0.000024	-0.013239
C	-3.037213	-0.000005	0.012164
C	-4.246620	0.000019	0.035347
C	-0.451445	-0.000030	-0.034293
H	3.800167	0.000038	-0.657548
H	3.507994	0.000041	1.091440
H	1.989120	-1.659106	-0.977871
H	1.853204	-1.815504	0.781931
H	1.989065	1.659111	-0.977878
H	1.853138	1.815510	0.781922
H	-5.309574	0.000044	0.056907

**Vibrational frequencies**

70.9569	80.9773	115.8143
221.5985	240.5819	422.9652
445.5049	490.2773	530.9371
566.3098	606.0927	668.6547
735.7683	752.9252	840.5727
931.5684	954.8107	1014.587
1015.286	1057.415	1130.349
1210.024	1225.306	1236.009
1270.269	1279.969	1460.003
1461.78	1469.517	1515.548
2054.501	2159.397	3051.694
3054.632	3098.39	3102.781
3103.844	3159.684	3479.602

**i46**

**Cartesian coordinates**

C	-1.850927	1.077963	0.092672
C	-2.710708	0.153631	-0.710385
C	-1.925405	-1.038106	-0.093769
C	-1.053405	-0.031475	0.737551
C	1.552112	-0.015401	0.198561
C	2.890740	0.003486	-0.102063
C	4.063875	0.021483	-0.367220
C	0.374448	-0.031009	0.456969
H	-1.680434	2.146479	0.064198
H	-2.614319	0.253364	-1.798088
H	-3.781431	0.175942	-0.474131
H	-2.518275	-1.712845	0.523790
H	-1.346927	-1.619957	-0.810150
H	-1.203951	-0.124890	1.821039
H	5.100956	0.038479	-0.600551

**Vibrational frequencies**

44.2909	90.8969	118.0544
221.1159	238.924	289.9223
434.4557	477.5653	532.1661
589.2133	655.0671	680.8831
694.0724	761.1821	805.9068
917.048	941.0458	973.423
993.684	1041.967	1087.124
1186.872	1197.136	1212.771
1244.051	1274.221	1302.599
1340.599	1467.515	1498.149
2200.079	2395.665	3020.196
3023.255	3055.714	3101.012
3165.348	3226.276	3486.508

**i47**

**Cartesian coordinates**

C	-1.914934	1.098446	-0.081285
C	-2.814914	0.000000	-0.554125
C	-1.914933	-1.098446	-0.081285
C	-1.058137	0.000000	0.636778
C	1.553748	0.000000	0.167058
C	2.902561	0.000000	-0.084325
C	4.085383	0.000000	-0.302940
C	0.368581	0.000000	0.389163
H	-2.344006	1.862083	0.576048
H	-1.362663	1.612279	-0.878649
H	-3.719622	-0.000001	-1.147215
H	-1.362662	-1.612278	-0.878648
H	-2.344006	-1.862083	0.576048
H	-1.242189	0.000001	1.713338
H	5.131025	-0.000001	-0.495159

**Vibrational frequencies**

68.8313	87.2281	139.7837
230.4151	235.0064	261.2624
439.3688	476.0591	542.0337
596.7858	620.1605	678.3937
701.9078	793.9161	813.3904
905.588	954.4906	980.2852
993.3751	1038.265	1045.317
1131.072	1206.135	1210.073
1237.78	1284.759	1303.657
1368.411	1461.025	1478.372
2200.537	2397.477	3017.944
3021.643	3067.785	3071.667
3103.438	3222.926	3484.1

**i48**

**Cartesian coordinates**

C	2.845430	-1.386479	-0.450670
C	2.049567	-0.607662	0.542691
C	1.902333	0.831487	0.143029
C	0.751540	1.450967	-0.142471
C	-1.621755	0.322556	-0.056088
C	-2.861218	-0.259135	-0.012575
C	-3.949122	-0.771716	0.026569
C	-0.525348	0.828748	-0.090216
H	3.535104	-2.158243	-0.133583
H	2.657931	-1.261352	-1.510414
H	1.050553	-1.051422	0.667856
H	2.822598	1.403356	0.060718
H	2.533607	-0.657078	1.524716
H	0.761922	2.497051	-0.433107
H	-4.910277	-1.224912	0.062195

**Vibrational frequencies**

56.4421	92.8384	114.1588
164.2352	205.9402	245.8509
351.6728	366.4404	495.3786
520.5197	533.6968	572.5668
603.8289	677.3389	713.8919
758.822	768.0637	812.3796
999.7963	1010.953	1058.612
1106.934	1173.726	1221.906
1280.607	1332.639	1427.159

1467.181	1472.096	1708.386
2200.014	2382.066	2998.099
3068.003	3160.987	3170.263
3191.218	3273.909	3486.347

**i49**

**Cartesian coordinates**

C	3.719098	0.812900	-0.357243
C	2.996076	-0.311726	0.309100
C	1.524010	-0.012148	0.420368
C	0.571999	-0.682949	-0.235772
C	-1.991236	-0.124824	-0.081610
C	-3.329047	0.159496	-0.003041
C	-4.503996	0.409382	0.067231
C	-0.810827	-0.372418	-0.145997
H	4.348033	1.492087	0.204110
H	3.523933	1.030656	-1.400464
H	3.125961	-1.242181	-0.257626
H	3.405531	-0.481439	1.309867
H	1.241766	0.825257	1.053153
H	0.840874	-1.518523	-0.878213
H	-5.542555	0.627864	0.130953

**Vibrational frequencies**

68.5798	78.7635	105.9462
174.8573	194.3392	224.9727
333.1893	359.3383	444.0607
476.3262	541.9472	559.9477
581.2856	681.1147	703.7772
766.0266	805.3931	856.4869
984.6364	1023.844	1060.99
1122.146	1214.607	1243.618
1308.66	1335.161	1347.943
1466.835	1483.449	1713.933
2199.637	2382.3	3032.488
3087.629	3159.69	3160.547
3178.399	3273.296	3485.279

**i50**

**Cartesian coordinates**

C	-1.734510	1.985197	0.003916
C	-2.117059	0.683539	-0.004864
C	-1.246705	-0.441054	-0.005286
C	-1.788838	-1.844299	0.002560
C	1.345766	-0.138599	0.000735
C	2.700430	0.015990	0.000166
C	3.898268	0.154195	-0.000934
C	0.135249	-0.273023	0.000117
H	-2.470460	2.779212	0.001982
H	-0.686863	2.265981	0.013098
H	-3.180521	0.456977	-0.013131
H	-1.544583	-2.350758	0.942117
H	-1.353475	-2.437020	-0.806776
H	-2.874086	-1.843124	-0.113542
H	4.954382	0.277057	-0.002206

**Vibrational frequencies**

56.5147	71.0653	101.6956
160.6531	208.2755	272.4509
276.4421	443.7887	462.4535
529.6747	548.7571	604.7279
631.5415	642.7605	647.3924
703.0362	884.4883	897.1717
980.0525	1036.813	1043.619
1103.044	1241.632	1277.686
1358.09	1412.15	1447.221
1481.736	1492.895	1569.331
2146.275	2241.5	3043.731
3107.107	3141.289	3160.563
3170.193	3264.623	3481.248

**i51**

**Cartesian coordinates**

C	0.099287	1.190156	-0.186986
C	1.547874	0.711696	-0.253198
C	1.545406	-0.820922	-0.376089
C	2.078302	-0.136669	0.862129
C	-0.714058	-0.108126	-0.156571
C</			



H 1.915273 -1.805597 -0.866949  
H 3.281782 0.179225 -0.000002  
H 1.963918 2.234275 -0.000001  
H -4.329567 -0.020742 -0.000001  
H -0.523653 2.162415 0.000001

**Vibrational frequencies**

116.9387 155.0623 173.8675  
353.0009 453.4967 464.9908  
529.6921 589.1595 602.0179  
661.8573 674.1709 700.2113  
753.4004 773.9753 802.1426  
910.6751 936.9518 977.5151  
990.4673 1038.742 1102.325  
1188.057 1191.176 1196.014  
1300.174 1329.397 1391.596  
1441.244 1450.858 1577.609  
1622.707 2241.587 2964.942  
2968.386 3190.116 3208.323  
3209.919 3228.92 3483.141

**i61**

**Cartesian coordinates**

C -3.033577 -0.254153 -0.642168  
C -3.033398 -0.254538 0.642298  
C -1.660147 -0.351561 -0.000152  
C -0.765370 0.817518 0.000056  
C 1.424616 -0.338642 -0.000128  
C 2.821634 -0.265421 -0.000035  
C 4.029912 -0.210374 0.000055  
C 0.607060 0.801053 0.000058  
H -3.552951 -0.196935 -1.582850  
H -3.552544 -0.197862 1.583140  
H -1.172045 -1.324952 -0.000523  
H -1.261153 1.785182 0.000276  
H 0.985814 -1.330459 -0.000351  
H 5.091745 -0.158593 0.000143  
H 1.116760 1.760319 0.000257

**Vibrational frequencies**

51.3968 106.7536 119.9639  
228.0359 246.5757 347.1595  
421.019 482.2015 498.4123  
567.1308 622.4048 659.5225  
689.1558 744.0419 750.6011  
821.9584 877.3635 930.9179  
977.7606 990.5187 1022.848  
1055.512 1098.081 1160.227  
1188.118 1245.32 1346.445  
1400.085 1496.297 1533.605  
1753.057 2130.077 3123.519  
3170.031 3190.817 3203.358  
3275.651 3326.108 3479

**i62**

**Cartesian coordinates**

C 2.038017 1.014661 -0.031218  
C 2.858779 -0.000218 -0.514083  
C 2.037860 -1.014755 -0.030930  
C 1.041665 0.000172 0.545862  
C -1.457450 -0.000026 0.605944  
C -2.745474 0.000022 -0.004141  
C -3.841543 -0.000128 -0.496886  
C -0.311163 0.000293 -0.080423  
H 2.046043 2.095241 -0.062982  
H 3.793180 -0.000345 -1.061531  
H 2.045387 -2.095305 -0.063488  
H 0.973353 0.000054 1.638749  
H -1.436930 -0.000307 1.693219  
H -4.807616 -0.000077 -0.940750  
H -0.337561 0.000617 -1.167958

**Vibrational frequencies**

75.8063 107.7312 131.0579  
220.113 338.0306 349.7237  
447.4349 495.6356 534.905  
584.4451 654.1021 655.431  
723.4616 850.6895 909.4085  
927.7827 933.045 954.4333  
958.5879 994.7735 1040.154  
1129.813 1155.318 1196.039  
1201.016 1239.787 1323.396  
1329.737 1369.872 1464.065  
1720.473 2239.579 3072.736  
3168.68 3176.168 3217.171  
3243.506 3258.555 3485.754

**i63**

**Cartesian coordinates**

C -1.974288 -0.679378 0.668724  
C -1.974453 -0.679333 -0.668533  
C -1.308720 0.680761 -0.755456  
C -1.308535 0.680708 0.755573  
C 0.974259 -0.442124 -0.000279  
C 2.336688 -0.246937 -0.000065

C 3.540127 -0.064912 0.000129  
C 0.026744 0.676625 -0.000121  
H -2.199341 -1.425828 1.420151  
H -2.199695 -1.425735 -1.419951  
H -1.577690 1.505196 -1.402496  
H -1.577329 1.505099 1.402743  
H 0.588223 -1.455245 -0.000528  
H 4.591917 0.089645 0.000367  
H 0.502988 1.654404 -0.000120

**Vibrational frequencies**

43.235 140.1297 241.8802  
266.387 391.5831 471.3624  
473.9353 506.467 532.5279  
674.2417 691.0419 769.3147  
781.3283 817.3797 845.9712  
890.7689 895.1912 957.6238  
1002.771 1028.767 1036.644  
1072.999 1101.789 1154.778  
1217.713 1221.304 1286.832  
1307.129 1327.801 1474.443  
1636.786 2044.971 3164.165  
3203.789 3204.286 3214.841  
3221.534 3241.48 3472.938

**i64**

**Cartesian coordinates**

C -3.201612 0.005933 -0.642411  
C -3.201410 0.004521 0.642752  
C -1.919931 -0.494400 -0.000593  
C -0.705770 0.336266 0.000115  
C 1.725434 0.617760 0.000397  
C 3.017220 0.083146 0.000104  
C 4.137503 -0.373359 -0.000187  
C 0.565843 -0.169852 -0.000140  
H -3.685382 0.212591 -1.581338  
H -3.684890 0.209053 1.582294  
H -1.729773 -1.569184 -0.001752  
H -0.849560 1.415763 0.000783  
H 1.629872 1.699932 0.000960  
H 5.120482 -0.778195 -0.000413  
H 0.695592 -1.250060 -0.000755

**Vibrational frequencies**

57.8185 101.8259 164.5016  
177.8205 227.6467 379.7153  
413.1608 444.7797 457.9587  
562.1619 590.4162 656.2451  
696.8419 734.3432 772.6137  
852.9828 888.2653 927.3643  
966.5779 1027.824 1029.262  
1061.08 1109.767 1164.738  
1196.73 1257.138 1302.876  
1367.703 1462.311 1540.673  
1750.789 2128.687 3095.308  
3156.175 3166.279 3177.432  
3272.602 3322.702 3478.639

**i65**

**Cartesian coordinates**

C 1.777461 -0.258198 1.014447  
C 2.730468 -0.270514 0.000043  
C 1.777613 -0.257784 -1.014498  
C 0.626665 -0.235805 -0.000108  
C -1.530112 1.067731 0.000141  
C -2.386878 -0.072665 -0.000013  
C -3.129291 -1.017982 -0.000126  
C -0.193813 1.008739 0.000100  
H 1.799616 -0.242299 2.095083  
H 3.813302 -0.288846 0.000120  
H 1.799932 -0.241440 -2.095124  
H -0.002327 -1.130216 -0.000332  
H -2.023088 2.034841 0.000311  
H -3.784789 -1.855033 -0.000225  
H 0.364680 1.941863 0.000245

**Vibrational frequencies**

45.2079 109.9982 193.6065  
194.7269 350.504 362.7631  
483.6252 564.7441 610.576  
611.5958 669.666 675.7032  
710.6073 780.5052 904.6936  
923.1531 929.7614 946.7057  
962.2838 985.9525 1015.174  
1104.398 1170.59 1197.945  
1211.703 1252.395 1321.624  
1330.579 1430.042 1467.571  
1707.59 2235.116 3089.368  
3164.045 3187.136 3210.708  
3237.398 3252.548 3487.058

**i66**

**Cartesian coordinates**

C -3.642984 -0.831333 0.000063  
C -3.139828 0.383947 -0.000004

C -1.721581 0.750070 -0.000034  
C -0.696504 -0.116150 0.000014  
C 1.718173 -0.570785 0.000027  
C 3.082259 -0.172410 -0.000007  
C 4.242353 0.143237 -0.000034  
C 0.689813 0.293531 -0.000020  
H -4.625448 -1.279581 -0.000093  
H -3.845838 1.220487 -0.000043  
H -1.504917 1.815220 -0.000100  
H -0.902393 -1.184765 0.000081  
H 1.523965 -1.640335 0.000094  
H 5.266754 0.427673 -0.000059  
H 0.897676 1.360664 -0.000088

**Vibrational frequencies**

38.9677 91.0736 94.1101  
181.7317 204.065 291.4358  
328.2268 415.804 477.719  
526.1861 638.0161 638.6633  
669.8195 710.9733 825.5086  
863.3306 869.4247 926.3377  
976.3228 1006.493 1033.094  
1057.571 1192.531 1247.578  
1275.896 1331.082 1349.458  
1362.66 1639.72 1681.056  
1717.96 2232.139 3066.408  
3157.433 3166.5 3170.928  
3174.913 3263.186 3486.178

**i67**

**Cartesian coordinates**

C -2.840501 1.396800 -0.000271  
C -2.830435 0.081503 0.000163  
C -1.652447 -0.789028 0.000051  
C -0.377380 -0.369884 0.000064  
C 2.040904 -0.910578 -0.000091  
C 2.491329 0.438729 0.000013  
C 2.890979 1.572726 0.000095  
C 0.747172 -1.278545 -0.000078  
H -3.583118 2.180834 -0.000256  
H -3.798621 -0.429350 0.000632  
H -1.852519 -1.857759 -0.000033  
H -0.160550 0.695514 0.000196  
H 2.812213 -1.673669 -0.000204  
H 3.243374 2.575829 0.000168  
H 0.521493 -2.341736 -0.000173

**Vibrational frequencies**

33.047 83.3918 138.4779  
185.6199 190.0674 326.4853  
327.7742 397.6883 535.1622  
583.4569 644.328 671.7217  
705.4902 709.0296 780.4893  
844.2652 856.45 919.5525  
952.7375 993.0041 1033.908  
1037.946 1151.695 1252.958  
1273.435 1304.664 1353.549  
1439.524 1640.254 1666.184  
1715.187 2229.57 3066.436  
3166.19 3166.971 3175.984  
3193.534 3262.97 3485.954

**i68**

**Cartesian coordinates**

C 0.933949 1.173342 -0.162490  
C 2.195952 0.815962 0.110803  
C 2.300865 -0.648552 0.083625  
C 1.101929 -1.173318 -0.203909  
C -1.055326 -0.146714 0.571722  
C -2.368895 -0.034594 0.188235

C -3.530209 0.066342 -0.165980  
 C 0.095707 -0.063941 -0.391435  
 H 0.528629 2.174502 -0.211266  
 H 3.019395 1.487806 0.316343  
 H 3.213714 -1.201515 0.264331  
 H 0.850134 -2.221194 -0.292304  
 H -0.819530 -0.258167 1.625084  
 H -4.545685 0.157958 -0.467334  
 H -0.290487 -0.070554 -1.418271

**Vibrational frequencies**

38.1187 100.5533 197.9111  
 292.2419 400.2992 464.9114  
 493.8852 553.8611 558.8963  
 655.1168 662.96 736.7059  
 743.6963 817.0366 839.4138  
 934.7407 971.811 978.5796  
 1013.541 1028.835 1041.924  
 1114.798 1127.692 1163.773  
 1212.207 1230.159 1312.399  
 1400.48 1410.777 1590.537  
 1673.068 2034.108 3064.923  
 3192.606 3218.814 3229.186  
 3249.515 3255.627 3474.065

**i69**

**Cartesian coordinates**

C 0.610415 0.084709 0.987914  
 C 0.848417 1.368053 0.233830  
 C 1.633582 0.805310 -0.688643  
 C 1.530566 -0.594657 -0.091530  
 C -0.603153 -0.775056 0.461601  
 C -1.798489 -0.067929 0.022885  
 C -2.777136 0.519820 -0.346626  
 C 0.327357 -1.355951 -0.576419  
 H 0.813008 0.035147 2.056609  
 H 0.430903 2.359956 0.354641  
 H 2.097745 1.167362 -1.598729  
 H 2.448780 -1.132455 0.151788  
 H -0.888273 -1.527000 1.209220  
 H -3.644879 1.039153 -0.674611  
 H 0.113370 -1.847952 -1.516984

**Vibrational frequencies**

103.2554 153.0605 261.3503  
 316.439 385.6651 447.5865  
 543.3325 551.7342 688.661  
 698.791 717.7193 801.8255  
 840.7066 857.559 916.1774  
 929.3726 968.0554 982.0328  
 989.7787 1027.352 1080.087  
 1101.229 1138.689 1177.346  
 1186.523 1218.078 1254.912  
 1279.774 1310.014 1337.869  
 1648.264 2244.75 3022.513  
 3104.68 3143.736 3199.603  
 3221.172 3232.05 3486.374

**i70**

**Cartesian coordinates**

C -2.875640 0.951869 -0.127320  
 C -2.737331 -0.349854 0.002125  
 C -1.506652 -1.147107 0.020643  
 C -0.232732 -0.717292 0.050693  
 C 1.483723 1.060984 0.059004  
 C 2.599912 0.181914 -0.021335  
 C 3.557103 -0.542648 -0.087720  
 C 0.199186 0.663043 0.086480  
 H -3.700754 1.648640 -0.161164

H -3.659061 -0.933301 0.101289  
 H -1.666596 -2.220718 0.014936  
 H 0.554021 -1.466239 0.056105  
 H 1.713187 2.120850 0.098377  
 H 4.403880 -1.182941 -0.147056  
 H -0.570089 1.428257 0.142098

**Vibrational frequencies**

12.396 97.3485 112.4677  
 169.9484 256.988 326.22  
 380.4076 400.5808 532.1458  
 639.8548 660.1602 676.0628  
 708.7032 747.4129 766.012  
 823.2872 849.3657 884.6094  
 943.9937 998.1479 1006.158  
 1029.793 1121.224 1245.94  
 1286.437 1296.214 1391.116  
 1474.087 1640.024 1658.718  
 1712.892 2229.239 3056.452  
 3162.87 3174.017 3190.467  
 3193.614 3254.839 3485.239

**i71**

**Cartesian coordinates**

C 0.216796 -0.753673 0.526855  
 C 1.542036 -1.142508 0.007095  
 C 2.268594 -0.000005 -0.304880  
 C 1.542044 1.142503 0.007095  
 C -0.683940 0.000004 -0.470057  
 C -2.099272 0.000012 -0.254190  
 C -3.284641 -0.000005 -0.059583  
 C 0.216803 0.753677 0.526855  
 H -0.295231 -1.333500 1.284173  
 H 1.861494 -2.164443 -0.142386  
 H 3.252180 -0.000008 -0.756955  
 H 1.861506 2.164436 -0.142387  
 H -0.360096 0.000002 -1.505293  
 H -4.335144 -0.000024 0.103542  
 H -0.295224 1.333510 1.284170

**Vibrational frequencies**

140.5631 147.8847 299.5507  
 364.4058 490.8686 494.9447  
 537.6161 637.0586 671.6154  
 709.7563 729.8575 749.3674  
 818.9317 841.4724 842.412  
 903.411 958.0754 965.298  
 1025.573 1040.057 1043.991  
 1080.892 1085.788 1095.846  
 1177.593 1283.015 1285.037  
 1338.29 1376.103 1406.034  
 1482.391 2235.893 3174.978  
 3203.351 3211.53 3226.253  
 3243.425 3255.054 3482.641

**PART2. 2-methyl-1,3-butadiene+ butadiynyl**

**i14**

**Cartesian coordinates**

C 2.735577 -0.692241 -1.017946  
 C 1.781191 -0.422460 -0.134584  
 C 0.873009 0.788347 -0.337816  
 C 1.134665 1.872875 0.670436  
 C -1.717602 0.130825 -0.206236  
 C -3.048253 -0.191992 -0.119035  
 C -4.214839 -0.474050 -0.040801  
 C -0.548255 0.413927 -0.283094  
 C 1.542075 -1.254515 1.092522  
 H 3.406613 -1.533708 -0.881905

H 2.880814 -0.084481 -1.904882  
 H 1.061108 1.190064 -1.339318  
 H 1.292703 1.622986 1.711769  
 H 0.959023 2.906942 0.403896  
 H -5.246622 -0.720636 0.030213  
 H 1.609692 -0.652625 2.004043  
 H 2.272038 -2.061814 1.164321  
 H 0.539230 -1.691034 1.071191

**Vibrational frequencies**

31.7668 66.7173 105.4115  
 146.2748 176.6788 203.1129  
 223.076 265.6201 359.7418  
 400.1092 438.545 508.9094  
 540.1692 542.9598 561.732  
 603.8784 686.065 700.4764  
 708.2052 762.7947 826.2343  
 935.1701 951.6484 1002.646  
 1066.129 1071.012 1098.911  
 1166.646 1294.182 1297.791  
 1308.121 1417.005 1453.317  
 1454.464 1489.504 1498.744  
 1747.2 2199.311 2393.945  
 3050.492 3061.207 3112.781  
 3145.746 3158.484 3169.601  
 3244.436 3285.205 3486.21

**i15**

**Cartesian coordinates**

C 2.615022 -1.017407 -0.970569  
 C 1.796560 -0.408779 -0.114522  
 C 0.915544 0.693356 -0.589186  
 C 0.474395 1.844363 0.312669  
 C -1.668553 0.302301 -0.038361  
 C -2.831186 -0.340735 -0.075436  
 C -3.914740 -0.907598 -0.088338  
 C -0.495178 0.810840 -0.092387  
 C 1.712801 -0.803127 1.333995  
 H 3.258611 -1.830809 -0.653878  
 H 2.667593 -0.723864 -2.013686  
 H 1.045190 0.955742 -1.635669  
 H 0.796751 1.845025 1.349049  
 H 0.388544 2.825850 -0.141902  
 H -4.853337 -1.406356 -0.106820  
 H 0.678780 -1.015739 1.621647  
 H 2.073968 0.000816 1.983358  
 H 2.315911 -1.689957 1.530717

**Vibrational frequencies**

29.9804 46.6709 90.3863  
 179.0663 190.1827 263.3778  
 330.2031 363.7094 381.308  
 424.4295 437.7512 483.7108  
 513.9408 538.8153 607.5103  
 667.3075 735.3635 753.5334  
 850.0355 906.0729 924.843  
 947.6027 1000.184 1027.994  
 1058.505 1061.657 1072.287  
 1112.95 1239.286 1315.885  
 1358.773 1416.628 1451.021  
 1466.11 1487.273 1505.856  
 1734.983 1921.896 2044.82  
 3046.798 3107.779 3127.969  
 3146.527 3153.904 3162.366  
 3218.163 3240.839 3474.366

**i16**

**Cartesian coordinates**

C -2.991117 0.149126 -0.819832  
 C -1.805366 0.200470 0.022893  
 C -0.731957 -0.911215 -0.251873  
 C -1.569799 -0.924644 1.000276  
 C 1.827915 -0.293936 -0.155388  
 C 3.158698 0.030516 -0.101861  
 C 4.326606 0.315784 -0.052126  
 C 0.657652 -0.586640 -0.199318  
 C -1.303944 1.582269 0.383041  
 H -3.354043 1.042607 -1.311411  
 H -3.478054 -0.795165 -1.033881  
 H -1.005373 -1.620450 -1.024775  
 H -1.067073 -0.676384 1.927650  
 H -2.325092 -1.697461 1.079386  
 H 5.359233 0.564647 -0.007746  
 H -0.391547 1.538073 0.979724  
 H -2.065808 2.116413 0.956641  
 H -1.084366 2.157339 -0.520466

**Vibrational frequencies**

70.8036 77.2443 174.9722  
 193.0358 204.8577 229.0657  
 296.7702 364.8815 374.9854  
 392.3176 467.9206 494.9435  
 529.9142 549.178 574.2156  
 669.2631 685.9623 697.9007  
 709.5544 767.2421 930.6014

941.3508	963.2961	987.8708	C	3.454161	0.140429	0.013614	234.3001	272.5681	364.8877
1058.631	1086.152	1098.331	C	4.596064	0.517776	0.144141	383.6403	449.6145	478.2694
1119.566	1228.215	1289.465	C	1.011079	-0.660676	-0.267912	504.5812	524.6282	564.5718
1346.76	1399.776	1428.063	C	-1.819986	1.614001	-0.080742	633.6864	696.7468	747.5422
1471.436	1487.896	1496.088	H	-4.333481	0.616609	-0.471861	785.0935	858.6449	904.7777
1508.91	2200.14	2385.629	H	-3.972917	-1.124178	0.042420	973.9094	1003.677	1068.098
3052.719	3125.653	3143.499	H	-0.568071	-1.575636	-1.314034	1085.618	1167.863	1230.548
3147.357	3162.834	3187.268	H	-0.876365	-0.430402	1.544564	1245.99	1345.692	1421.718
3242.47	3272.68	3487.129	H	-1.859185	-1.731911	0.860372	1425.923	1450.888	1471.861
			H	5.599668	0.849451	0.259734	1485.086	1492.176	1493.898
			H	-1.401655	2.008406	0.851516	1569.675	2133.248	2218.432
			H	-2.601036	2.293829	-0.424471	3025.321	3039.067	3078.263
			H	-1.008988	1.616626	-0.815642	3091.737	3138.899	3158.565
							3172.232	3190.045	3481.911

**i17**

**Cartesian coordinates**

C	3.064233	-0.837395	-0.972471
C	2.128263	-0.281793	-0.125338
C	1.417887	0.854045	-0.508284
C	0.351799	1.506524	0.332603
C	-2.003438	0.289901	0.026680
C	-3.208698	-0.344859	-0.140427
C	-4.265404	-0.900264	-0.286547
C	-0.948059	0.852398	0.173241
C	1.870866	-0.906297	1.227183
H	3.625020	-1.721392	-0.693403
H	3.261002	-0.403090	-1.946188
H	1.589567	1.270711	-1.495320
H	0.621749	1.484697	1.394374
H	0.248068	2.560428	0.057724
H	-5.200066	-1.389789	-0.416940
H	0.808814	-1.129052	1.361885
H	2.170948	-0.230986	2.034594
H	2.430198	-1.835096	1.343442

**Vibrational frequencies**

	39.048	62.4255	140.6231
	153.4424	182.6795	257.6276
	279.1535	338.5712	403.7626
	451.8753	486.1828	540.0724
	547.5124	569.1029	589.1669
	679.9869	706.6534	714.4282
	769.5859	809.9039	815.1328
	924.426	989.0403	1024.238
	1063.952	1114.029	1170.833
	1229.175	1286.836	1328.203
	1392.663	1433.086	1451.397
	1472.44	1498.927	1510.19
	1534.319	2201.92	2401.807
	3048.568	3051.8	3095.476
	3116.116	3148.698	3155.209
	3188.024	3253.435	3485.467

**i18**

**Cartesian coordinates**

C	1.790026	-0.822643	-1.279500
C	2.086701	-0.273177	-0.053034
C	1.407179	0.830927	0.463802
C	0.291036	1.554238	-0.244286
C	-2.040768	0.282502	0.002520
C	-3.236505	-0.377574	0.136486
C	-4.285485	-0.954168	0.253769
C	-0.992837	0.864761	-0.115701
C	3.174481	-0.887686	0.801825
H	2.338876	-1.678790	-1.652890
H	0.989653	-0.443343	-1.903334
H	1.659035	1.179739	1.460237
H	0.184926	2.562010	0.168195
H	0.520226	1.677566	-1.308906
H	-5.213469	-1.462147	0.358678
H	2.742166	-1.375031	1.680194
H	3.874207	-0.126557	1.156061
H	3.741419	-1.636527	0.246474

**Vibrational frequencies**

	25.7157	55.0106	60.1949
	139.2887	150.0861	251.2604
	286.794	341.2086	385.8999
	458.969	479.413	540.4335
	544.0644	562.7988	586.1225
	659.6298	697.4257	709.6606
	765.3333	815.5564	821.794
	939.4396	998.1905	1039.518
	1065.239	1111.315	1173.447
	1230.587	1284.82	1333.106
	1353.501	1420.832	1464.393
	1489.031	1493.002	1506.376
	1553.587	2202.057	2402.945
	3049.389	3054.503	3092.612
	3121.744	3143.076	3170.67
	3193.454	3263.83	3485.291

**i19**

**Cartesian coordinates**

C	-3.613417	-0.112289	-0.114746
C	-2.349683	0.222758	0.125036
C	-0.274371	-1.066681	-0.400255
C	-1.342245	-0.796224	0.624370
C	2.175403	-0.279560	-0.132273

**Vibrational frequencies**

	25.7635	56.6942	108.3229
	128.632	203.2126	229.3475
	242.4945	381.4873	389.3255
	422.3397	491.8087	494.9099
	529.0678	568.3445	611.4854
	670.9267	684.4047	720.614
	761.1999	836.8532	944.2389
	953.0137	986.1409	1031.44
	1069.417	1089.438	1207.511
	1251.427	1305.228	1322.064
	1421.952	1451.773	1455.43
	1479.848	1490.865	1503.383
	1746.956	2045.738	2153.047
	3041.934	3052.977	3102.925
	3106.003	3142	3149.098
	3178.16	3234.912	3478.602

**i20**

**Cartesian coordinates**

C	-0.003308	-0.959270	0.000137
C	-1.423813	-0.452036	-0.000084
C	-1.731192	0.842661	-0.000175
C	-0.715461	1.965168	0.000051
C	1.044566	0.146958	0.000086
C	2.418343	-0.247703	-0.000004
C	3.554407	-0.638055	-0.000117
C	0.645599	1.403567	0.000068
C	-2.478803	-1.521791	-0.000010
H	0.157893	-1.603526	-0.873826
H	0.157721	-1.603324	0.874283
H	-2.775442	1.145297	-0.000356
H	-0.864109	2.608939	-0.875746
H	-0.864236	2.608664	0.876032
H	4.565964	-0.965219	-0.000229
H	-3.483509	-1.095719	-0.000521
H	-2.378435	-2.165641	0.880382
H	-2.377879	-2.166463	-0.879729

**Vibrational frequencies**

	40.8922	107.1169	132.3687
	159.7629	236.383	335.7778
	338.8965	421.6588	431.4398
	491.2508	530.8901	541.4251
	657.2854	682.5956	697.7493
	786.7186	840.2862	901.6598
	943.1446	958.1791	965.4676
	1059.819	1068.339	1076.165
	1142.282	1199.259	1202.006
	1221.68	1302.734	1341.845
	1395.709	1416.427	1464.656
	1464.734	1479.366	1491.674
	1748.364	1776.697	2238.405
	3028.668	3033.693	3038.991
	3057.878	3059.823	3096.944
	3140.515	3161.154	3485.85

**i21**

**Cartesian coordinates**

C	-3.083491	1.186895	0.002657
C	-2.414402	-0.154311	-0.004743
C	-1.059983	-0.338975	-0.005834
C	-0.070780	0.667685	-0.003101
C	2.479983	0.145765	-0.000750
C	3.815399	-0.120024	0.001139
C	4.998976	-0.355057	0.003209
C	1.283144	0.385530	-0.002371
C	-3.341656	-1.332501	0.003135
H	-3.612135	1.339606	0.950845
H	-3.837671	1.238216	-0.789696
H	-0.694758	-1.362944	-0.005940
H	-0.350180	1.716161	0.001999
H	-2.394034	2.019100	-0.134704
H	6.042067	-0.560450	0.004983
H	-4.020180	-1.286519	0.863045
H	-2.802496	-2.280240	0.042298
H	-3.973746	-1.332969	-0.892876

**Vibrational frequencies**

	49.907	65.7505	108.3887
	126.8683	172.1085	195.1072

**i22**

**Cartesian coordinates**

C	-2.010766	1.426687	-0.558854
C	-2.264578	0.204414	-0.087555
C	-1.424720	-0.961242	-0.418428
C	-0.086910	-1.048027	-0.365260
C	2.130605	-0.090643	0.050262
C	3.431579	0.140906	0.147494
C	4.647793	0.287790	0.204114
C	0.818579	-0.005406	0.102827
C	-3.463784	-0.091783	0.775338
H	-2.651692	2.266713	-0.312258
H	-1.176357	1.615450	-1.224682
H	-1.970402	-1.859246	-0.702594
H	0.381059	-1.982827	-0.658355
H	5.698833	0.435540	0.266542
H	0.368506	0.887534	0.539711
H	-3.153835	-0.507197	1.738997
H	-4.106147	-0.838164	0.296113
H	-4.056754	0.806025	0.956888

**Vibrational frequencies**

	34.1873	44.7774	100.3841
	161.0331	176.954	243.7206
	261.9052	341.4451	379.4297
	388.3532	435.7692	445.9477
	495.8821	544.3484	640.9715
	646.7504	720.9304	804.3104
	836.2912	874.2938	945.7827
	951.5363	980.2727	1014.154
	1030.257	1066.318	1119.158
	1264.357	1275.799	1303.458
	1407.485	1442.515	1459.913
	1482.889	1498.766	1695.949
	1723.081	1796.568	1998.551
	3043.646	3105.303	3115.087
	3142.484	3150.066	3156
	3193.846	3247.076	3472.355

**i23**

**Cartesian coordinates**

C	1.032836	-1.418266	-0.380535
C	1.856944	-0.433716	-0.081027
C	1.542391	0.996480	-0.200849
C	0.372638	1.650484	-0.077272
C	-1.513219	0.014168	-0.295901
C	-2.841371	-0.394014	0.010105
C	-3.960199	-0.761170	0.252052
C	-0.970423	1.151489	0.168470
C	3.262270	-0.732515	0.417400
H	1.082745	-2.498611	-0.358134
H	2.422490	1.625134	-0.321761
H	0.441435	2.735899	-0.093855
H	-0.945514	-0.630018	-0.961663
H	-4.951273	-1.079557	0.468439
H	-1.604241	1.804467	0.763970
H	3.		

C	-2.592543	-1.084321	-0.876204
C	-1.856008	-0.435030	0.100474
C	-1.645854	1.032623	-0.035718
C	-0.494907	1.709099	0.041212
C	1.330817	0.063859	-0.375734
C	2.668154	-0.395944	-0.217235
C	3.791165	-0.807710	-0.098378
C	0.864444	1.183667	0.192357
C	-1.364702	-1.104091	1.212871
H	-2.788412	-2.148109	-0.805483
H	-2.988965	-0.552222	-1.732658
H	-2.551610	1.608759	-0.208564
H	-0.557429	2.793468	-0.014694
H	4.785061	-1.169220	0.010701
H	1.552599	1.792383	0.773501
H	0.679794	-0.543817	-0.996805
H	-1.527948	-2.169135	1.331135
H	-0.806489	-0.585021	1.980993

**Vibrational frequencies**

47.0312	80.3528	125.6982
146.3175	191.384	278.5566
298.383	417.7473	436.9675
484.0836	548.486	559.4182
567.8707	586.8282	672.2434
703.6201	737.5079	770.4978
786.9605	815.2986	876.524
919.3327	982.1974	1002.541
1014.473	1027.318	1046.855
1062.725	1237.477	1301.055
1326.478	1349.9	1371.881
1453.778	1482.675	1534.202
1712.673	1723.502	2235.348
3153.15	3159.894	3166.457
3172.234	3180.603	3187.54
3263.22	3269.775	3482.972

**i25**

**Cartesian coordinates**

C	-0.085598	-0.945147	0.000053
C	-1.483026	-0.394108	-0.000007
C	-1.700242	0.943472	-0.000019
C	-0.629370	1.881595	0.000005
C	1.003099	0.096741	0.000014
C	2.342623	-0.354787	-0.000008
C	3.471575	-0.778297	-0.000032
C	0.694641	1.442486	0.000011
C	-2.591814	-1.398653	-0.000023
H	0.044204	-1.611790	-0.867878
H	0.044165	-1.611670	0.868085
H	-2.720396	1.315604	-0.000051
H	-0.845164	2.942844	-0.000001
H	4.471015	-1.140773	-0.000053
H	1.503391	2.164456	0.000004
H	-3.571523	-0.917760	-0.000142
H	-2.528583	-2.050290	0.879366
H	-2.528438	-2.050432	-0.879295

**Vibrational frequencies**

58.8049	103.9649	136.6651
175.3847	260.2401	335.9559
401.1648	443.286	504.5033
513.5579	541.9866	556.6108
606.8521	691.8855	715.4988
728.9876	857.9566	879.4276
930.1872	931.0726	955.7674
1007.804	1049.688	1072.797
1119.234	1175.138	1209.645
1241.879	1292.878	1321.967
1393.094	1417.264	1439.178
1447.86	1478.017	1491.935
1530.565	1653.965	2180.56
2977.289	2987.53	3027.15
3079.772	3138.931	3183.563
3205.578	3222.943	3480.056

**i26**

**Cartesian coordinates**

C	2.518396	-1.448106	0.101461
C	1.531097	-0.535398	-0.048724
C	1.787917	0.868041	-0.089371
C	0.734568	1.804221	-0.128317
C	-0.895022	0.007481	0.427984
C	-2.279838	-0.336007	0.104725
C	-3.410901	-0.624489	-0.169065
C	-0.562595	1.439688	0.080948
C	0.092023	-0.955371	-0.259723
H	2.308787	-2.511564	0.121563
H	3.553533	-1.140990	0.205116
H	2.816372	1.212515	-0.099060
H	0.969207	2.851292	-0.289807
H	-0.772623	-0.105034	1.516891
H	-4.415705	-0.877349	-0.407875
H	-1.362487	2.169986	0.075403
H	-0.073276	-1.974615	0.093981

H	-0.117675	-0.942439	-1.335722
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**Vibrational frequencies**

96.7682	133.9258	146.0006
256.8568	367.6808	385.0678
434.1609	494.0553	527.7306
553.6748	563.4169	639.0524
698.0422	704.0904	713.3796
743.5102	797.1775	868.3225
878.1212	936.3137	978.1847
981.8415	985.8285	1062.526
1086.118	1112.216	1184.647
1204.213	1285.461	1317.801
1319.201	1334.431	1377.572
1443.741	1446.41	1473.687
1555.698	1606.355	2252.996
2987.088	3053.853	3125.949
3157.347	3185.799	3201.309
3223.844	3250.709	3488.383

**i27**

**Cartesian coordinates**

C	-0.188903	-0.863966	0.447993
C	-1.396012	-0.426078	0.008387
C	-1.576718	0.949164	-0.315338
C	-0.505198	1.860961	-0.200872
C	0.998256	0.047062	0.642152
C	2.189024	-0.482222	-0.043765
C	3.158122	-0.916631	-0.600317
C	0.720615	1.471082	0.233563
C	-2.559681	-1.368875	-0.151592
H	-0.034293	-1.912115	0.681787
H	-2.542388	1.291730	-0.669812
H	-0.665454	2.898873	-0.473376
H	1.248987	0.048885	1.718548
H	4.015146	-1.302223	-1.097508
H	1.541803	2.174658	0.303974
H	-2.932751	-1.353096	-1.179698
H	-3.387072	-1.074670	0.501047
H	-2.281010	-2.395020	0.093777

**Vibrational frequencies**

60.9836	95.8609	123.8088
202.1136	279.9588	335.581
407.8704	449.7928	495.6696
540.6874	556.2676	628.6087
688.8263	697.0748	713.6901
767.2379	782.8762	840.6737
896.2425	962.3233	979.9743
992.3067	1043.85	1062.411
1085.014	1126.237	1188.811
1209.498	1275.611	1299.757
1337.454	1352.878	1416.639
1445.595	1489.083	1495.637
1582.135	1643.28	2244.363
2935.847	3048.21	3113.61
3138.09	3187.803	3194.82
3202.19	3217.211	3484.623

**i28**

**Cartesian coordinates**

C	0.581771	1.533332	0.188660
C	-0.867727	1.768429	-0.135667
C	-1.455161	-0.616384	0.016561
C	-1.771346	0.792501	-0.236525
C	0.934524	0.074997	0.213580
C	2.198002	-0.357552	-0.120508
C	3.314790	-0.739453	-0.418496
C	-0.123049	-0.880144	0.689692
C	-2.303986	-1.597217	-0.291130
H	0.809461	1.989794	1.165927
H	1.213917	2.059988	-0.532971
H	-1.163719	2.797532	-0.314955
H	-0.262474	-0.735335	1.770311
H	-2.793136	1.028581	-0.518804
H	4.288823	-1.074509	-0.681547
H	0.190804	-1.913905	0.537654
H	-2.061087	-2.638262	-0.107960
H	-3.269500	-1.384941	-0.738271

**Vibrational frequencies**

62.123	93.8993	161.784
266.7175	309.3311	384.3406
396.5995	472.449	475.4029
494.1503	545.2465	569.4407
668.473	670.273	709.0028
804.9506	842.4153	889.0751
912.6863	943.9601	954.8137
974.7032	1008.528	1018.989
1164.491	1185.836	1195.507
1263.637	1283.892	1322.542
1331.743	1403.794	1425.663
1459.613	1465.938	1474.426
1701.411	1752.171	2045.155
2981.011	2984.719	3084.74

3129.453	3154.134	3172.636
3196.58	3241.613	3474.419

**i29**

**Cartesian coordinates**

C	-2.578980	-1.572213	0.071756
C	-1.642211	-0.881223	-0.559863
C	-0.979583	0.398022	-0.067228
C	-1.195439	1.489366	-1.085165
C	1.668641	-0.016345	0.012925
C	3.025115	-0.218031	0.041698
C	4.214628	-0.394924	0.067070
C	0.475256	0.157698	-0.008367
C	-1.475556	0.848050	1.316583
H	-2.996012	-2.468837	-0.372120
H	-2.966393	-1.281825	1.041876
H	-1.283947	-1.221275	-1.529075
H	-1.249494	1.244618	-2.138951
H	-1.053910	2.523111	-0.792340
H	5.265936	-0.551714	0.090357
H	-0.956372	1.759843	1.617184
H	-1.283322	0.079848	2.068023
H	-2.547752	1.053840	1.278600

**Vibrational frequencies**

62.8801	76.9435	118.5168
123.9382	216.7616	221.156
304.1165	308.9216	319.3837
366.4367	437.8737	485.4151
498.2252	539.4474	576.5092
585.1986	640.2166	677.4322
706.6722	728.7097	843.6367
936.2523	967.785	977.5362
1039.995	1042.66	1074.512
1206.802	1220.688	1257.107
1341.037	1407.005	1448.73
1460.719	1506.916	1508.756
1736.659	2195.249	2386.281
3058.714	3144.775	3146.874
3157.242	3159.442	3174.675
3254.402	3276.155	3483.707

**i30**

**Cartesian coordinates**

C	2.550735	1.619645	-0.074758
C	1.659380	0.806757	-0.630522
C	1.037053	-0.369296	0.025229
C	0.618406	-1.521890	-0.890884
C	-1.622321	-0.247305	-0.206539
C	-2.805873	0.300852	0.056728
C	-3.913599	0.771189	0.271362
C	-0.405501	-0.621424	-0.335750
C	1.458612	-0.704500	1.437261
H	2.954542	2.461285	-0.624852
H	2.908693	1.479451	0.939464
H	1.328670	0.996571	-1.649647
H	0.841333	-1.439661	-1.950604
H	0.679847	-2.526439	-0.483424
H	-4.869944	1.193459	0.463955
H	2.531909	-0.913498	1.477822
H	0.921703	-1.582181	1.801813
H	1.241895	0.126851	2.112716

**Vibrational frequencies**

36.1262	69.5284	113.7055
204.5162	235.3567	262.5311
287.6776	365.0187	370.3182
417.3196	439.5204	456.3909
487.6385	540.8356	563.695
679.7349	707.0856	736.993
836.2071	922.1945	944.8889
955.4929	974.7066	1031.405
1049.029	1059.46	1096.774
1146.143	1292.23	1312.647
1355.541	1413.754	1457.697
1460.241	1494.251	1510.17
1725.803	1919.795	2043.694



H 0.930026 -0.933323 2.000946  
H 2.399771 0.116315 1.712662  
H -5.397778 -0.415204 -0.283716  
H 0.853024 2.513746 0.315252  
H 1.100815 1.877562 -1.320740  
H 2.405867 1.792287 -0.129383

**Vibrational frequencies**

76.1987 86.5026 181.0887  
184.8504 202.3132 224.8534  
275.0587 309.0998 351.3276  
449.0687 474.5383 498.879  
523.7809 579.8576 583.2138  
613.522 682.2855 690.3994  
714.8002 814.2699 899.5265  
917.6648 988.1759 1040.106  
1078.449 1095.313 1108.146  
1121.773 1216.508 1297.49  
1335.874 1400.104 1425.826  
1479.083 1486.192 1496.552  
1509.027 2200.033 2384.917  
3059.088 3134.032 3145.804  
3148.668 3174.062 3182.481  
3243.205 3280.834 3488.527

**i32**

**Cartesian coordinates**

C 3.474714 0.445769 -0.980877  
C 2.468381 -0.406130 -0.586685  
C 1.453197 -0.127421 0.322644  
C 0.400691 -1.170929 0.615556  
C -2.048316 -0.306409 0.010460  
C -3.303323 0.154978 -0.299178  
C -4.403045 0.560357 -0.568793  
C -0.947487 -0.713118 0.282278  
C 1.299707 1.193922 1.008633  
H 4.217799 0.124656 -1.699584  
H 3.560819 1.456123 -0.599243  
H 2.458032 -1.397573 -1.035771  
H 0.610507 -2.093823 0.066907  
H 0.418808 -1.426141 1.684467  
H -5.375079 0.919947 -0.806027  
H 2.258688 1.695198 1.151246  
H 0.828678 1.073388 1.988282  
H 0.654630 1.862107 0.425492

**Vibrational frequencies**

36.2994 63.8055 139.0631  
142.2057 173.0379 226.2591  
305.8152 340.0385 351.4521  
383.4325 431.5897 543.5689  
549.747 576.4684 614.4517  
682.8542 687.0237 737.1729  
785.4109 802.9497 917.6722  
981.5918 1006.736 1036.375  
1061.158 1167.583 1208.443  
1234.668 1247.062 1326.083  
1389.236 1429.186 1461.218  
1463.863 1502.365 1508.862  
1538.63 2202.097 2403.548  
3015.197 3032.697 3092.4  
3094.153 3135.149 3157.306  
3171.698 3265.305 3485.649

**i33**

**Cartesian coordinates**

C 2.066775 -1.996467 -0.137968  
C 2.254545 -0.690975 -0.528105  
C 1.634430 0.436558 0.000984  
C 0.662333 0.337586 1.155785  
C -1.842897 0.050300 0.290026  
C -3.126910 -0.099117 -0.170823  
C -4.252672 -0.230261 -0.573283  
C -0.715837 0.178272 0.695940  
C 1.830846 1.797295 -0.585130  
H 2.608743 -2.799417 -0.620960  
H 1.360909 -2.276552 0.635277  
H 2.952752 -0.512603 -1.343634  
H 0.919641 -0.496707 1.815233  
H 0.722500 1.246982 1.764608

H -5.246716 -0.348004 -0.931505  
H 2.536766 1.781330 -1.417240  
H 2.202150 2.504236 0.167024  
H 0.879577 2.201594 -0.953360

**Vibrational frequencies**

28.349 68.2997 134.6293  
161.329 181.2082 227.2483  
293.2234 336.4134 347.5802  
383.3468 472.2837 538.8853  
550.5961 563.9145 594.5736  
678.3438 702.5119 734.9844  
790.6527 811.9246 914.12  
972.473 997.9448 1038.563  
1068.437 1168.883 1182.307  
1236.903 1276.45 1322.561  
1379.575 1424.524 1461.007  
1475.485 1481.323 1510.391  
1539.365 2201.546 2402.08  
3017.213 3046.347 3066.688  
3093.757 3136.905 3156.813  
3170.245 3262.139 3484.407

**i34**

**Cartesian coordinates**

C 3.576684 -0.876233 -0.403595  
C 2.273642 -1.039656 -0.217734  
C 0.488953 0.629051 0.241781  
C 1.466573 -0.348638 0.851976  
C -2.019911 0.016961 0.032659  
C -3.330622 -0.304935 -0.083812  
C -4.500890 -0.592153 -0.189923  
C -0.827582 0.310041 0.130476  
C 1.029263 1.921300 -0.291252  
H 4.103774 -1.388935 -1.200385  
H 4.164631 -0.228552 0.240778  
H 1.709438 -1.691358 -0.881339  
H 0.922438 -1.090298 1.442683  
H 2.141022 0.190728 1.527255  
H -5.529820 -0.841996 -0.285594  
H 1.452714 2.520693 0.523731  
H 0.258283 2.508571 -0.789322  
H 1.840864 1.726718 -1.001261

**Vibrational frequencies**

41.8386 80.9607 98.7176  
106.7932 123.633 210.6485  
229.3786 311.4652 339.9276  
423.8708 455.8249 493.2002  
509.2489 583.8669 599.3357  
623.5544 678.4615 716.8408  
907.76 916.8351 959.4878  
971.3279 1014.988 1043.916  
1057.394 1128.956 1219.312  
1263.608 1306.409 1332.389  
1404.092 1437.704 1456.136  
1475.873 1483.538 1508.932  
1732.89 2053.041 2157.578  
3029.079 3046.487 3085.823  
3109.565 3141.968 3154.757  
3167.131 3233.838 3480.762

**i35**

**Cartesian coordinates**

C -0.490299 1.262569 0.000076  
C 1.008753 1.174490 0.000045  
C 1.721854 0.051374 0.000012  
C 1.057827 -1.317536 0.000077  
C -1.165027 -0.103687 0.000043  
C -2.593829 -0.137750 -0.000067  
C -3.794651 -0.105891 -0.000078  
C -0.407761 -1.182684 0.000055  
C 3.222812 0.032431 -0.000121  
H -0.834662 1.828163 -0.874456  
H -0.834635 1.828130 0.874642  
H 1.535784 2.125520 0.000024  
H 1.392778 -1.888709 -0.875699  
H 1.392773 -1.888617 0.875911  
H -4.857775 -0.095962 -0.000165  
H 3.637174 1.042187 0.000202  
H 3.605159 -0.494975 -0.880827  
H 3.605335 -0.495630 0.880111

**Vibrational frequencies**

49.929 136.137 157.9596  
168.4597 250.3568 334.4426  
345.174 382.0892 438.8579  
509.7638 537.3439 597.3066  
653.4025 671.9912 698.1412  
761.9525 808.6981 914.0476  
949.2037 966.5257 974.85  
1065.81 1070.612 1089.994  
1151.773 1190.54 1211.738  
1215.845 1323.218 1359.896  
1370.811 1420.508 1469.25  
1475.477 1479.27 1498.067  
1749.614 1782.041 2238.162  
3021.693 3032.774 3038.441  
3048.066 3061.104 3095.943  
3138.284 3170.692 3483.615

**i36**

**Cartesian coordinates**

C 3.529360 -1.022489 -0.003756  
C 2.765463 0.261082 -0.001333  
C 1.410763 0.434762 0.003379  
C 0.504304 -0.661267 0.006431  
C -2.081378 -0.371627 0.002977  
C -3.433338 -0.217487 -0.001430  
C -4.632141 -0.077583 -0.005886  
C -0.867234 -0.509297 0.005706  
C 0.830548 1.827547 0.001135  
H 4.295347 -1.009464 0.777725  
H 4.054262 -1.153395 -0.956918  
H 3.374955 1.161564 -0.016398  
H 2.906315 -1.902591 0.156162  
H 0.882708 -1.677201 0.003775  
H -5.688113 0.045949 -0.010150  
H 1.617651 2.582743 -0.002472  
H 0.201775 1.987376 0.881456  
H 0.197018 1.983172 -0.876520

**Vibrational frequencies**

54.7965 65.1193 97.7327  
105.2485 170.7947 200.7985  
237.8906 248.317 376.488  
402.4947 467.9982 497.1685  
513.7031 523.21 559.8371  
630.7425 697.859 737.2217  
793.9146 797.1567 834.4678  
975.1763 1047.127 1062.364  
1066.254 1119.041 1233.898









H 1.896761 -2.543166 -0.755198

**Vibrational frequencies**

87.1295	138.9421	147.5048
213.9364	346.4208	392.4933
396.7881	423.4941	530.3827
553.2564	555.2051	632.1542
658.7362	718.4815	735.1096
798.3768	839.0268	918.7325
940.1536	949.3978	950.3139
1005.911	1042.043	1075.73
1152.008	1172.473	1212.125
1233.162	1301.197	1322.911
1332.266	1368.452	1455.24
1475.31	1481.129	1502.741
1743.082	1753.162	2238.11
3035.77	3050.297	3051.609
3090.985	3100.969	3117.476
3152.264	3238.761	3484.91

**i88**

**Cartesian coordinates**

C	0.139538	-1.102756	-0.101407
C	-1.116644	-0.677943	0.088037
C	-1.097849	0.803670	0.413066
C	-1.864941	1.634455	-0.564148
C	1.076124	0.020958	0.078947
C	2.490048	-0.086804	-0.052509
C	3.679916	-0.203371	-0.168567
C	0.378252	1.130270	0.388220
C	-2.382850	-1.462407	0.006474
H	0.448380	-2.111214	-0.345482
H	-1.491665	0.962397	1.426414
H	-2.404535	2.518079	-0.247848
H	-1.717211	1.465180	-1.624516
H	4.733636	-0.300250	-0.271570
H	0.782508	2.115563	0.571450
H	-3.056679	-1.038225	-0.745050
H	-2.917397	-1.443944	0.961847
H	-2.186595	-2.504016	-0.253929

**Vibrational frequencies**

95.1635	138.2684	143.9491
156.3624	179.1462	232.0401
290.4211	353.9645	454.0425
502.5852	538.7424	579.3039
581.9445	652.8473	663.5902
691.8551	719.3058	797.1694
841.0221	879.8081	950.0528
997.7449	1011.435	1027.685
1074.017	1119.97	1148.047
1189.096	1227.033	1271.638
1323.741	1364.427	1422.094
1458.231	1481.422	1496.278
1632.381	1710.215	2247.293
3038.402	3040.847	3098.503
3135.052	3156.284	3229.668
3250.822	3271.126	3489.078

**i89**

**Cartesian coordinates**

C	-0.055019	-0.916743	0.246868
C	1.294030	-0.327481	0.080312

C	1.028175	1.084380	-0.416284
C	1.574902	0.857442	0.990216
C	-1.033659	0.015240	-0.098201
C	-2.440981	-0.201085	0.007250
C	-3.624412	-0.385994	0.092126
C	-0.436620	1.203323	-0.528151
C	2.437998	-1.182945	-0.405156
H	-0.244189	-1.918435	0.609188
H	1.682066	1.566825	-1.133700
H	2.618106	1.106413	1.150941
H	0.913850	1.041440	1.829102
H	-4.672042	-0.549484	0.169743
H	-0.967592	2.086593	-0.854378
H	2.670451	-1.967739	0.320855
H	3.340321	-0.583083	-0.547798
H	2.192552	-1.659349	-1.357831

**Vibrational frequencies**

111.9228	147.6207	209.8798
236.4781	295.9802	347.2859
418.7985	492.3546	520.9292
545.3373	557.1469	628.0012
676.4668	677.3455	727.948
750.7276	777.0805	819.6737
869.1024	937.2844	950.1064
976.0812	1004.254	1045.656
1061.841	1083.996	1111.069
1172.41	1217.948	1260.408
1299.602	1336.163	1397.101
1427.964	1481.005	1492.871
1510.453	1545.471	2245.916
3047.326	3119.081	3130.64
3141.444	3188.412	3236.951
3239.391	3245.333	3485.555

**i90**

**Cartesian coordinates**

C	0.112598	-1.098901	0.109844
C	1.346563	-0.531034	-0.081699
C	1.184949	0.909969	-0.414070
C	0.556070	1.770445	0.666812
C	-0.921238	-0.157745	-0.108668
C	-2.294811	-0.386377	-0.012955
C	-3.488047	-0.569905	0.062410
C	-0.306151	1.160882	-0.421701
C	2.678105	-1.182975	0.058045
H	-0.059126	-2.122187	0.419745
H	1.854210	1.384129	-1.123151
H	0.727994	2.838739	0.608903
H	0.481752	1.359945	1.667318
H	-4.535742	-0.734418	0.134542
H	-0.781803	1.824838	-1.132343
H	3.260081	-0.714048	0.859765
H	3.262837	-1.075756	-0.862373
H	2.581573	-2.247392	0.279483

**Vibrational frequencies**

102.1711	141.2017	156.1983
186.4751	308.3433	345.9727
373.4289	502.3472	520.495
545.7232	569.14	613.9795
641.737	714.1604	790.3238
805.7729	861.4825	885.0742
917.9853	931.6574	997.6235
1011.067	1041.766	1054.879
1074.544	1092.617	1152.144
1187.495	1219.855	1265.26
1320.513	1378.504	1417.208

1424.457	1474.418	1480.911
1483.328	1543.949	2132.436
3030.561	3084.588	3136.533
3143.341	3182.825	3204.109
3228.318	3241.964	3480.21

**i91**

**Cartesian coordinates**

C	-0.647359	1.430900	0.227738
C	0.813899	1.744117	0.088277
C	1.485074	-0.616821	-0.468794
C	1.750850	0.858025	-0.227369
C	-0.960742	-0.031353	-0.067766
C	-2.330220	-0.437357	-0.010353
C	-3.495627	-0.721872	0.050938
C	0.029352	-0.849940	-0.367421
C	2.286343	-1.493632	0.507224
H	-1.235589	2.064853	-0.446735
H	-0.991716	1.674193	1.240296
H	1.099455	2.778194	0.258941
H	1.811757	-0.862815	-1.488387
H	2.788611	1.171361	-0.311960
H	-4.523445	-0.988998	0.101166
H	3.357123	-1.301052	0.399550
H	2.106413	-2.553306	0.314286
H	1.997968	-1.274835	1.538003

**Vibrational frequencies**

79.4085	105.3417	142.5301
262.8135	283.6199	286.6341
419.1968	431.3508	499.4519
518.7349	549.8504	587.4642
665.0161	698.4033	708.2399
750.7816	862.1249	908.4645
945.7361	963.6499	996.8475
1019.386	1066.618	1097.377
1145.47	1163.716	1201.917
1217.04	1311.656	1338.421
1362.57	1402.168	1419.442
1475.118	1502.311	1511.419
1737.791	1765.325	2239.657
3025.638	3038.466	3051.382
3067.9	3132.114	3139.155
3163.478	3189.947	3487.001

**i92**

**Cartesian coordinates**

C	0.021215	-0.938625	0.547000
C	1.425459	-0.659543	0.075861
C	1.888194	0.758306	0.296466
C	0.840029	1.750530	-0.120246
C	-0.947822	0.113302	0.056115
C	-2.305907	-0.208424	-0.049049
C	-3.474701	-0.509964	-0.129254
C	-0.475012	1.410693	-0.236359
C	2.180541	-1.581413	-0.508422
H	-0.306006	-1.931171	0.230563
H	0.001475	-0.935422	1.647744
H	2.111575	0.906675	1.364714
H	2.823880	0.942434	-0.238402
H	1.152627	2.768895	-0.322969
H	-4.503619	-0.765998	-0.207200
H	-1.196855	2.155634	-0.553481
H	1.817579	-2.591654	-0.667034
H	3.187363	-1.358565	-0.846604

**Vibrational frequencies**

63.4568	124.0664	149.2103
215.32	379.3743	392.0496
410.4601	428.446	530.4528



989.6548	1004.643	1040.963	<b>Vibrational frequencies</b>			C	-1.069628	-0.062154	-0.000073		
			45.9856	116.2535	131.2818	C	-2.500666	-0.060683	0.000077		
1143.057	1198.172	1209.369				C	-3.701393	-0.013574	0.000233		
			150.8419	278.5236	322.4103	C	-0.381274	-1.205924	-0.000030		
1238.569	1284.465	1345.765				C	3.211613	0.057673	0.000302		
			390.654	425.9704	457.0874	H	-0.747984	1.860893	-0.870863		
1411.081	1431.194	1436.993				H	-0.748210	1.861231	0.870047		
			497.4093	528.9647	568.2732	H	1.627608	2.162429	0.000129		
1458.07	1483.487	1486.068				H	1.435750	-1.872906	-0.872416		
			612.076	663.6485	674.2951	H	1.435968	-1.873355	0.871577		
1511.602	1658.607	2177.305				H	-4.764224	0.015611	0.000386		
			715.8308	764.8752	855.2032	H	-0.924986	-2.145439	0.000120		
2987.469	2998.16	3032.27				H	3.760909	0.992000	0.000431		
			873.2462	933.3938	941.2387	H	3.782273	-0.863962	0.000396		
3088.604	3135.914	3170.291				<b>Vibrational frequencies</b>					
			991.9257	997.7492	1016.67		30.7517	143.2045	154.9058		
3188.472	3196.293	3483.054									
			1105.429	1166.196	1175.342		196.8908	348.8154	362.677		
			1200.678	1233.58	1273.286		394.225	462.0883	525.3105		
<b>i98</b>			1315.573	1350.519	1386.559		527.0911	538.8737	601.7134		
<b>Cartesian coordinates</b>			1432.214	1464.12	1476.425		654.5852	693.5623	700.9463		
C	0.016052	-0.836879	-0.824677	1676.723	1735.362	2241.121	726.8784	770.7773	775.5945		
C	-1.450148	-0.806275	-0.368383	2878.719	3011.476	3097.123	856.4795	931.0679	950.6889		
C	-1.944253	0.626371	-0.261729	3155.018	3188.196	3197.835	954.5938	990.1836	1057.712		
C	-1.105343	1.617044	0.064524	3216.84	3263.282	3484.717	1103.266	1156.645	1217.554		
C	0.866360	0.196951	-0.115934	<b>i100</b>			1239.164	1246.723	1332.98		
C	2.254639	-0.073174	0.053683	<b>Cartesian coordinates</b>			1343.684	1412.044	1431.276		
C	3.420595	-0.340087	0.177678	C	0.617631	1.459142	-0.062249	1461.241	1468.922	1487.935	
C	0.314710	1.361781	0.268917	C	-0.830497	1.751034	-0.234217	1527.758	1749.164	2237.017	
C	-1.664813	-1.429349	0.974375	C	-1.468150	-0.648320	0.028326	3014.623	3029.007	3033.185	
H	0.067504	-0.629011	-1.901855	C	-1.845893	0.795096	0.288950	3054.506	3156.096	3181.389	
H	-2.053140	-1.337368	-1.110330	C	0.921452	-0.021634	0.000598	3193.308	3255.64	3483.317	
H	-3.008709	0.807967	-0.365179	C	2.301985	-0.386720	0.018571	<b>i102</b>			
H	-1.476301	2.625256	0.212886	C	3.474642	-0.650196	0.035113	<b>Cartesian coordinates</b>			
H	4.453548	-0.562902	0.294606	C	-0.041073	-0.958671	0.015988	C	-3.485482	-0.055343	-0.373019
H	0.928794	2.126967	0.729689	C	-2.383106	-1.604227	-0.146842	C	-2.342262	-0.723484	-0.071097
H	-0.978161	-1.199953	1.781961	H	1.012586	1.929882	0.855093	C	-1.053498	-0.160559	0.075404
H	0.431696	-1.835437	-0.673028	H	1.199951	1.902774	-0.878302	C	-0.669393	1.200680	-0.084561
H	-2.612024	-1.893827	1.220529	H	-1.132132	2.750630	-0.523524	C	1.300165	0.092462	0.621236
				H	-1.939384	0.917705	1.383657	C	2.540536	-0.201885	-0.095656
<b>Vibrational frequencies</b>				H	-2.834987	1.006841	-0.124195	C	3.555799	-0.442188	-0.687092
	89.5513	150.14	160.8303	H	4.509328	-0.894463	0.049876	C	0.644354	1.385026	0.181046
				H	0.242377	-2.006524	0.015149	C	0.179681	-0.966941	0.406330
198.6659	240.9139	331.2869		H	-2.095156	-2.639147	-0.298380	H	-4.429072	-0.578240	-0.465106
				H	-3.444514	-1.380718	-0.144806	H	-3.500157	1.017308	-0.532470
353.451	447.3351	511.1593		<b>Vibrational frequencies</b>			H	-2.411387	-1.799329	0.078623	
				88.0845	126.0545	140.8459	H	-1.347075	1.991326	-0.381860	
543.2656	551.5396	579.7764		153.9279	307.4588	350.4111	H	1.544248	0.163371	1.689329	
				377.8603	422.9289	514.2061	H	4.455584	-0.653770	-1.212439	
608.0939	676.3513	714.4544		521.3592	549.3941	553.3856	H	1.185353	2.320135	0.125221	
				651.0851	660.8818	712.4841	H	0.441288	-1.629502	-0.425347	
731.2927	764.5088	848.0673		719.8273	860.0603	873.198	H	0.041811	-1.597913	1.288500	
				900.9401	919.2856	925.3675	<b>Vibrational frequencies</b>				
869.3909	923.8024	946.5618		944.9384	993.2299	1021.387		39.1063	135.7758	151.895	
				1119.891	1156.091	1184.129		212.3521	230.2247	278.3562	
998.3937	1009.059	1036.909		1228.993	1306.444	1331.605		410.0752	440.2177	536.0859	
				1347.488	1394.212	1402.262		554.3637	609.1542	653.2098	
1099.61	1123.418	1177.717		1455.122	1456.753	1464.744		698.6863	713.9036	718.0104	
				1689.423	1733.907	2233.719		769.535	855.4319	864.3537	
1201.395	1254.585	1300.612		2933.84	2958.845	3057.497		869.1676	956.5756	967.7544	
				3098.072	3155.817	3185.484		1012.739	1034.337	1041.785	
1323.853	1349.681	1394.528		3207.212	3244.213	3485.582		1063.474	1116.467	1183.332	
				<b>i101</b>				1218.652	1243.805	1260.343	
1422.474	1455.102	1480.841		<b>Cartesian coordinates</b>				1299.117	1316.117	1340.136	
				C	-0.398129	1.289134	-0.000251		1422.045	1460.784	1475.574
1422.474	1455.102	1480.841		C	1.092099	1.217424	-0.000027				
1652.749	1715.081	2229.799		C	1.825544	0.046441	0.000027				
				C	1.112317	-1.291088	-0.000227				
3030.862	3080.56	3108.647									
3155.704	3187.672	3206.882									
3217.097	3268.676	3483.341									
<b>i99</b>											
<b>Cartesian coordinates</b>											
C	0.024536	-0.931924	0.124954								
C	1.463192	-0.523852	0.326189								
C	1.734919	0.842131	-0.324687								
C	0.645321	1.830515	-0.007403								
C	-0.950014	-0.010045	0.078219								
C	-2.326771	-0.376792	-0.053998								
C	-3.490743	-0.652674	-0.163545								
C	-0.610692	1.422970	0.173818								
C	2.433823	-1.561699	-0.116391								
H	-0.218574	-1.988037	0.072553								
H	1.584970	-0.378503	1.420348								
H	2.707691	1.216568	0.004747								
H	1.798592	0.718544	-1.415792								
H	0.887320	2.887724	0.018436								
H	-4.518975	-0.903856	-0.263666								
H	-1.413548	2.126041	0.362251								
H	2.156701	-2.608710	-0.149962								
H	3.474389	-1.301555	-0.271852								



1549.235	1583.51	2248.581	680.8164	719.4655	729.0965
3028.114	3056.901	3103.682	767.6192	827.8464	881.8826
3154.899	3165.895	3219.887	913.0545	962.9362	980.4486
3243.99	3257.69	3483.838	989.6566	1008.997	1039.99

H	4.739866	-0.000002	0.431549
H	0.921245	-2.160107	-0.088981
H	-3.518442	0.885728	0.653444
H	-2.408486	-0.000002	1.715846
H	-3.518442	-0.885730	0.653443

**i103**

**Cartesian coordinates**

C	0.452715	1.192698	0.000002
C	-1.039822	1.253374	0.000000
C	-1.719844	-0.085607	-0.000001
C	-0.984667	-1.232959	0.000000
C	1.131704	0.007997	0.000002
C	2.566176	-0.004474	0.000000
C	3.766780	-0.027887	-0.000002
C	0.425652	-1.228643	0.000001
C	-3.215379	-0.078413	-0.000001
H	1.001961	2.127131	0.000001
H	-1.388749	1.840713	-0.867174
H	-1.388752	1.840714	0.867172
H	-1.499851	-2.189016	0.000000
H	4.829826	-0.045869	-0.000005
H	0.979873	-2.157958	0.000002
H	-3.604216	0.448753	-0.879490
H	-3.604218	0.448826	0.879443
H	-3.625764	-1.089819	0.000040

**Vibrational frequencies**

74.6747	143.6775	145.3381
168.2468	263.615	333.7359
392.0484	404.4891	467.5338
529.7336	600.6865	609.6679
658.3861	691.6744	700.9296
749.1981	783.9276	789.0982
895.6633	941.6347	966.1763
1001.893	1051.556	1060.051
1126.811	1179.062	1202.429
1221.644	1300.251	1332.018
1371.903	1418.987	1436.059
1447.541	1476.698	1493.709
1583.414	1632.256	2241.234
2953.314	2956.036	3027.003
3078.239	3136.1	3184.803
3208.594	3229.678	3483.553

**i104**

**Cartesian coordinates**

C	-3.101858	0.075565	0.591681
C	-2.328674	-0.713822	-0.141522
C	-0.980325	-0.336789	-0.722838
C	-0.615220	1.124214	-0.605768
C	1.083434	0.020784	0.610227
C	2.481853	-0.172939	0.205883
C	3.624265	-0.335696	-0.120995
C	0.488715	1.323094	0.102129
C	0.146706	-0.997681	0.018877
H	-4.045504	-0.279029	0.990703
H	-2.818473	1.097270	0.823942
H	-2.645426	-1.735312	-0.342067
H	-1.209358	1.906311	-1.063297
H	1.055798	-0.002636	1.711585
H	4.635789	-0.479931	-0.414942
H	0.950305	2.280264	0.309095
H	-0.984008	-0.642194	-1.781968
H	0.267503	-2.065127	0.140905

**Vibrational frequencies**

43.9425	106.57	115.956
177.4024	250.7441	319.0661
373.6781	393.0356	501.1859
530.586	582.7557	658.8177

1048.081	1068.357	1109.14
1138.728	1243.617	1260.788
1277.119	1305.029	1312.06
1333.852	1402.765	1449.351
1714.901	1728.035	2244.859
2971.455	2982.079	3148.624
3165.888	3210.895	3236.876
3240.65	3241.247	3485.475

**i105**

**Cartesian coordinates**

C	0.345047	1.258645	-0.168163
C	-1.141022	1.211098	-0.005659
C	-1.832727	-0.002112	-0.046577
C	-1.027116	-1.234185	-0.164245
C	1.023960	0.019338	0.448724
C	2.443390	-0.035320	0.098889
C	3.604704	-0.071302	-0.197565
C	0.287048	-1.243416	0.048248
C	-3.208698	-0.079392	0.014504
H	0.762618	2.165710	0.274733
H	0.595454	1.290139	-1.239422
H	-1.695744	2.141604	0.050622
H	-1.545955	-2.155458	-0.409259
H	0.956515	0.105644	1.543315
H	4.635192	-0.106189	-0.456941
H	0.858024	-2.163012	-0.014379
H	-3.813337	0.815039	0.108963
H	-3.720277	-1.033600	-0.026570

**Vibrational frequencies**

71.8281	139.9648	203.5067
243.0256	328.3166	366.2148
397.1565	493.949	518.2535
554.5406	593.8342	632.8397
679.9625	693.6733	701.0872
719.6224	769.4612	798.7528
819.9177	945.303	951.2039
980.0704	1007.114	1054.989

1067.938	1126.8	1182.802
1221.426	1285.53	1297.534
1319.954	1345.9	1380.794
1439.796	1449.111	1479.498
1525.782	1724.634	2252.705
2996.257	3010.546	3106.164
3162.772	3186.311	3194.852
3210.92	3262.189	3487.438

**i106**

**Cartesian coordinates**

C	0.367103	1.229992	-0.147928
C	-0.972800	1.244845	-0.313850
C	-1.807040	0.000000	-0.376919
C	-0.972799	-1.244845	-0.313850
C	1.093463	0.000001	-0.049449
C	2.488878	0.000001	0.132928
C	3.686058	-0.000001	0.291186
C	0.367104	-1.229991	-0.147928
C	-2.882307	-0.000001	0.731392
H	0.921243	2.160108	-0.088980
H	-1.495954	2.193568	-0.386947
H	-2.351032	0.000000	-1.335918
H	-1.495952	-2.193569	-0.386948

**Vibrational frequencies**

61.9124	144.1501	165.67
215.906	277.4367	353.9087
431.0141	436.9658	488.1216
541.046	613.6552	614.8922
651.1461	687.1395	729.7936
760.6639	776.5322	812.5026
942.9009	968.6595	988.2209
990.5692	1039.901	1079.314
1112.116	1183.15	1191.238
1262.985	1277.282	1298.915
1356.107	1400.929	1421.252
1471.841	1493.731	1500.785
1559.909	1648.721	2149.549
2972.803	3046.553	3125.787
3136.214	3180.886	3182.181
3208.38	3210.484	3478.2

**i107**

**Cartesian coordinates**

C	-0.311313	-1.086455	0.834681
C	0.826302	-1.264825	-0.108950
C	1.693426	-0.026839	-0.196272
C	0.996717	1.254948	-0.056001
C	-1.115116	0.180594	0.761632
C	-2.251971	0.012256	-0.162556
C	-3.163281	-0.153152	-0.925369
C	-0.269110	1.365645	0.346213
C	3.005837	-0.086966	-0.423169
H	-0.750270	-1.943311	1.331437
H	0.425103	-1.459942	-1.119895
H	1.426633	-2.136898	0.159494
H	1.558349	2.152177	-0.299982
H	-1.537756	0.394226	1.752322
H	-3.968462	-0.295056	-1.605090
H	-0.745788	2.338693	0.400961
H	3.521562	-1.035985	-0.522795
H	3.601688	0.814855	-0.517709

**Vibrational frequencies**

49.2961	109.9136	158.5056
237.0361	316.0803	374.3107
401.2499	440.5545	480.4684
567.6954	569.9822	627.5883
692.1703	697.1269	706.6088
759.1368	804.6462	862.2384
885.4953	935.9353	948.6331
985.9447	1005.586	1016.84
1029.77	1136.952	1184.162
1216.059	1285.875	1310.939
1322.959	1350.318	1389.853
1417.12	1454.92	1469.8
1701.787	1753.656	2235.704
2946.351	3028.33	3097.674
3154.445	3172.308	3202.659
3211.654	3242.732	3483.35

**i108**

**Cartesian coordinates**

C	2.446855	-0.420485	-0.748222	1197.678	1233.137	1301.732	148.6547	215.1645	234.5493
C	1.728963	0.560170	0.132999	1354.779	1428.414	1460.223	267.4909	356.4361	367.8392
C	0.831416	-0.495012	0.753355						
C	1.607083	-1.555319	-0.100948	1472.048	1496.9	1504.486	468.8277	501.834	522.5086
C	-1.752141	-0.189023	0.194260						
C	-3.079247	-0.012185	-0.105536	1511.762	2058.225	2157.23	585.3528	594.3312	646.7945
C	-4.243033	0.143785	-0.367106						
C	-0.586202	-0.347176	0.459985	3046.288	3121.427	3127.69	695.6635	788.6023	827.2568
C	1.534757	2.022082	0.028310						
H	3.531107	-0.493974	-0.603659	3140.671	3145.93	3158.367	845.1283	881.1661	955.783
H	2.266963	-0.283721	-1.822911						
H	0.959113	-0.622508	1.836170						
H	2.181099	-2.254659	0.507045	3227.591	3241.509	3481.082	1018.759	1023.491	1050.67
H	0.974675	-2.113002	-0.790482						
H	-5.271983	0.283097	-0.595197				1074.198	1100.417	1131.187
H	0.768730	2.272802	-0.721875						
H	2.460445	2.522324	-0.270200						
H	1.199141	2.448615	0.978534						

**Vibrational frequencies**

	44.0899	58.8399	97.1591
	106.5748	152.8673	225.2285
	255.3317	312.1349	434.0535
	490.978	536.5443	584.8854
	631.8646	677.0652	696.4732
	703.0994	761.8766	869.9825
	927.8204	939.2647	962.7249
	972.494	1032.214	1090.942
	1169.907	1197.175	1211.305
	1223.451	1237.244	1289.681
	1327.427	1355.254	1414.103
	1468.318	1473.574	1486.545
	1498.697	2198.061	2392.518
	2986.879	3015.125	3020.391
	3053.455	3071.281	3102.607
	3119.059	3165.69	3485.122

**i109**

**Cartesian coordinates**

C	-2.847317	-0.266690	-0.748025	1216.533	1248.065	1289.754	137.2196	168.0648	195.8265
C	-1.575802	0.107382	-0.000043	1302.575	1334.492	1364.954	214.9774	278.9777	345.9508
C	-0.500492	-0.899990	-0.000016						
C	-2.847302	-0.266640	0.748014	1410.724	1467.51	1493.817	381.511	452.4189	484.949
C	2.024417	-0.326190	0.000077						
C	3.346302	-0.029514	0.000042	1500.661	2199.913	2395.98	497.3706	548.0264	568.8093
C	4.526404	0.235851	-0.000048						
C	0.824597	-0.602079	0.000044	3026.102	3030.478	3049.748	587.7428	682.1519	704.3686
C	-1.150162	1.557780	-0.000009						
H	-3.359704	0.537173	-1.263694	3068.732	3092.25	3129.015	794.1486	812.8563	853.8811
H	-2.869427	-1.220418	-1.261666						
H	-0.787927	-1.948643	-0.000061	3132.819	3222.545	3484.81	867.7937	1022.199	1025.022
H	-3.359636	0.537298	1.263638						
H	-2.869429	-1.220303	1.261773				1064.266	1110.282	1190.05
H	5.564212	0.466498	-0.000253						
H	-0.550043	1.786910	0.884646				1221.221	1233.024	1350.327
H	-2.022717	2.215276	-0.000476						
H	-0.549201	1.786749	-0.884124						

**Vibrational frequencies**

	38.5211	68.3785	136.8856
	200.3856	214.4577	308.7964
	327.3083	358.4991	379.467
	400.3698	474.0664	479.2838
	546.0034	602.9087	685.5624
	687.0049	758.5039	778.995
	812.2422	825.9147	933.2592
	954.1965	964.9808	1044.639
	1074.409	1080.996	1115.223

**i110**

**Cartesian coordinates**

C	2.649058	-0.269503	-0.456047				1199.678	1214.415	1291.779
C	1.825589	0.609787	0.437598						
C	0.863272	-0.627194	0.634759				1363.814	1410.251	1448.814
C	1.675267	-1.404085	-0.455000						
C	-1.723140	-0.249986	0.179561				1464.715	1489.241	1507.837
C	-3.058119	-0.046773	-0.062533						
C	-4.228662	0.132479	-0.273870				1518.041	2070.775	2163.825
C	-0.550016	-0.428838	0.394307						
C	1.216327	1.850787	-0.211423				3032.499	3088.569	3154.051
H	3.569057	-0.093948	-0.999002						
H	2.315559	0.901950	1.374843				3157.465	3158.925	3192.147
H	1.001567	-1.073169	1.622168						
H	2.044906	-2.387657	-0.145566				3237.97	3252.064	3479.537
H	1.120208	-1.535592	-1.392443						
H	-5.263339	0.291190	-0.459417						
H	0.700069	1.597223	-1.140730						
H	2.000948	2.575856	-0.442486						
H	0.493575	2.324097	0.458517						

**Vibrational frequencies**

	56.7982	71.2102	107.8876
	202.0332	224.2989	238.2883
	254.3662	338.5065	410.348
	441.7691	497.6477	542.1812
	596.5979	675.2986	703.7739
	714.8999	747.6532	868.9583
	895.9315	910.2451	967.1273
	992.3969	1038.078	1059.622
	1090.121	1126.859	1204.145
	1216.533	1248.065	1289.754
	1302.575	1334.492	1364.954
	1410.724	1467.51	1493.817
	1500.661	2199.913	2395.98
	3026.102	3030.478	3049.748
	3068.732	3092.25	3129.015
	3132.819	3222.545	3484.81
	59.4794	68.3739	95.8585
	137.2196	168.0648	195.8265
	214.9774	278.9777	345.9508
	381.511	452.4189	484.949
	497.3706	548.0264	568.8093
	587.7428	682.1519	704.3686
	794.1486	812.8563	853.8811
	867.7937	1022.199	1025.022
	1064.266	1110.282	1190.05
	1221.221	1233.024	1350.327
	1380.285	1429.838	1462.45
	1468.912	1485.34	1488.667
	1721.712	2197.253	2378.493
	2988.038	3043.673	3055.456
	3101.898	3154.536	3158.988
	3169.377	3268.227	3485.076
	52.1675	73.2027	107.2343

**i111**

**Cartesian coordinates**

C	2.880303	-0.562134	-0.695538				1221.221	1233.024	1350.327
C	1.486190	-0.715887	-0.121630						
C	0.562875	0.433157	-0.017938				1380.285	1429.838	1462.45
C	2.715032	-0.819422	0.768000						
C	-1.995333	0.001899	-0.012045				1468.912	1485.34	1488.667
C	-3.332276	-0.224030	-0.004472						
C	-4.524715	-0.425611	0.003550				1721.712	2197.253	2378.493
C	-0.782675	0.206317	-0.016814						
C	1.088150	1.837381	0.063152				2988.038	3043.673	3055.456
H	3.245063	-1.362320	-1.327441						
H	3.192128	0.429786	-0.999693				3101.898	3154.536	3158.988
H	0.993819	-1.658415	-0.329232						
H	2.954442	-1.801592	1.155992				3169.377	3268.227	3485.076
H	2.911533	-0.004823	1.454632						
H	-5.572893	-0.602546	0.011242						
H	0.295340	2.537132	0.325396						
H	1.511535	2.148544	-0.899083						
H	1.883731	1.924216	0.810602						

**Vibrational frequencies**

**i112**

**Cartesian coordinates**

C	3.614110	-0.067304	0.831789						
C	1.372539	0.032493	-0.275276						
C	0.384854	-0.873498	-0.211843						
C	2.811930	-0.411485	-0.378940						
C	-2.172000	-0.305962	0.002581						
C	-3.506641	-0.020014	0.118744						
C	-4.678698	0.233029	0.221593						
C	-0.993374	-0.553668	-0.096927						
C	1.139678	1.511755	-0.234772						
H	4.676582	0.127231	0.756999						
H	3.172247	-0.162515	1.817048						
H	0.625725	-1.932576	-0.248555						
H	3.266875	0.049540	-1.264531						
H	2.842233	-1.498085	-0.554669						
H	-5.714604	0.453137	0.314979						
H	1.516764	1.974840	-1.153025						
H	1.695918	1.957354	0.596065						
H	0.083875	1.759001	-0.126012						

**Vibrational frequencies**

	59.4794	68.3739	95.8585
	137.2196	168.0648	195.8265
	214.9774	278.9777	345.9508
	381.511	452.4189	484.949
	497.3706	548.0264	568.8093
	587.7428	682.1519	704.3686
	794.1486	812.8563	853.8811
	867.7937	1022.199	1025.022
	1064.266	1110.282	1190.05
	1221.221	1233.024	1350.327
	1380.285	1429.838	1462.45
	1468.912	1485.34	1488.667
	1721.712	2197.253	2378.493
	2988.038	3043.673	3055.456
	3101.898	3154.536	3158.988
	3169.377	3268.227	3485.076

**i113**

**Cartesian coordinates**



H 4.538583 -1.046488 0.220002  
H 3.789902 -1.638420 -1.257814  
H 3.212327 -2.218481 0.313532

**Vibrational frequencies**

47.3664 77.0512 117.836  
170.7258 191.4478 203.4317  
216.9307 255.2668 287.7517  
363.5921 403.5267 476.0376  
547.2362 567.6579 597.686  
616.5009 677.9148 707.4844  
744.0707 831.5322 887.2205  
969.6658 1017.689 1045.363  
1078.804 1113.579 1146.841  
1177.161 1278.946 1306.77  
1330.301 1343.76 1418.257  
1455.748 1481.75 1499.244  
1767.876 2198.801 2393.253  
3029.78 3042.653 3103.673  
3130.679 3158.758 3163.587  
3164.48 3279.578 3486.177

**i119**

**Cartesian coordinates**

C -1.382260 -2.360049 -0.000014  
C -2.051440 1.430117 0.000013  
C -2.116217 0.066246 0.000023  
C -1.065714 -0.884692 0.000008  
C 1.485158 -0.333634 -0.000009  
C 2.818940 -0.055739 0.000001  
C 3.999112 0.194151 0.000016  
C 0.284653 -0.545948 -0.000009  
C -0.819605 2.278949 -0.000022  
H -2.460498 -2.528368 0.000401  
H -0.955196 -2.849728 0.880353  
H -0.955872 -2.849562 -0.880802  
H -3.003735 1.951849 0.000038  
H -3.113453 -0.366707 0.000050  
H 5.039907 0.411083 0.000022  
H -0.194479 2.078177 0.875788  
H -1.077916 3.338681 -0.000024  
H -0.194525 2.078167 -0.875865

**Vibrational frequencies**

14.6318 67.3636 70.1692  
111.1756 208.8485 209.6151  
252.8409 259.552 311.9648  
388.8669 489.535 503.2205  
568.328 588.8666 612.426  
639.2729 686.6071 695.4621  
701.7929 930.5481 957.6162  
984.706 1028.03 1041.487  
1060.96 1115.765 1233.033  
1273.716 1340.273 1402.035  
1421.166 1470.055 1476.232  
1492.578 1497.028 1500.229  
1560.386 2140.536 2232.455  
3042.445 3045.753 3100.042  
3107.966 3134.913 3143.376  
3167.868 3191.714 3482.493

**i120**

**Cartesian coordinates**

C 0.730342 2.066401 -0.000018  
C 2.721552 -0.176557 -0.000151  
C 1.386027 -0.406541 0.000112  
C 0.379951 0.603050 0.000019  
C -2.135218 -0.079742 0.000159  
C -3.449934 -0.431656 0.000082  
C -4.615769 -0.743924 -0.000194  
C -0.953962 0.232144 0.000107  
C 3.757192 -1.252149 -0.000030  
H 1.325700 2.322619 -0.882788  
H -0.167480 2.683376 -0.000557  
H 1.324780 2.322791 0.883332  
H 3.085648 0.848007 -0.000528  
H 1.036124 -1.436156 0.000421  
H -5.643079 -1.017549 -0.000427  
H 4.406900 -1.171387 0.878263  
H 4.406380 -1.172123 -0.878788  
H 3.303944 -2.245731 0.000558

**Vibrational frequencies**

31.5198 63.3326 105.2682  
140.2333 165.2096 186.3811  
197.3163 252.357 333.9528  
364.6791 410.3601 476.2098  
508.4017 513.7774 609.6851  
636.1499 684.9521 722.2802  
793.1981 911.1053 972.1892  
980.7328 1026.054 1041.331  
1046.866 1137.98 1269.764  
1309.238 1336.173 1399.553  
1407.145 1416.608 1476.411  
1486.633 1490.729 1498.171  
1593.775 2122.054 2209.115  
3032.637 3034.309 3089.334  
3091.397 3132.369 3150.414  
3168.175 3177.077 3485.378

**i121**

**Cartesian coordinates**

C 2.014180 1.942994 -0.462984  
C 1.582841 -0.442920 0.126981  
C 0.509859 -1.190915 -0.173035  
C 1.476019 0.998404 0.559548  
C -1.985719 -0.374831 -0.059993  
C -3.289638 0.040956 -0.001763  
C -4.434546 0.407930 0.051272  
C -0.833188 -0.735493 -0.107179  
C 2.970911 -1.001372 0.028376  
H 2.469527 2.880283 -0.169325  
H 1.810296 1.773602 -1.513971  
H 0.647784 -2.220953 -0.490289  
H 2.016981 1.127633 1.504783  
H 0.423097 1.234103 0.772648  
H -5.446342 0.730942 0.098790  
H 3.460770 -0.972671 1.007771  
H 3.579155 -0.390217 -0.646137  
H 2.974423 -2.031245 -0.331610

**Vibrational frequencies**

55.1296 83.1069 89.2799  
163.3572 196.0566 211.5636  
224.1513 250.8683 361.8189  
367.8325 440.2671 488.688  
511.322 548.8459 562.8335  
609.7729 674.318 681.8615  
787.8862 806.8993 846.3662  
851.4145 1021.886 1040.168  
1066.794 1109.994 1171.808  
1217.578 1274.693 1333.14

1390.676 1424.605 1461.357  
1468.113 1480.244 1494.355  
1719.681 2197.757 2378.113  
3001.36 3040.224 3062.935  
3099.727 3143.007 3158.263  
3176.382 3270.976 3486.211

**i122**

**Cartesian coordinates**

C -1.802216 -1.266240 -0.544790  
C -1.845034 0.219226 -0.300422  
C -0.791676 1.011572 -0.056680  
C -2.422558 -2.003420 0.596631  
C 1.679392 0.095137 -0.012972  
C 2.969151 -0.366371 0.013755  
C 4.101492 -0.772723 0.036521  
C 0.538130 0.490937 -0.040150  
C -0.924133 2.489697 0.216235  
H -2.333986 -1.490904 -1.474554  
H -0.760140 -1.578211 -0.681088  
H -2.833098 0.673107 -0.286426  
H -3.381505 -2.496976 0.501920  
H -1.953706 -1.964054 1.572653  
H 5.101696 -1.132798 0.057319  
H -0.522073 2.735748 1.202809  
H -1.970636 2.796874 0.178529  
H -0.361836 3.070327 -0.519942

**Vibrational frequencies**

45.6591 79.4144 102.9498  
134.0351 135.7388 165.3226  
209.7584 268.0804 291.5029  
384.2282 432.1992 510.4209  
522.925 526.684 605.0091  
623.6939 639.2421 674.1008  
683.5423 790.0842 877.3618  
971.5479 1031.47 1067.229  
1071.876 1085.579 1122.94  
1229.949 1285.036 1311.8  
1395.908 1416.359 1465.24  
1478.928 1485.251 1496.187  
1717.082 2196.32 2377.712  
3043.22 3052.36 3094.29  
3121.719 3143.131 3159.883  
3176.167 3272.366 3483.665

**Transition states**  
**PART1. 1,3-butadiene+ butadiynyl**

**i4 - i2**

**Cartesian coordinates**

C 2.465862 -1.707136 -0.081801  
C 1.947974 -0.559994 0.380058  
C 1.356363 0.457189 -0.448779  
C 0.919014 1.787038 0.088662  
C -1.402615 0.454891 0.053757  
C -2.531808 -0.282878 0.016294  
C -3.561915 -0.922468 -0.007441  
C -0.274151 0.976176 0.027319  
H 2.897300 -2.439416 0.589209  
H 2.473338 -1.936800 -1.142508  
H 1.951952 -0.369623 1.451861  
H 1.397797 0.345316 -1.525949  
H 1.269562 2.040975 1.088083  
H 0.960962 2.628179 -0.599939  
H -4.463251 -1.485542 -0.029179

**Vibrational frequencies**

-694.489 54.4131 108.9161  
130.4989 195.2341 286.4971

314.4529	372.9219	429.9644	438.1309	494.7488	546.8008	685.1218	697.7778	703.2229
485.4564	536.9983	543.3129	554.3655	580.7022	625.7011	757.8026	870.1997	915.4615
638.503	665.4092	695.5532	678.495	715.2537	764.1428	948.4195	966.2426	1024.916
817.0557	872.5846	902.5874	858.8336	917.8049	923.5685	1103.322	1153.815	1210.781
977.4586	1011.552	1055.643	952.6915	1018.105	1130.171	1240.705	1319.652	1398.567
1104.672	1174.746	1230.35	1188.296	1238.929	1330.333	1465.547	1492.694	1636.809
1244.467	1320.296	1355.868	1382.415	1462.97	1479.912	2023.86	2256.804	3027.947
1462.624	1470.758	1643.411	2017.489	2207.181	2413.388	3095.846	3148.275	3157.738
2041.421	2132.169	3101.708	3035.941	3074.916	3154.159	3203.393	3239.815	3485.386
3152.553	3161.971	3177.441	3167.645	3249.474	3486.633			
3205.664	3251.737	3479.349						
<b><i>i4 - p5</i></b>			<b><i>i4 - i5</i></b>			<b><i>i7 - i12</i></b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C	-3.175645	-1.356904	C	1.887694	1.791944	C	-0.098753	1.227170
C	-2.003059	-0.714428	C	2.489748	0.607058	C	-1.429315	1.177701
C	-1.888601	0.715769	C	1.951353	-0.615916	C	-2.087959	0.032596
C	-0.719721	1.412701	C	0.975514	-1.484310	C	-1.497104	-1.218034
C	1.652153	0.280007	C	-1.466612	-0.415349	C	0.626554	-0.095044
C	2.888233	-0.308950	C	-2.710686	0.156644	C	1.994615	-0.099879
C	3.973045	-0.828860	C	-3.800286	0.659381	C	3.158686	-0.062154
C	0.560375	0.795777	C	-0.374966	-0.919663	C	-0.124461	-1.235140
H	-3.232485	-2.431933	H	2.328966	2.656790	H	0.515911	2.046243
H	-4.113138	-0.823722	H	0.934860	1.930994	H	-0.265408	1.445706
H	-1.079339	-1.272162	H	3.443870	0.515593	H	-1.854985	2.117331
H	-2.810405	1.278374	H	2.120701	-0.816989	H	-3.045120	0.010201
H	-0.732328	2.476515	H	1.269126	-1.575773	H	-0.645448	-1.912722
H	-0.684878	2.090274	H	0.954753	-2.494043	H	-2.145326	-2.024821
H	4.931892	-1.288023	H	-4.762829	1.104689	H	4.186795	-0.045230
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
						-1696.42	101.372	152.1085
			-226.451	44.1289	87.8195	232.9121	368.4351	414.4786
-778.903	64.6281	117.5079	143.7563	180.542	271.2298	497.1429	508.5308	563.6254
144.5684	187.8518	247.9366	333.0703	340.794	438.4823	592.9546	622.7046	694.9005
287.7919	311.5906	360.2963	522.9344	550.2393	568.0991	696.3858	743.9868	827.7442
414.4937	487.2492	546.7676	681.3405	694.2648	713.1001	886.3252	922.8882	955.2157
560.7637	633.7375	678.0288	714.0037	853.9149	988.3204	986.7803	1013.238	1157.779
687.4904	717.2742	774.8083	1000.646	1027.112	1056.534	1174.45	1189.771	1213.392
844.1464	947.1728	966.6398	1138.445	1167.336	1221.06	1261.993	1326.034	1390.831
993.5923	1049.281	1129.591	1302.864	1324.146	1365.411	1400.838	1470.396	1492.144
1197.758	1260.966	1325.532	1460.622	1463.005	1710.436	1685.417	2125.378	2188.08
1396.729	1471.804	1581.556	2201.499	2399.648	3043.023	3010.422	3100.979	3167.533
1680.233	2199.65	2375.688	3094.116	3100.414	3154.124	3181.313	3214.166	3485.81
3157.722	3181.924	3189.019	3192.078	3245.22	3487.104			
3200.251	3252.787	3485.656						
<b><i>i4 - p22</i></b>			<b><i>i7 - i5</i></b>			<b><i>i1 - p6</i></b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C	-1.912617	-1.977802	C	-0.201206	1.388342	C	-1.696011	1.909747
C	-2.030571	-0.686946	C	-1.465658	1.250619	C	-2.142081	0.664267
C	-2.135507	0.615873	C	-2.171524	0.108881	C	-1.284443	-0.545191
C	-0.992686	1.594254	C	-1.632247	-1.229187	C	-1.801603	-1.777643
C	1.412969	0.461040	C	0.824806	-0.502468	C	1.332329	-0.183052
C	2.650633	-0.132044	C	2.175732	-0.222301	C	2.688265	0.014056
C	3.734854	-0.652135	C	3.342108	0.063009	C	3.877671	0.189586
C	0.327003	0.979876	C	-0.168346	-1.248394	C	0.140383	-0.360979
H	-1.946453	-2.658702	H	-0.123260	1.093496	H	-2.386926	2.741681
H	-1.763809	-2.393963	H	0.457579	2.200296	H	-0.634956	2.133819
H	-2.012996	-0.584101	H	-1.834524	2.118065	H	-3.209205	0.463646
H	-3.121430	1.049274	H	-3.120623	0.095026	H	-1.165256	-2.649719
H	-1.048811	2.329370	H	-1.881455	-1.417693	H	-2.872327	-1.912263
H	-1.123704	2.158977	H	-2.096771	-2.035656	H	4.929271	0.344823
H	4.692735	-1.113551	H	4.377070	0.295453	H	-1.347652	-0.586736
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
						-1074.4	75.0728	100.9645
			-688.208	97.9297	131.7384	128.3617	213.2248	279.4166
-809.2	57.6482	75.1835	161.8395	323.1866	361.583	309.4831	396.299	445.1243
107.7501	150.415	170.0373	391.9642	463.0977	486.5193	473.074	492.4858	533.7277
264.3421	331.9835	406.715	517.5162	629.0141	672.0191	556.8131	603.8038	651.2936

675.0825	681.5065	717.8798	974.3236	1038.213	1041.212	1015.109	1044.874	1084.71
749.7493	892.8405	899.9483	1070.668	1113.59	1242.362	1108.784	1137.679	1214.278
964.7696	1019.048	1052.909	1350.088	1425.406	1458.974	1359.207	1442.024	1476.411
1102.117	1329.646	1339.223	1483.646	1497.12	1645.607	1784.382	2202.592	2397.803
1414.373	1455.824	1567.297	1947.124	2238.081	3054.1	3144.806	3151.339	3169.885
1724.235	2201.431	2389.518	3119.499	3122.021	3145.611	3238.904	3247.604	3484.378
3162.958	3171.261	3186.108	3172.973	3214.727	3482.697			
3258.438	3276.789	3482.81						
<b><i>i1 - p17</i></b>			<b><i>i52 - i53</i></b>			<b><i>i5 - i8</i></b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C -2.871610	-1.360005	0.386874	C -0.226351	1.429520	0.000011	C 2.623396	1.203573	-0.095301
C -1.817358	-1.189369	-0.365200	C 1.281217	1.309142	-0.000032	C 2.712843	-0.069681	0.668643
C -0.976201	0.947423	-0.505874	C 1.559896	-0.002019	0.000047	C 1.775242	-0.958701	0.353301
C -1.663628	1.686055	0.406144	C 2.536996	-1.131017	-0.000057	C 0.867785	-0.478395	-0.747727
C 1.520448	0.197089	-0.118333	C -0.746067	-0.008384	0.000047	C -1.675789	-0.096393	-0.187182
C 2.821142	-0.187022	0.078423	C -2.119363	-0.344432	-0.000005	C -2.994059	0.121911	0.106398
C 3.963160	-0.523792	0.251503	C -3.295995	-0.591525	-0.000051	C -4.154548	0.313963	0.364137
C 0.375712	0.541138	-0.285105	C 0.361279	-0.779599	0.000109	C -0.510184	-0.295068	-0.448798
H -3.332870	-2.338920	0.515206	H -0.593770	1.969300	-0.881080	H 3.440843	1.455803	-0.769809
H -3.326511	-0.526528	0.918410	H -0.593733	1.969327	0.881103	H 2.205422	2.067298	0.421284
H -1.192297	-1.840561	-0.961869	H 1.950586	2.158447	-0.000129	H 3.482740	-0.246123	1.413816
H -1.316668	0.920907	-1.536456	H 1.306608	-1.862518	0.000006	H 1.652524	-1.931559	0.815073
H -1.278581	1.839606	1.406580	H 3.077264	-1.351128	0.918639	H 1.495786	0.670869	-0.829584
H -2.635974	2.095372	0.162009	H 3.077093	-1.351054	-0.918869	H 1.034118	-0.947588	-1.720817
H 4.972914	-0.818974	0.405532	H -4.333717	-0.822485	-0.000084	H -5.179543	0.484037	0.589203
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
-425.99	47.3884	79.5374	-2381.01	124.8948	145.7592	-1885.84	63.5739	90.2293
108.0215	159.1801	188.3532	220.7187	334.1382	338.2642	168.4881	216.5702	312.5023
250.1638	284.689	346.9945	412.6682	514.266	520.7293	360.0181	443.3232	473.0213
417.8572	490.2924	529.575	570.4952	589.4511	649.3824	532.6194	573.1587	597.4483
568.4131	609.9455	671.8006	695.208	716.6711	760.3013	677.5018	694.4261	702.9656
689.648	710.0098	802.7417	874.9731	904.0391	963.1966	765.6762	819.3409	912.7965
873.3571	902.3721	937.2893	988.9944	1017.146	1039.403	941.8645	996.3122	1025.188
953.3946	1034.005	1092.477	1123.547	1157.764	1166.563	1061.974	1084.02	1158.803
1192.506	1277.259	1392.66	1196.027	1259.868	1361.627	1211.201	1309.359	1357.076
1427.083	1561.805	1676.226	1417.861	1424.843	1595.694	1391.839	1454.195	1632.582
2200.275	2384.143	3098.663	1668.979	1821.304	2236.141	1710.472	2183.608	2328.587
3170.016	3178.252	3179.969	3052.638	3094.204	3111.384	3092.678	3104.586	3176.268
3235.876	3273.796	3486.226	3209.947	3237.996	3485.565	3187.037	3210.6	3484.81
<b><i>i2 - i50</i></b>			<b><i>i3 - p24</i></b>			<b><i>i5 - i9</i></b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C 0.044687	1.652379	-0.047531	C 2.325500	1.551363	0.089860	C -1.562087	1.733914	0.004252
C -1.321239	1.143122	0.043044	C 2.042356	0.256482	-0.009082	C -2.475745	0.739478	-0.000194
C -1.496657	-0.194761	-0.008834	C 1.027890	-0.698083	-0.523712	C -2.253874	-0.671659	-0.039521
C -2.799751	-0.927264	0.010745	C 1.932389	-1.023522	0.690942	C -1.042832	-1.365103	-0.039523
C 0.947643	-0.395443	0.025396	C -1.534232	-0.174965	-0.161884	C 1.440097	-0.402380	-0.123723
C 2.324032	-0.407515	0.020992	C -2.864495	0.097399	0.030023	C 2.703098	0.072652	-0.028744
C 3.527995	-0.377325	0.025682	C -4.031374	0.335696	0.198926	C 3.832124	0.506068	0.028854
C -0.215805	-0.856985	-0.052676	C -0.364703	-0.416603	-0.327095	C 0.283805	-0.830542	0.011501
H 0.405846	2.368150	0.685985	H 1.905865	2.266120	-0.608785	H -1.886599	2.766828	0.048339
H 0.501329	1.724952	-1.031943	H 3.031027	1.910933	0.830400	H -0.496748	1.554314	-0.047626
H -2.160655	1.821243	0.178595	H 3.512463	-0.237509	-1.263652	H -3.523749	1.026657	0.041283
H -2.827981	-1.647863	0.832402	H 1.269017	-1.238524	-1.433393	H -3.135030	-1.302954	-0.022602
H -2.940741	-1.487020	-0.918353	H 1.465789	-1.020074	1.669899	H -0.254035	-1.179787	1.137930
H -3.634418	-0.233131	0.123441	H 2.678934	-1.791706	0.528917	H -1.073866	-2.448047	-0.119472
H 4.591187	-0.363587	0.028970	H -5.063082	0.544154	0.348745	H 4.822503	0.888423	0.084979
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
-662.807	106.1677	120.6361	-763.774	75.3987	97.2562	-1841.3	63.9083	67.8916
161.2071	223.0696	256.7589	358.8595	374.0541	444.9476	119.0596	195.7591	249.6762
319.8789	411.7363	443.2194	471.5181	516.4252	542.5116	297.203	409.7923	417.3179
488.2307	532.8797	581.6045	577.4235	600.1955	698.7765	449.6348	533.4532	552.3695
608.1967	635.734	698.9032	714.3108	715.8109	774.1767	633.2838	652.736	692.7121
753.4263	772.8349	812.1824	910.4844	927.0614	936.0479	707.9732	784.4792	796.5941
						900.97	953.8301	992.0848
						1018.841	1087.214	1165.926

1270.813	1323.324	1411.63	1448.655	1666.662	1710.263	1682.894	2199.612	2374.54			
1457.518	1494.194	1619.564	2074.75	2253.561	3071.348	3154.919	3164.396	3174.148			
1873.824	2091.651	2199.895	3156.84	3171.37	3253.126	3182.613	3255.268	3486.356			
3157.593	3173.765	3178.144	3255.347	3420.773	3483.824						
3198.88	3274.676	3480.195									
<b><i>i8 - i9</i></b>			<b><i>i12 - i9</i></b>			<b><i>i5 - p4</i></b>					
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>					
C	1.533216	-1.522887	0.085259	C	-0.470490	1.566404	-0.352668	C	-3.708009	-0.508155	-0.010505
C	2.541087	-0.556462	-0.052484	C	-1.610225	1.193484	0.280600	C	-2.981897	0.612689	0.012000
C	2.250023	0.803456	0.112042	C	-2.219016	-0.087917	0.062822	C	-1.533160	0.678149	-0.097014
C	0.946050	1.256911	0.053359	C	-1.501474	-1.225093	-0.132727	C	-0.687424	-0.341816	0.198992
C	-1.425355	0.352731	-0.020659	C	0.836686	-0.375794	-0.015204	C	1.926646	-0.114305	0.063010
C	-2.710674	-0.017903	-0.012689	C	2.169835	-0.126779	0.063099	C	3.289533	0.003724	-0.001691
C	-3.893454	-0.311094	0.028157	C	3.337730	0.210290	0.097718	C	4.486727	0.108918	-0.059170
C	-0.151447	0.386263	-0.154951	C	-0.064905	-1.356287	0.000249	C	0.724449	-0.215026	0.114786
H	0.958217	-1.550761	1.007842	H	0.055382	2.474158	-0.078532	H	-4.786818	-0.476655	0.083815
H	1.690887	-2.503487	-0.357590	H	-0.202764	1.127999	-1.305669	H	-3.252913	-1.483870	-0.147063
H	3.493668	-0.824603	-0.500550	H	-2.040357	1.837070	1.044104	H	-3.493425	1.568496	0.086299
H	3.052242	1.532024	0.079258	H	-3.294649	-0.179934	0.185457	H	-1.104395	1.609283	-0.454811
H	0.760112	2.322029	-0.034280	H	-2.047024	-2.158548	-0.226570	H	-1.063852	-1.233810	0.691217
H	-4.924169	-0.569659	0.058063	H	4.367142	0.472826	0.139006	H	-0.944323	-1.531361	-1.469677
H	0.432366	-0.751643	-0.480951	H	0.293427	-2.363419	0.218866	H	5.544532	0.202843	-0.112232
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>					
			-410.384	108.4436	111.6422	-709.006	67.0597	72.8405			
-1748.03	70.6191	93.3693	237.0236	284.0154	307.2221	163.0908	195.5843	219.2188			
225.4608	290.2675	384.9401	450.542	462.461	491.6534	260.0192	302.5417	361.9876			
441.1897	445.2635	466.5393	535.7677	561.3247	647.5265	438.5341	461.4227	542.992			
511.3458	518.6307	549.051	649.7988	751.3061	785.6549	559.1545	567.4677	647.4489			
641.1993	694.0594	746.3666	849.1013	885.2243	951.3614	683.7466	705.9617	805.179			
782.2113	899.0019	925.8268	976.1087	991.6342	1000.441	894.0306	969.6169	987.896			
981.1696	1023.583	1040.633	1076.264	1104.045	1240.894	1002.059	1035.224	1079.134			
1103.537	1165.526	1225.433	1288.783	1315.391	1422.142	1219.511	1302.312	1330.276			
1261.088	1274.037	1417.44	1481.56	1545.703	1634.856	1352.256	1455.909	1613.569			
1476.221	1496.569	1511.706	1712.83	2069.792	3119.059	1694.073	2199.568	2375.671			
1588.999	1878.309	2053.886	3160.639	3167.553	3176.596	3155.394	3173.186	3183.836			
3118.304	3177.404	3193.935	3198.691	3257.356	3478.307	3191.964	3250.64	3486.384			
3200.172	3214.806	3477.765									
<b><i>i9 - p33</i></b>			<b><i>i4 - p4</i></b>			<b><i>i43 - i3</i></b>					
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>					
C	-2.491575	1.279250	-0.497054	C	-3.944524	-0.732424	0.032828	C	1.858585	1.469865	-0.342607
C	-2.867721	0.119054	0.038354	C	-2.965022	0.165788	-0.109752	C	2.112714	0.011947	-0.331326
C	-2.103246	-1.136772	-0.040393	C	-1.564612	-0.154191	0.035633	C	0.985110	-0.946882	-0.536569
C	-0.791745	-1.252649	-0.071219	C	-0.571668	0.765155	-0.096351	C	2.340679	-0.296672	1.101867
C	1.715178	0.400443	0.403958	C	1.978202	0.132321	-0.039348	C	-1.497547	-0.297919	-0.137391
C	2.981678	0.134193	-0.034038	C	3.307631	-0.195546	-0.014726	C	-2.796397	0.048879	0.064980
C	4.100156	-0.094998	-0.418418	C	4.475395	-0.484429	0.007916	C	-3.949461	0.358129	0.246340
C	0.554191	0.540868	0.734725	C	0.805484	0.419519	-0.056558	C	-0.330224	-0.616998	-0.321763
H	-1.571924	1.364871	-1.066881	H	-4.986024	-0.459257	-0.085887	H	2.701626	2.147803	-0.379065
H	-3.102617	2.168627	-0.394161	H	-3.728552	-1.769730	0.269007	H	0.888544	1.854964	-0.050227
H	-3.821460	0.058983	0.557268	H	-3.211182	1.198767	-0.344920	H	2.973953	-0.263065	-0.942572
H	-2.698253	-2.055172	-0.058328	H	-1.303253	-1.177961	0.288417	H	1.240068	-1.973486	-0.773582
H	-0.126680	-2.102098	-0.132312	H	-0.811003	1.769807	-0.434718	H	1.566582	-0.024047	1.806915
H	5.087881	-0.294337	-0.758267	H	-0.593316	1.678363	1.721163	H	3.254154	-0.750961	1.471540
H	-0.348437	0.922796	1.157190	H	5.508013	-0.737148	0.029089	H	-4.965686	0.626699	0.405798
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>					
			-801.914	68.2813	93.2539	-512.472	74.7583	80.2311			
-355.62	17.926	63.4848	147.2097	194.4261	219.0466	172.2708	198.9363	264.6899			
107.08	138.3441	206.3301	292.855	312.0766	370.63	320.3395	378.9041	409.2206			
251.5735	272.6217	295.4879	414.0688	456.1291	513.0173	510.5847	521.0353	542.0536			
505.9626	519.8051	535.4572	563.0846	576.9892	667.4608	557.3063	581.2985	637.0491			
634.4567	665.6655	692.3913	680.3216	700.9729	788.3877	649.3955	688.5991	693.6958			
703.8655	748.1894	756.3324	893.2762	959.294	970.8755	753.269	881.8284	923.3501			
849.7199	899.9844	917.6928	978.0813	1047.224	1198.65	1065.289	1122.494	1167.647			
970.0618	997.585	1045.789	1213.447	1287.889	1302.532	1245.899	1272.367	1365.776			
1090.273	1266.869	1337.394	1336.914	1456.681	1606.646	1415.361	1456.715	1468.956			
						2111.981	2199.437	3097.881			

3155.166	3165.732	3199.021	3215.977	3271.737	3485.16		
3280.797	3283.342	3483.404					
<b><i>i1 - i3</i></b>			<b><i>i6 - p25</i></b>				
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>				
C	1.813854	1.663886	0.190455	C	-4.023897	0.200520	0.333738
C	2.124747	0.451672	-0.361984	C	-3.103032	-0.501762	-0.400588
C	1.186937	-0.718967	-0.478075	C	-0.241904	1.141273	-0.127571
C	1.942255	-1.151509	0.728709	C	-1.916891	-1.021841	0.112317
C	-1.400539	-0.227968	-0.158901	C	2.162088	0.324038	-0.024702
C	-2.738434	0.024319	0.011779	C	3.397260	-0.125781	0.031205
C	-3.911030	0.244938	0.161723	C	4.550527	-0.548972	0.083422
C	-0.2226973	-0.454251	-0.308726	C	0.949917	0.776918	-0.079903
H	2.566404	2.437066	0.273201	H	-4.928736	0.590439	-0.115543
H	0.825084	1.865912	0.586049	H	-3.875487	0.373734	1.394968
H	3.086780	0.306878	-0.839351	H	-3.298488	-0.648820	-1.460410
H	1.371796	-1.326394	-1.363807	H	-1.160674	1.677157	-0.182442
H	1.559600	-0.904203	1.707771	H	-1.238740	-1.595848	-0.504847
H	2.793373	-1.810291	0.630925	H	-1.689502	-0.946131	1.169746
H	-4.947940	0.438314	0.295332	H	5.547221	-0.916885	0.131020
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>				
			-185.969	36.3345	41.9414		
-615.992	77.588	100.001	72.8221	122.0264	135.1347		
196.645	232.6576	279.537	172.0036	381.3132	398.5046		
366.5144	465.4314	498.5238	427.7959	443.9815	446.8818		
514.135	531.7582	559.4184	471.3136	497.3163	511.1253		
602.2	669.1836	707.9992	517.7255	579.156	606.5613		
710.6555	731.6313	787.8659	765.1494	804.9118	850.0793		
904.4806	944.4515	983.1054	951.7926	1031.838	1043.995		
1075.131	1113.751	1194.787	1204.656	1286.839	1430.429		
1209.303	1294.598	1389.169	1512.13	1541.802	1567.052		
1414.402	1448.615	1536.102	1645.293	1972.217	3154.042		
2203.854	2405.077	3119.187	3163.79	3169.356	3256.83		
3164.554	3184.882	3200.66	3273.091	3437.443	3465.681		
3265.883	3312.65	3484.355					
<b><i>i6 - i3</i></b>			<b><i>i42 - p22</i></b>				
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>				
C	1.831885	1.668295	0.017496	C	-3.163636	-1.096298	0.000289
C	2.284384	0.369650	-0.205733	C	-1.816859	-1.262459	-0.000294
C	1.069664	-0.965201	-0.397606	C	-0.888009	0.752264	-0.000142
C	2.045567	-0.778934	0.712781	C	-1.749856	1.747918	0.000128
C	-1.447277	-0.307420	-0.135302	C	1.628040	0.188568	-0.000136
C	-2.761243	0.041460	0.013632	C	2.943093	-0.163100	0.000009
C	-3.917714	0.350355	0.147642	C	4.107347	-0.477940	0.000194
C	-0.287603	-0.634891	-0.261246	C	0.460599	0.545251	-0.000196
H	2.055999	2.456412	-0.689172	H	-3.718278	-0.994809	0.926564
H	1.164043	1.895710	0.839991	H	-3.719101	-0.994305	-0.925434
H	3.010130	0.208407	-0.994973	H	-1.294868	-1.502868	0.919199
H	1.354217	-1.595012	-1.231465	H	-1.295554	-1.502479	-0.920288
H	1.611682	-0.525905	1.675815	H	-1.412177	2.781405	0.000226
H	2.837219	-1.518783	0.782881	H	-2.818900	1.560583	0.000214
H	-4.939271	0.619294	0.266946	H	5.134571	-0.752757	0.000413
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>				
			-534.993	18.2197	64.0138		
-630.248	68.2596	100.949	107.336	176.3641	214.0345		
177.894	229.5343	304.0104	249.4278	292.0064	346.5205		
394.0206	437.8537	469.5058	440.0837	462.6805	528.1072		
488.2001	533.9951	558.2462	529.9771	636.7908	654.9535		
654.6245	690.4508	701.9523	663.0965	681.3486	831.7681		
711.4955	750.2096	894.9454	879.3117	923.2669	933.4741		
925.9978	994.0364	1029.667	1029.038	1039.911	1164.173		
1131.071	1180.501	1193.62	1245.391	1306.625	1435.601		
1239.205	1258.437	1404.969	1465.996	1586.441	1759.283		
1412.001	1490.91	1509.96	2140.87	2231.439	3130.843		
2185.81	2329.345	3128.9	3150.46	3160.738	3222.012		
3167.397	3189.494	3198.209	3235.942	3260.724	3484.699		

***i7 - i55***

**Cartesian coordinates**

C	0.082946	1.140615	0.597180
C	1.274835	1.189821	-0.330232
C	2.078371	0.062632	-0.453679
C	1.526761	-1.241948	0.058916
C	-0.651588	-0.154616	0.266202
C	-2.028334	-0.149349	-0.080135
C	-3.199625	-0.097667	-0.349794
C	0.155161	-1.225348	0.211165
H	-0.566957	2.005245	0.458947
H	0.417590	1.147010	1.648110
H	1.519784	2.099805	-0.861863
H	2.961959	0.057136	-1.082492
H	2.299827	-0.284082	0.738437
H	2.170518	-2.102548	0.174334
H	-4.233885	-0.067410	-0.593217

**Vibrational frequencies**

	-1785.61	110.2575	153.0717
	255.948	367.8533	436.0118
	493.3225	528.4602	549.7754
	575.4717	639.7757	659.4428
	704.1957	713.0454	746.3626
	842.5869	921.9135	927.5375
	956.0848	993.8434	1133.015
	1144.438	1163.75	1224.557
	1247.438	1293.131	1333.53
	1362.918	1460.938	1496.494
	1674.541	2034.654	2224.409
	2960.458	3131.753	3189.189
	3230.329	3242.098	3486.794

***i48 - i6***

**Cartesian coordinates**

C	-3.154248	1.376175	-0.124076
C	-1.983458	0.662003	0.086915
C	-1.849253	-0.801837	0.011497
C	-0.649785	-1.505769	-0.047334
C	1.676312	-0.322830	-0.023648
C	2.887903	0.305648	-0.010638
C	3.956040	0.864558	0.001615
C	0.598648	-0.887087	-0.040310
H	-3.155613	2.453331	-0.034736
H	-4.096880	0.876234	-0.313841
H	-1.044831	1.200402	0.191307
H	-2.778657	-1.356088	-0.082499
H	-2.029656	-0.085626	1.165981
H	-0.686439	-2.588509	-0.061995
H	4.899113	1.355077	0.011645

**Vibrational frequencies**

	-1842.83	60.9762	115.044
	169.4153	190.6636	284.8088
	307.9824	415.3198	445.3723
	519.6539	541.6109	559.2536
	637.5157	638.7119	679.1585
	710.7255	715.5235	768.0499
	877.1552	911.5085	1003.694
	1104.765	1194.454	1209.458
	1258.632	1276.413	1369.568
	1446.265	1507.846	1591.852
	1879.753	2168.359	2281.933
	3169.282	3178.418	3188.59
	3208.566	3275.76	3484.315

***i4 - i6***

**Cartesian coordinates**

C	-3.176178	1.385655	-0.038883
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C -2.020712 0.698864 0.036540  
 C -1.929414 -0.729969 -0.003846  
 C -0.645977 -1.486168 -0.033315  
 C 1.685558 -0.310518 -0.022844  
 C 2.900187 0.311031 -0.007101  
 C 3.971975 0.863143 0.007781  
 C 0.605957 -0.869496 -0.043131  
 H -3.185486 2.467949 -0.013694  
 H -4.132420 0.881786 -0.138207  
 H -1.083115 1.242401 0.126923  
 H -2.821154 -1.321562 -0.176919  
 H -1.329591 -1.246978 1.047100  
 H -0.714054 -2.547865 -0.236944  
 H 4.917446 1.349018 0.020535

**Vibrational frequencies**

-1869.71 59.4892 111.1739  
 146.1118 181.199 265.5157  
 295.2397 388.2175 415.5625  
 500.1042 543.4474 598.3504  
 627.2411 636.9143 685.6002  
 719.6005 748.9955 872.8258  
 891.4413 920.2818 1014.663  
 1068.691 1186.518 1223.415  
 1262.72 1312.016 1351.357  
 1413.072 1478.042 1633.584  
 2152.736 2172.469 2285.173  
 3156.954 3173.793 3202.477  
 3214.606 3256.202 3484.223

***i1 - i50***

**Cartesian coordinates**

C -1.733934 -1.949712 0.071350  
 C -2.137797 -0.684731 -0.035378  
 C -1.255252 0.489920 -0.102245  
 C -1.820437 1.849252 0.150062  
 C 1.350747 0.157112 -0.024285  
 C 2.707527 -0.018167 0.004398  
 C 3.901270 -0.173451 0.029924  
 C 0.151100 0.313272 -0.047241  
 H -2.453771 -2.757836 0.108378  
 H -0.681824 -2.207082 0.130740  
 H -3.201328 -0.462282 -0.082983  
 H -1.566389 1.198987 -1.065793  
 H -1.149061 2.687879 0.254148  
 H -2.882153 1.950808 0.322290  
 H 4.955183 -0.311439 0.053717

**Vibrational frequencies**

-1854.81 71.3257 104.5905  
 122.272 208.3164 267.5734  
 290.7605 399.8251 432.3426  
 483.339 528.7217 549.5928  
 583.0894 603.7944 634.205  
 647.7481 718.2587 745.9718  
 877.8437 937.0119 1012.367  
 1019.139 1095.284 1172.474  
 1241.475 1337.425 1376.194  
 1424.834 1451.209 1697.408  
 2188.304 2235.941 2342.72  
 3160.93 3172.605 3188.3  
 3260.863 3321.112 3483.208

***i1 - i42***

**Cartesian coordinates**

C 3.207323 -0.935694 -0.132892  
 C 1.847288 -0.865906 0.035540  
 C 1.027626 0.389234 0.076222  
 C 1.552114 1.672259 -0.055717

C -1.587720 0.033088 0.018804  
 C -2.944603 -0.155354 -0.024869  
 C -4.135254 -0.322313 -0.063322  
 C -0.393540 0.199340 0.049850  
 H 3.696501 -1.899795 -0.145738  
 H 3.827868 -0.053316 -0.221582  
 H 1.256883 -1.775916 0.044855  
 H 1.457280 -0.255118 1.177449  
 H 0.892804 2.527604 -0.030888  
 H 2.616884 1.838509 -0.145320  
 H -5.187623 -0.469889 -0.100473

**Vibrational frequencies**

-1860.52 75.7889 90.9737  
 174.4105 223.5435 289.6148  
 299.0473 413.076 473.9925  
 498.7763 514.574 553.5803  
 595.3482 642.3002 672.0888  
 680.5517 713.7421 721.1512  
 736.8663 874.1409 903.5234  
 1047.812 1076.08 1141.693  
 1266.111 1290.983 1393.39  
 1429.178 1518.374 1566.701  
 1781.061 2201.313 2387.511  
 3181.703 3187.673 3196.193  
 3281.427 3292.937 3483.685

***i3 - i51***

**Cartesian coordinates**

C 0.366677 1.409345 -0.187086  
 C 1.666023 0.704542 -0.277085  
 C 1.520854 -0.836997 -0.355203  
 C 2.115930 -0.159622 0.859332  
 C -0.919178 -0.442012 -0.160742  
 C -2.258034 -0.184554 0.043791  
 C -3.416564 0.092305 0.219458  
 C 0.108326 -1.138082 -0.294585  
 H -0.020166 1.880104 -1.084186  
 H 0.056998 1.848072 0.755448  
 H 2.428472 1.141434 -0.913731  
 H 2.172369 -1.415273 -0.996966  
 H 1.520607 -0.156147 1.765383  
 H 3.181383 -0.284509 1.010844  
 H -4.443858 0.316763 0.375926

**Vibrational frequencies**

-614.632 103.2509 128.5888  
 241.3916 359.9635 435.2317  
 464.278 470.4256 519.9737  
 582.2337 620.7322 668.6444  
 700.0962 716.4373 770.1269  
 822.9448 837.8663 870.5583  
 983.836 985.6283 1072.877  
 1082.987 1107.494 1155.985  
 1191.257 1204.688 1359.385  
 1385.766 1470.278 1493.834  
 1990.346 2245.256 3143.686  
 3149.178 3174.417 3206.449  
 3238.128 3251.205 3484.181

***i43 - i48***

**Cartesian coordinates**

C 2.001728 -0.812725 0.706762  
 C 2.023310 0.603546 0.241433  
 C 0.916943 1.328855 -0.132240  
 C 2.329245 -1.174347 -0.691663  
 C -1.514636 0.368228 -0.044107  
 C -2.780372 -0.144903 -0.002670  
 C -3.894413 -0.602438 0.034335

C -0.389752 0.823984 -0.076509  
 H 2.773394 -1.051901 1.436181  
 H 1.021081 -1.144381 1.044797  
 H 2.991629 1.088013 0.193349  
 H 1.047900 2.333578 -0.519377  
 H 1.534467 -1.306770 -1.412484  
 H 3.356248 -1.252921 -1.022607  
 H -4.877039 -1.006821 0.068102

**Vibrational frequencies**

-547.793 62.3495 94.1857  
 156.9868 204.2166 311.5709  
 361.2102 450.1791 485.0257  
 530.6829 538.4956 598.5583  
 647.9981 652.0039 694.529  
 725.597 767.8343 825.2514  
 915.4455 939.4674 1092.764  
 1121.152 1197.389 1229.434  
 1236.927 1259.305 1425.373  
 1457.264 1495.468 1510.776  
 2174.284 2299.34 3104.597  
 3172.649 3176.235 3188.281  
 3215.211 3294.062 3484.053

***i53 - p26***

**Cartesian coordinates**

C -0.110514 1.323560 -0.111400  
 C 1.236054 1.175678 -0.123555  
 C 1.540759 -0.252581 -0.012567  
 C 2.754609 -0.814292 0.036762  
 C -0.731821 -0.022786 -0.036327  
 C -2.133321 -0.251761 -0.027392  
 C -3.322232 -0.423860 -0.024466  
 C 0.249678 -0.948540 0.028669  
 H -0.668138 2.234538 -0.276735  
 H -0.488516 1.795489 1.887560  
 H 1.976871 1.959039 -0.192387  
 H 2.876613 -1.888836 0.115832  
 H 3.655189 -0.211168 -0.000158  
 H -4.373498 -0.583175 -0.018794  
 H 0.122206 -2.018395 0.106340

**Vibrational frequencies**

-649.564 116.6787 148.2  
 202.1778 268.9609 303.4429  
 345.5022 434.4881 527.1818  
 544.2739 620.5225 656.6413  
 662.9055 692.6178 704.616  
 726.8887 803.4826 872.3774  
 926.3533 943.8329 960.3476  
 973.7122 976.8777 1098.001  
 1182.13 1237.958 1339.204  
 1368.262 1454.786 1538.566  
 1648.966 1719.797 2243.047  
 3159.552 3241.612 3252.299  
 3256.505 3261.614 3482.198

***i1 - i2***

**Cartesian coordinates**

C 3.166432 -1.059714 -0.071834  
 C 2.087404 -0.468439 0.419333  
 C 1.192249 0.423467 -0.382255  
 C 0.766983 1.717628 0.239746  
 C -1.427817 -0.103254 -0.156188  
 C -2.756856 -0.326288 -0.012784  
 C -3.941901 -0.536142 0.110401  
 C -0.235712 0.194448 -0.250805  
 H 3.793256 -1.691649 0.546319  
 H 3.460476 -0.934123 -1.109458

H 1.803199 -0.610817 1.459200  
H 1.516207 0.515010 -1.420148  
H 0.789758 1.828700 1.314991  
H 0.515586 2.561870 -0.385334  
H -4.983167 -0.719216 0.220739

**Vibrational frequencies**

-670.331 65.6255 97.3086  
116.9411 222.5699 283.4461  
311.9104 383.3946 424.3254  
442.6638 526.8138 587.4525  
597.5407 627.7899 672.5452  
711.2757 793.7329 856.3724  
975.3342 990.1339 1041.926  
1093.906 1160.305 1215.467  
1228.053 1309.874 1342.941  
1444.117 1467.122 1741.591  
2085.415 2171.66 3109.386  
3153.236 3177.609 3178.813  
3244.309 3302.803 3481.515

***i12 - p1***

**Cartesian coordinates**

C 0.116253 1.184140 -0.036548  
C 1.517315 1.170010 -0.114801  
C 2.206130 -0.027678 -0.053401  
C 1.507753 -1.230934 0.042638  
C -0.591337 -0.038797 -0.020716  
C -2.019173 -0.037015 -0.040960  
C -3.220196 -0.028459 -0.055072  
C 0.119618 -1.237337 0.046589  
H -0.428943 2.103279 -0.213985  
H -0.071097 1.661013 1.774244  
H 2.052768 2.108643 -0.192958  
H 3.289451 -0.032369 -0.089368  
H 2.047668 -2.169153 0.094240  
H -4.283454 -0.021898 -0.068693  
H -0.424569 -2.173099 0.090146

**Vibrational frequencies**

-893.258 133.128 153.1732  
280.5001 361.4503 405.072  
452.9039 481.6861 541.1521  
564.3303 635.1414 663.8623  
704.4199 733.1079 773.652  
777.7588 882.5965 968.6528  
1007.251 1013.507 1032.456  
1057.203 1100.104 1186.138  
1204.434 1228.384 1312.14  
1349.841 1471.476 1532.517  
1623.736 1654.804 2238.62  
3198.225 3207.354 3214.596  
3222.243 3228.223 3482.643

***i6 - i55***

**Cartesian coordinates**

C 0.118319 -1.381163 0.035577  
C 1.470151 -1.143065 0.271747  
C 2.128671 -0.061304 -0.479538  
C 1.501992 1.267631 0.096487  
C -0.730144 0.350780 0.168014  
C -2.095063 0.207587 -0.014312  
C -3.278306 -0.002777 -0.139829  
C 0.173969 1.300362 0.180417  
H -0.416565 -2.050712 0.703043  
H -0.203674 -1.449116 -1.002682  
H 1.910551 -1.437270 1.219597  
H 1.906347 -0.103828 -1.550543  
H 3.208886 -0.028848 -0.337534

H 2.180265 1.999676 0.516284  
H -4.323353 -0.158209 -0.259544

**Vibrational frequencies**

-656.762 100.9286 151.3539  
218.7086 343.5866 383.2856  
420.1142 481.7136 508.865  
530.5561 599.3986 645.5884  
683.678 708.9586 742.9588  
788.3356 816.5093 912.3842  
952.0883 1003.775 1057.496  
1092.22 1170.95 1213.075  
1241.416 1270.943 1409.286  
1443.176 1500.695 1533.031  
1679.292 2145.664 3061.177  
3116.176 3144.443 3186.356  
3211.653 3215.432 3480.444

***i50 - p6***

**Cartesian coordinates**

C 1.647401 -1.974763 -0.075370  
C 2.110114 -0.732674 0.035385  
C 1.275621 0.477088 0.099594  
C 1.822404 1.704918 0.186776  
C -1.340897 0.175127 0.027578  
C -2.700532 0.008889 -0.004951  
C -3.893889 -0.139762 -0.032582  
C -0.143903 0.326607 0.058941  
H 2.325176 -2.818751 -0.117520  
H 0.583711 -2.182096 -0.128155  
H 3.180807 -0.553737 0.083538  
H 1.208482 2.593174 0.260121  
H 2.094833 2.335360 -2.062304  
H 2.897807 1.825304 0.250113  
H -4.948732 -0.271823 -0.058023

**Vibrational frequencies**

-393.684 75.8581 99.1673  
121.0272 156.6261 195.4562  
214.7375 297.9219 306.4183  
448.9868 487.7608 530.7591  
567.6302 605.8872 653.7765  
680.2064 713.6976 739.1203  
791.4062 903.4372 945.6231  
971.3387 1022.6 1057.105  
1107.412 1336.449 1358.864  
1428.521 1460.67 1637.003  
1719.077 2199.27 2381.737  
3162.96 3170.964 3183.654  
3258.361 3271.244 3483.083

***i51 - i55***

**Cartesian coordinates**

C 0.081521 1.250586 -0.294336  
C 1.540087 1.015028 -0.036047  
C 1.489546 -1.138421 -0.271602  
C 1.974233 -0.158810 0.785010  
C -0.669670 -0.095129 -0.264712  
C -2.054594 -0.134538 0.050568  
C -3.229370 -0.117034 0.305598  
C 0.156658 -1.127751 -0.418685  
H -0.069724 1.776707 -1.240775  
H -0.350040 1.882745 0.493927  
H 2.280071 1.534813 -0.633889  
H 2.188018 -1.586422 -0.969426  
H 1.439701 -0.263365 1.731074  
H 3.049795 -0.186540 0.953321  
H -4.268289 -0.121521 0.531014

**Vibrational frequencies**

-242.129 120.4011 156.5824  
257.7557 332.9553 466.8834  
518.4606 527.5265 554.7927  
584.338 594.6792 659.2963  
703.4443 776.4537 816.8841  
870.3816 894.8198 949.9906  
1051.268 1114.677 1121.113  
1144.703 1181.409 1229.741  
1244.602 1300.644 1370.392  
1397.542 1460.113 1494.989  
1764.561 2232.929 3033.796  
3085.005 3098.947 3158.476  
3197.928 3213.889 3485.16

***i42 - p6***

**Cartesian coordinates**

C 1.685510 1.876595 -0.172235  
C 2.123532 0.618859 0.033424  
C 1.256991 -0.582070 -0.020953  
C 1.773361 -1.815254 -0.092226  
C -1.349951 -0.194413 0.001630  
C -2.703775 0.017777 0.015229  
C -3.891593 0.206734 0.027106  
C -0.158768 -0.386360 -0.008831  
H 2.382701 2.703948 -0.213891  
H 0.627652 2.099262 -0.255269  
H 3.190048 0.413842 0.016957  
H 1.139020 -2.690504 -0.147154  
H 2.847257 -1.964591 -0.092536  
H -4.941772 0.373425 0.038884  
H 2.343250 0.613406 1.954139

**Vibrational frequencies**

-874.938 75.7059 90.9357  
118.5457 214.7413 276.6147  
304.1297 362.0008 431.0707  
459.9711 507.1236 534.2066  
566.8197 607.5858 653.4348  
678.9728 715.7175 721.019  
756.5906 896.2961 931.8294  
950.5191 1028.989 1055.868  
1104.014 1314.61 1348.335  
1424.89 1458.957 1618.91  
1698.209 2200.474 2388.204  
3167.398 3170.056 3183.42  
3267.546 3268.566 3482.217

***i8 - i10***

**Cartesian coordinates**

C -3.816117 -0.653911 -0.285429  
C -2.921655 0.343996 0.368030  
C -1.481370 0.094131 0.497455  
C -0.556537 0.560738 -0.350676  
C 2.019740 0.094890 -0.116690  
C 3.363886 -0.141070 0.003296  
C 4.544419 -0.347722 0.109995  
C 0.833789 0.301322 -0.214108  
H -4.816953 -0.248676 -0.445832  
H -3.922044 -1.563987 0.325086  
H -3.409250 -0.976299 -1.250110  
H -3.357216 1.148729 0.953177  
H -1.142674 -0.522982 1.333781  
H -0.856435 1.177765 -1.193758  
H 5.587639 -0.528796 0.206417

**Vibrational frequencies**

-295.602 65.1473 71.1884

94.5802	172.7698	193.3349	215.3587	258.7671	281.5966	427.1712	467.4092	541.71
254.2022	328.3048	418.504	414.913	460.9503	538.6926	547.2905	645.0609	677.7591
457.0075	502.0582	555.555	556.2246	570.3286	676.6518	686.6472	690.1648	792.5436
571.4208	695.9643	707.5621	677.4488	701.9668	808.2229	808.6959	947.23	965.8168
786.3928	853.8957	932.3142	890.8752	964.069	986.0447	1007.39	1032.697	1105.008
967.029	977.1781	1105.391	1002.067	1032.882	1080.346	1180.238	1271.26	1343.805
1132.906	1211.999	1279.905	1221.341	1311.755	1327.499	1437.104	1470.7	1634.436
1327.753	1363.993	1404.682	1351.468	1453.821	1658.069	1692.105	2194.553	2364.955
1479.277	1484.284	1702.27	1697.387	2198.264	2374.435	3162.733	3172.004	3180.114
2199.653	2383.367	2988.65	3161.167	3170.157	3177.151	3191.719	3272.683	3482.886
3064.215	3097.33	3128.56	3191.32	3256.251	3485.566			
3167.78	3178.777	3485.167						

**i50 – p27**

**Cartesian coordinates**

C	-2.760435	1.580107	-0.146242
C	-1.947420	0.581605	0.041500
C	-1.088135	-0.426386	-0.040523
C	-1.539219	-1.867899	-0.071159
C	1.504602	0.005817	-0.008463
C	2.858368	0.210071	0.001430
C	4.048548	0.387077	0.009880
C	0.308410	-0.163842	-0.017736
H	-3.242575	2.094964	0.675781
H	-2.967637	1.922126	-1.156435
H	-2.265568	0.291597	2.083648
H	-1.215544	-2.382813	0.837430
H	-1.092195	-2.380360	-0.926357
H	-2.624953	-1.929000	-0.144395
H	5.100161	0.544187	0.018210

**Vibrational frequencies**

-660.656	68.3466	93.3396
119.6975	141.8026	184.8362
236.0972	244.1468	373.2849
425.5728	454.6993	521.3223
527.8454	574.3827	577.7778
652.2963	670.6043	679.0759
713.4379	913.1943	919.2299
1006.523	1059.926	1060.994
1246.224	1329.105	1410.94
1461.132	1482.045	1499.708
2011.844	2194.687	2365.546
3055.573	3127.835	3146.396
3158.679	3236.037	3482.302

**i8 – p4**

**Cartesian coordinates**

C	3.645683	-0.424760	-0.360998
C	2.930093	0.620200	0.074963
C	1.475053	0.713869	0.049051
C	0.641667	-0.338528	0.110068
C	-1.972995	-0.134011	0.019121
C	-3.337458	-0.029799	-0.028731
C	-4.536350	0.063966	-0.071345
C	-0.768162	-0.217614	0.059496
H	3.683096	-1.828291	1.464974
H	4.727827	-0.420497	-0.311242
H	3.178660	-1.270515	-0.854463
H	3.454332	1.483761	0.475451
H	1.046179	1.710782	0.002067
H	1.040283	-1.343379	0.223989
H	-5.595571	0.148202	-0.110528

**Vibrational frequencies**

-428.684	61.6205	69.5689
127.5237	172.9012	191.0838

**i8 – p20**

**Cartesian coordinates**

C	-3.290975	1.183539	0.287138
C	-2.682144	0.083571	-0.540885
C	-1.641185	-0.602405	-0.163255
C	-0.578353	-1.111235	0.447945
C	1.856150	-0.189879	0.118462
C	3.126623	0.292081	-0.047836
C	4.243022	0.716564	-0.194952
C	0.730151	-0.604964	0.259327
H	-4.342701	0.966116	0.493029
H	-3.251653	2.129950	-0.259486
H	-2.765873	1.306917	1.234544
H	-3.142125	-0.133701	-1.500052
H	-1.613298	-1.976806	-1.715595
H	-0.692483	-1.989923	1.078061
H	5.228406	1.093824	-0.326166

**Vibrational frequencies**

-711.607	49.4433	89.4127
132.8708	164.4957	185.2553
218.8197	255.6783	350.0547
413.7332	444.9085	516.2827
561.0048	563.1063	578.468
681.5774	710.2215	768.0465
782.4888	892.7536	903.0113
1070.336	1090.726	1125.495
1214.694	1315.576	1418.504
1438.969	1493.703	1503.554
2015.257	2195.764	2364.209
3051.396	3117.055	3152.789
3164.248	3183.299	3483.88

**i8 – p5**

**Cartesian coordinates**

C	1.530053	1.659721	-0.243129
C	2.421168	0.693500	0.025775
C	2.199666	-0.744690	0.013536
C	1.039669	-1.430979	-0.000325
C	-1.401219	-0.472772	-0.000115
C	-2.676270	0.024120	-0.004850
C	-3.795465	0.466489	-0.010964
C	-0.264557	-0.886129	0.000197
H	1.832241	2.700222	-0.218839
H	0.491063	2.008617	1.793825
H	0.517870	1.447895	-0.561982
H	3.434914	0.992502	0.278769
H	3.102989	-1.347044	0.042561
H	1.086661	-2.516031	0.000355
H	-4.784013	0.858273	-0.015437

**Vibrational frequencies**

-417.655	16.1562	67.0125
116.2483	156.1911	206.9945
236.127	303.4206	312.9863

**i9 – i11**

**Cartesian coordinates**

C	-0.921114	1.708822	-0.000056
C	-2.051579	1.011211	0.000067
C	-2.187935	-0.435541	-0.000005
C	-1.228991	-1.388442	-0.000023
C	0.909035	-0.106219	-0.000078
C	2.297823	0.079476	-0.000006
C	3.479194	0.319419	0.000042
C	0.212086	-1.253193	0.000025
H	-0.777008	2.782664	0.000009
H	0.215619	0.920927	-0.000224
H	-2.991618	1.565057	0.000241
H	-3.213750	-0.791787	-0.000017
H	-1.581593	-2.415612	-0.000048
H	4.524962	0.511560	0.000090
H	0.772276	-2.186006	0.000159

**Vibrational frequencies**

-1285.31	101.1607	139.9507
162.8774	261.7405	325.8219
469.187	472.2488	504.6569
534.7978	608.1628	636.7028
656.4229	690.5603	781.994
816.7423	914.0174	919.976
934.0775	1006.738	1013.01
1014.689	1062.567	1133.842
1287.015	1315.732	1337.649
1458.524	1471.358	1623.068
1682.409	1718.197	2199.371
3118.793	3155.894	3173.977
3194.741	3224.218	3480.703

**i5 – i6**

**Cartesian coordinates**

C	-3.665796	0.582736	-0.276529
C	-2.996637	-0.573895	-0.112091
C	-1.582056	-0.721354	0.095276
C	-0.650235	0.413068	0.300499
C	1.936770	0.154891	0.046678
C	3.288101	0.011589	-0.084122
C	4.480904	-0.117576	-0.199735
C	0.733641	0.285982	0.150090
H	-4.741581	0.586730	-0.398985
H	-3.167177	1.545047	-0.311931
H	-3.556314	-1.504877	-0.121566
H	-1.117821	-1.687993	-0.059731
H	-1.075702	1.403230	0.414084
H	-1.142096	-0.322431	1.262469
H	5.532541	-0.232356	-0.304727

**Vibrational frequencies**

-1867.01	63.4847	75.5888
165.0348	208.5471	255.6501
264.1887	396.2586	461.2951
521.8186	544.0735	567.5856
611.1105	661.1182	717.9835

773.8604	798.0531	836.5812	795.8691	920.3884	937.7519	1000.836	1048.408	1130.811
881.4215	983.713	1006.058	999.6913	1055.868	1132.703	1203.292	1265.366	1327.078
1042.974	1193.122	1216.802	1198.418	1265.53	1304.075	1401.469	1470.705	1580.165
1249.927	1324.075	1352.693	1385.576	1468.869	1606.771	1715.221	2188.081	2339.332
1449.187	1497.033	1630.144	1689.263	2199.122	2376.446	3151.35	3174.316	3182.126
2156.632	2176.808	2292.153	3158.552	3177.372	3184.791	3192.879	3247.245	3485.708
3167.457	3178.181	3200.055	3200.155	3257.221	3485.617			
3210.11	3258.44	3488.192						
<b><i>i42 – i45</i></b>								
<b>Cartesian coordinates</b>			<b><i>i6 – p17</i></b>				<b><i>i48 – p18</i></b>	
C 2.787740 -0.500404 -0.720893			<b>Cartesian coordinates</b>				<b>Cartesian coordinates</b>	
C 1.927032 -0.953606 0.443473			C -2.030571 1.806397 0.230738				C 1.638870 -1.846751 -0.538402	
C 0.997436 0.239691 0.379794			C -2.889404 0.912591 -0.178587				C 2.006313 -1.253020 0.609756	
C 1.794956 1.321443 0.013674			H -2.306166 2.856250 0.344604				C 2.142833 1.070899 0.072072	
C -1.584839 0.055096 0.088843			H -1.002555 1.542392 0.472569				C 0.992984 1.682045 -0.155098	
C -2.934700 -0.057010 -0.064613			H -3.930626 0.914638 -0.473020				C -1.366675 0.526295 -0.025752	
C -4.128787 -0.157522 -0.201424			C -1.768337 -1.367484 -0.504062				C -2.595175 -0.077032 0.035575	
C -0.378072 0.157839 0.220056			C -0.806911 -1.391717 0.437325				C -3.672574 -0.610053 0.088765	
H 2.384126 -0.663652 -1.714210			C 1.575283 -0.341154 0.106125				C -0.278017 1.045795 -0.079508	
H 3.870965 -0.482492 -0.636307			C 2.815867 0.211987 -0.062015				H 2.373247 -2.219205 -1.244128	
H 1.418671 -1.911708 0.309949			C 3.906088 0.700082 -0.210178				H 0.594436 -1.927529 -0.817879	
H 2.494077 -0.995234 1.378388			C 0.477148 -0.828905 0.248612				H 1.266401 -0.959092 1.346024	
H 1.371350 2.203889 -0.459262			H -1.570552 -0.992093 -1.500237				H 3.043302 -1.237052 0.927102	
H 2.757111 1.464808 0.491228			H -2.724567 -1.842332 -0.324926				H 3.155308 1.450961 0.023944	
H -5.180896 -0.248768 -0.323236			H -1.010091 -1.819776 1.414275				H 0.981202 2.742517 -0.417020	
			H 4.869581 1.130135 -0.341019				H -4.625246 -1.079663 0.137513	
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>				<b>Vibrational frequencies</b>	
-840.837	75.777	92.7284	-182.106	41.9065	53.8002	-297.181	53.1141	60.762
161.1933	233.7397	306.2149	111.3811	126.4786	179.3427	107.3712	140.3604	162.3746
397.6181	495.9514	497.0284	202.6044	256.7681	265.9611	229.0371	280.7773	345.2591
532.6018	554.3064	597.4374	366.2513	493.7109	536.148	347.2499	505.7504	537.635
661.1875	697.1581	704.9172	564.791	686.3355	692.9614	569.506	683.014	693.0632
761.2229	804.769	859.1268	697.1525	720.5355	753.9262	695.2682	715.3741	839.1166
952.0962	958.6941	1027.102	862.8035	930.55	952.0227	897.5379	906.8117	939.7627
1032.985	1095.903	1208.739	984.6236	1050.8	1071.54	974.8412	1045.664	1195.041
1275.718	1297.393	1427.887	1211.086	1307.805	1393.062	1242.504	1259.669	1341.632
1456.095	1490.64	1542.174	1442.142	1619.624	1671.305	1467.711	1621.485	1653.407
2153.283	2245.848	3060.314	2189.043	2346.656	3083.772	2199.835	2382.076	3092.941
3107.941	3130.515	3142.995	3169	3169.885	3179.379	3148.853	3161.302	3234.895
3232.645	3244.11	3487.255	3235.561	3270.413	3486.162	3236.84	3259.416	3486.084
<b><i>i48 – p5</i></b>			<b><i>i6 – p5</i></b>				<b><i>i9 – p5</i></b>	
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>				<b>Cartesian coordinates</b>	
C 3.180749 -1.263462 -0.159221			C 3.146728 1.347758 -0.072771				C -1.723530 1.676474 -0.106170	
C 1.988655 -0.650924 0.018204			C 1.981769 0.709369 0.023247				C -2.538273 0.626261 0.025019	
C 1.852239 0.803513 0.010973			C 1.863654 -0.743657 -0.024597				C -2.185165 -0.782338 -0.106156	
C 0.685484 1.467284 -0.022400			C 0.686419 -1.417293 -0.129145				C -0.971108 -1.356872 -0.051160	
C -1.673158 0.313624 -0.021294			C -1.680534 -0.298422 -0.037354				C 1.455127 -0.384247 0.008331	
C -2.904986 -0.284432 -0.018866			C -2.919223 0.280194 0.008590				C 2.738441 0.072652 -0.028316	
C -3.986640 -0.811547 -0.016725			C -4.008413 0.790958 0.049228				C 3.873368 0.476692 -0.068859	
C -0.584305 0.837838 -0.023926			C -0.582511 -0.806300 -0.077123				C 0.284127 -0.708993 0.129379	
H 3.252752 -2.340507 -0.244558			H 3.200918 2.429515 -0.052284				H -2.103942 2.683033 0.024848	
H 4.106963 -0.698420 -0.180300			H 4.083215 0.807165 -0.172425				H -0.676726 1.573627 -0.362555	
H 1.071682 -1.228727 -0.056050			H 1.058120 1.271538 0.127145				H -3.586787 1.813301 0.241763	
H 1.703352 -0.858920 1.917475			H 2.782190 -1.308119 -0.155028				H -3.023192 -1.460016 -0.239893	
H 2.772701 1.380069 0.020273			H 0.701239 -2.497214 -0.234051				H -0.903101 -2.435249 -0.161365	
H 0.686922 2.552277 -0.043428			H -4.971102 1.240984 0.085359				H 4.874344 0.833986 -0.105021	
H -4.942604 -1.277139 -0.013881			H 2.218081 -1.119508 1.960835				H -0.178522 0.273557 1.789814	
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>				<b>Vibrational frequencies</b>	
-883.152	64.502	89.5571	-742.567	63.0553	107.1349	-804.712	67.7225	95.2845
129.6992	186.6309	279.3727	135.3247	184.8163	230.979	147.9147	189.8708	269.4041
310.3713	366.037	407.4753	309.2499	328.6779	367.8428	313.565	346.4143	429.0689
439.5177	475.1991	540.8589	413.8362	453.5711	542.5496	456.4316	467.0106	539.2666
551.9515	631.4646	672.3993	555.1992	636.3721	689.6482	553.2498	662.7752	668.6801
676.4218	715.0076	774.2064	699.2398	708.743	772.7073	674.4704	676.9822	796.3685
			809.9469	939.3328	967.8327	815.6826	952.7082	993.9095
						1008.859	1049.149	1106.715

1171.751	1269.505	1358.412	1445.209	1488.849	1503.176	1715.122	2191.79	2345.702			
1436.37	1475.635	1672.494	2012.205	2195.751	2362.628	3158.179	3169.092	3170.427			
1714.319	2153.957	2268.163	3052.68	3119.137	3134.125	3183.548	3255.222	3485.616			
3162.765	3172.53	3179.227	3155.887	3165.952	3484.918						
3197.314	3270.782	3481.15									
<b><i>i10 - p4</i></b>			<b><i>i43 - i49</i></b>			<b><i>i6 - i47</i></b>					
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>					
C	-3.896143	-0.600481	-0.190117	C	3.111797	0.963135	-0.378383	C	-2.144471	1.144300	0.423835
C	-2.892515	0.280003	-0.063001	C	3.094967	-0.333412	0.336741	C	-2.266692	0.519489	-0.820781
C	-1.494684	-0.094197	-0.083902	C	1.629629	-0.110539	0.496265	C	-1.977269	-0.925834	-0.516897
C	-0.491021	0.790684	0.052544	C	0.674253	-0.652461	-0.328331	C	-1.045980	-0.588203	0.666143
C	2.051960	0.147168	0.019388	C	-1.879714	-0.140393	-0.101962	C	1.496974	-0.169455	0.198766
C	3.381071	-0.180904	0.004525	C	-3.215417	0.117828	0.023518	C	2.820225	0.063510	-0.051452
C	4.549179	-0.469653	-0.008285	C	-4.393252	0.345867	0.136418	C	3.986866	0.268110	-0.272507
C	0.877518	0.432275	0.032372	C	-0.692343	-0.369174	-0.207972	C	0.323897	-0.383778	0.422784
H	-4.369032	-1.205775	1.956775	H	3.236330	1.893964	0.158166	H	-2.740052	0.793098	1.263311
H	-3.702572	-1.654993	-0.358493	H	2.938132	0.997754	-1.444680	H	-1.822496	2.179820	0.520733
H	-4.930578	-0.280035	-0.206319	H	3.341452	-1.196906	-0.280173	H	-1.987859	0.994464	-1.752939
H	-3.117379	1.334759	0.075709	H	3.648895	-0.353667	1.273673	H	-1.496497	-1.477030	-1.327482
H	-1.259867	-1.146890	-0.217786	H	1.314015	0.524262	1.316723	H	-2.845905	-1.499812	-0.178351
H	-0.714674	1.846091	0.188534	H	0.974271	-1.334846	-1.119778	H	-1.285134	-1.006579	1.641311
H	5.581905	-0.722533	-0.019561	H	-5.432615	0.544328	0.238305	H	5.016642	0.447208	-0.465931
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>					
			-559.261	68.951	83.3928	-966.751	72.2631	93.6099			
-432.637	66.1393	93.7388	180.6978	220.8066	250.5562	172.0847	216.5237	263.5931			
139.6001	179.6596	198.3128	352.1148	418.6809	462.4541	407.711	468.3288	492.3578			
227.4078	274.2942	307.308	522.2955	541.6484	558.7887	678.9874	681.4913	709.096			
414.2253	433.7254	510.3617	645.9228	667.6981	703.4911	756.108	895.7826	911.1512			
565.83	572.0087	679.3428	775.2515	788.7267	821.0703	947.5468	972.4783	1008.207			
698.6943	702.6246	790.3859	917.2816	972.8079	1076.027	1071.023	1149.523	1218.838			
896.5883	964.0636	967.3314	1165.068	1222.972	1228.377	1232.196	1282.368	1363.086			
990.9589	1051.578	1199.547	1231.564	1289.873	1335.669	1377.514	1480.801	1533.251			
1222.497	1293.615	1319.13	1459.675	1495.782	1535.867	2175.29	2304.632	3054.362			
1340.839	1455.062	1654.631	2173.952	2296.014	3095.979	3113.022	3117.201	3155.867			
1684.631	2198.126	2371.015	3164.061	3167.776	3181.708	3191.696	3224.748	3484.394			
3158.219	3170.127	3173.031	3206.8	3297.63	3484.211						
3185.836	3254.929	3486.388									
<b><i>i10 - p20</i></b>			<b><i>i6 - p4</i></b>			<b><i>i47 - p21</i></b>					
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>					
C	3.548605	1.018497	-0.273327	C	3.937933	0.658445	-0.166244	C	-1.906626	0.968223	-0.252540
C	2.582025	0.215151	0.544885	C	2.955858	-0.231232	-0.033561	C	-2.582384	-0.065783	-0.784835
C	1.597811	-0.527012	0.123614	C	1.547024	0.132894	0.071054	C	-1.903738	-1.112326	0.063769
C	0.497204	-1.254666	-0.019980	C	0.544949	-0.781320	-0.005114	C	-1.069065	0.078941	0.669025
C	-1.913373	-0.218397	-0.018872	C	-1.998300	-0.158801	-0.025316	C	1.541452	0.034851	0.180065
C	-3.171474	0.320944	-0.014422	C	-3.328236	0.161599	-0.037237	C	2.888452	0.010413	-0.079650
C	-4.276618	0.797386	-0.009939	C	-4.498175	0.444237	-0.047894	C	4.069429	-0.011967	-0.306279
C	-0.798014	-0.683619	-0.020441	C	-0.820969	-0.438124	-0.016648	C	0.357531	0.053253	0.405710
H	3.465413	2.077710	-0.014382	H	4.971815	0.349484	-0.261704	H	-3.232099	1.651722	1.128609
H	3.358874	0.902439	-1.340548	H	3.736272	1.725067	-0.182641	H	-1.809452	2.016883	-0.501997
H	4.576021	0.708545	-0.063261	H	3.185111	-1.294010	-0.015484	H	-3.354866	-0.133737	-1.540274
H	2.705418	0.254860	1.627317	H	1.299164	1.189855	0.028212	H	-1.301753	-1.845097	-0.477866
H	2.171033	-0.849775	-1.874859	H	1.513965	0.452476	2.093045	H	-2.537381	-1.629016	0.790125
H	0.578350	-2.323958	-0.197168	H	0.785406	-1.840876	-0.038506	H	-1.248358	0.238031	1.735420
H	-5.252108	1.220468	-0.006202	H	-5.532231	0.691815	-0.057165	H	5.113595	-0.032421	-0.505607
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>					
			-766.372	63.4992	68.9673	-656.639	82.867	85.5139			
-637.722	45.1844	77.6562	134.962	194.7494	212.9558	185.0917	228.9114	264.4156			
118.9731	139.6113	175.7618	292.1043	325.1176	373.796	335.6749	381.5178	456.6145			
228.0984	297.4422	353.2672	413.4949	426.9478	509.897	656.3238	681.8311	703.2264			
413.2789	487.6076	518.5917	561.8228	572.2136	670.2156	813.5172	862.0275	906.4679			
545.8794	553.9524	592.8146	677.8675	699.2101	789.3212	937.6099	969.8288	1004.096			
669.8836	707.5584	756.9973	860.3003	953.4773	961.1694	1010.906	1106.829	1130.314			
786.273	887.192	901.8622	982.9082	1035.989	1192.287	1187.222	1212.878	1241.982			
1065.355	1087.151	1145.194	1223.553	1285.37	1303.485	1315.005	1355.261	1469.682			
1214.541	1308.036	1412.945	1340.571	1452.133	1606.3	1593.593	2201.613	2399.226			

3073.204	3089.463	3131.406	3223.72	3467.868	3483.261		
3214.965	3243.177	3484.262					
<b><i>i12 – i13</i></b>			<b><i>i43 – p23</i></b>				
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>				
C	0.154730	-1.263612	0.055965	C	3.220331	-0.041148	0.155038
C	1.566716	-1.187313	-0.072346	C	1.791561	0.189574	-0.075239
C	2.232894	0.001098	-0.076542	C	0.768352	1.039826	0.069622
C	1.486143	1.246610	-0.022600	C	2.224948	-1.204422	0.026593
C	-0.639433	0.031641	0.128991	C	-1.739237	0.270406	0.026610
C	-2.043651	0.014474	-0.020105	C	-3.048288	-0.129895	0.008840
C	-3.245057	-0.008010	-0.123222	C	-4.198703	-0.482926	-0.007013
C	0.140295	1.262516	0.050112	C	-0.581668	0.618245	0.043000
H	-0.395694	-2.184863	-0.070556	H	3.916720	0.105327	-0.662656
H	2.112540	-2.119702	-0.168597	H	3.615506	0.192075	1.138430
H	3.311664	0.027702	-0.158311	H	1.875571	0.386863	-2.161970
H	2.026543	2.184800	-0.073681	H	0.959764	2.103489	0.176452
H	-0.259743	-0.665351	1.140783	H	1.946454	-1.749432	0.922571
H	-4.302772	-0.023728	-0.226526	H	2.277637	-1.802606	-0.875716
H	-0.408351	2.196721	0.035361	H	-5.215429	-0.793687	-0.021809
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>				
			-657.862	64.9099	92.7		
-2300.73	115.5779	147.5609	180.9336	202.2987	275.0464		
274.9656	379.0122	441.1248	346.2165	350.7725	408.0294		
485.1118	522.8315	558.8439	451.7255	472.8002	549.6247		
603.0931	628.0595	695.6911	560.8844	677.935	684.749		
714.0572	721.0367	754.948	750.6681	774.8165	788.6559		
812.6706	953.9694	973.5908	811.6224	940.8188	1017.203		
976.2425	993.8506	1050.722	1050.936	1065.914	1089.123		
1148.817	1161.283	1190.553	1095.56	1167.225	1220.98		
1234.58	1268.252	1339.519	1364.916	1445.554	1474.668		
1417.989	1470.384	1541.38	1775.498	2195.707	2362.747		
1667.099	2182.966	2188.822	3137.085	3141.633	3179.745		
3196.712	3201.375	3220.432	3221.416	3231.978	3486.651		
3228.871	3246.373	3482.889					
<b><i>i11 – p31</i></b>			<b><i>i49 – p18</i></b>				
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>				
C	-2.572908	1.682510	-0.085428	C	-3.810699	-0.835397	-0.000015
C	-2.511598	0.472354	0.014083	C	-3.647787	0.497427	0.000057
C	-2.045122	-0.883231	-0.017720	C	-1.279907	0.879387	-0.000028
C	-0.744771	-1.223576	-0.026952	C	-0.523907	-0.202976	-0.000002
C	1.647602	-0.713783	-0.023969	C	2.106444	-0.112832	-0.000019
C	2.761091	0.168449	0.010294	C	3.475540	-0.065582	-0.000004
C	3.716137	0.897624	0.037426	C	4.677993	-0.023874	0.000021
C	0.370260	-0.301743	0.010082	C	0.899331	-0.151857	-0.000018
H	-2.769115	2.727818	-0.122013	H	-3.862627	-1.398865	0.925219
H	-4.231729	0.090490	0.671913	H	-3.862883	-1.398714	-0.925320
H	-2.799122	-1.659988	-0.037523	H	-3.682773	1.065655	-0.922797
H	-0.504258	-2.282646	-0.064983	H	-3.682591	1.065561	0.922971
H	1.872692	-1.775883	-0.083847	H	-1.042914	1.936088	-0.000099
H	4.556276	1.549056	0.061342	H	-0.988819	-1.187936	0.000032
H	0.151112	0.759531	0.068225	H	5.740564	0.012444	0.000044
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>				
			-258.757	48.3448	52.555		
-866.459	22.1846	85.5953	56.2557	122.1476	165.7893		
119.4032	131.9372	188.4991	221.4638	265.0288	320.7375		
304.9245	329.9668	413.0771	377.651	476.4027	548.6483		
442.5635	522.251	557.4118	559.408	691.0605	697.8261		
580.2785	647.6916	689.6367	711.7835	746.2384	836.7041		
691.987	699.2402	730.3572	894.9107	923.1971	930.8701		
781.0174	893.669	943.4827	979.6869	1038.748	1196.895		
987.1006	1023.367	1040.583	1240.896	1277.111	1341.641		
1150.433	1257.391	1309.284	1466.512	1620.939	1650.965		
1341.38	1440.593	1660.512	2196.152	2375.21	3135.672		
1717.567	2119.226	2236.795	3144.76	3158.014	3228.891		
3170.07	3177.061	3204.159	3229.209	3253.859	3487.169		

<b><i>i49 – p4</i></b>			
<b>Cartesian coordinates</b>			
C	3.906060	0.725630	-0.110574
C	2.930837	-0.207071	-0.019549
C	1.514162	0.142444	0.053244
C	0.525300	-0.749400	-0.105032
C	-2.027144	-0.144020	-0.030465
C	-3.361161	0.162780	0.007121
C	-4.533358	0.432419	0.040369
C	-0.849099	-0.410703	-0.061055
H	3.686423	1.780985	0.011024
H	4.941151	0.445528	-0.260469
H	3.165934	-1.246148	-0.235847
H	3.110961	-0.750263	1.815576
H	1.269998	1.186234	0.230083
H	0.761683	-1.797013	-0.275601
H	-5.569727	0.668203	0.070884
<b>Vibrational frequencies</b>			
	-888.442	69.4408	98.2107
	151.1708	194.1871	210.5537
	306.6208	368.4131	399.0375
	444.4186	460.9864	512.4901
	567.4793	572.6256	654.2027
	679.3949	702.5627	789.2864
	894.7604	926.2941	960.4781
	999.5857	1064.918	1187.263
	1218.812	1291.516	1303.541
	1336.1	1450.298	1610.903
	1703.701	2199.048	2375.602
	3162.09	3167.565	3167.984
	3186.194	3264.109	3485.478
<b><i>i13 – i11</i></b>			
<b>Cartesian coordinates</b>			
C	-0.629910	1.645590	-0.043585
C	-1.840470	1.116074	-0.118265
C	-2.188132	-0.283048	0.089752
C	-1.337325	-1.335603	-0.010057
C	0.810010	-0.217375	0.397477
C	2.185079	0.010668	0.100242
C	3.343807	0.218666	-0.140685
C	0.079102	-1.207541	-0.193358
H	-0.227058	2.632609	-0.222960
H	-2.668976	1.756588	-0.431098
H	-3.249004	-0.498231	0.170558
H	-1.768166	-2.330876	-0.075629
H	0.436317	0.250230	1.300935
H	4.369768	0.397527	-0.354724
H	0.574153	-1.892438	-0.876210
<b>Vibrational frequencies</b>			
	-339.009	121.8079	130.4579
	234.1151	278.6298	300.3165
	451.8867	487.0882	507.6485
	552.9572	658.5941	689.3776
	726.2957	728.0596	760.9725
	796.7142	900.2649	906.0346
	917.1944	986.0508	992.4798
	1039.03	1092.163	1235.101
	1265.916	1287.537	1305.747
	1457.755	1536.172	1625.778
	1658.122	2233.383	3091.966
	3167.497	3182.498	3193.793
	3197.215	3249.633	3484.054
<b><i>i45 – p19</i></b>			
<b>Cartesian coordinates</b>			
C	-3.037852	0.003139	-0.110651

C -1.886621 0.983113 -0.195365  
 C -0.940634 0.029893 -0.038744  
 C -1.950269 -1.092524 0.129994  
 C 1.674405 0.012347 -0.017369  
 C 3.042766 -0.007473 -0.005883  
 C 4.246003 -0.024614 0.004064  
 C 0.465624 0.036954 -0.030766  
 H -3.594359 -0.120617 -1.043248  
 H -3.743636 0.155635 0.708026  
 H -1.829783 2.036764 -0.437899  
 H -1.954377 1.747713 1.852345  
 H -1.902024 -1.877451 -0.627789  
 H -1.965599 -1.546850 1.123308  
 H 5.309244 -0.040194 0.013577

**Vibrational frequencies**

-555.548 77.2141 82.5776  
 190.6254 220.1753 233.9664  
 282.9685 353.721 448.5059  
 485.3919 500.3115 571.3383  
 579.8712 679.8937 685.1773  
 790.3273 887.0351 901.3081  
 919.4507 939.9818 1037.348  
 1045.177 1098.721 1177.157  
 1209.324 1227.047 1274.017  
 1307.015 1471.656 1495.101  
 1628.969 2196.578 2363.827  
 3076.651 3081.701 3126.415  
 3139.943 3227.117 3483.013

**i13 - i70**

**Cartesian coordinates**

C -0.105676 1.334875 0.961052  
 C -1.142124 1.373175 0.136950  
 C -1.592206 0.291035 -0.720535  
 C -1.286637 -1.021483 -0.554054  
 C 0.805455 -0.851474 0.760223  
 C 1.627219 -0.132852 -0.163444  
 C 2.387678 0.411531 -0.918433  
 C -0.365027 -1.485352 0.437887  
 H 0.329012 2.032655 1.662218  
 H -1.765721 2.270006 0.128006  
 H -2.360081 0.544796 -1.444275  
 H -1.878727 -1.757145 -1.091248  
 H 1.327212 -1.177420 1.656476  
 H 3.041037 0.904120 -1.596812  
 H -0.664818 -2.333737 1.047757

**Vibrational frequencies**

-434.584 119.058 129.0647  
 233.7638 310.668 325.0262  
 429.1868 458.1658 466.5801  
 598.2263 633.0502 663.1702  
 715.4875 734.7634 793.496  
 806.8514 873.4374 904.3955  
 948.0167 967.0191 993.8879  
 1002.091 1069.757 1230.195  
 1232.279 1266.16 1402.037  
 1469.587 1514.773 1604.222  
 1654.169 2231.975 3091.842  
 3157.025 3173.181 3179.66  
 3200.628 3252.023 3488.194

**i13 - p1**

**Cartesian coordinates**

C -0.137071 1.218610 0.014495  
 C -1.515069 1.207241 -0.059870  
 C -2.212528 0.000000 -0.076455  
 C -1.515069 -1.207241 -0.059870

C 0.578662 0.000000 0.146962  
 C 2.010957 0.000000 -0.012328  
 C 3.199104 0.000000 -0.176220  
 C -0.137071 -1.218610 0.014495  
 H 0.413913 2.150814 0.016580  
 H -2.054795 2.145230 -0.120840  
 H -3.294577 0.000000 -0.136241  
 H -2.054795 -2.145230 -0.120840  
 H 0.691609 0.000000 1.912718  
 H 4.253237 0.000000 -0.315208  
 H 0.413913 -2.150814 0.016580

**Vibrational frequencies**

-1151.96 137.4333 150.0709  
 330.7368 394.6479 464.0595  
 480.3936 523.6463 539.0936  
 573.8214 631.428 689.9121  
 693.3016 704.3033 759.4327  
 801.4586 848.4298 935.7788  
 996.1729 1012.736 1013.832  
 1051.47 1112.829 1183.011  
 1200.651 1226.471 1299.682  
 1352.631 1480.147 1516.055  
 1608.647 1653.04 2249.221  
 3197.111 3205.599 3217.469  
 3225.66 3229.619 3483.072

**i46 - i47**

**Cartesian coordinates**

C -1.849195 -1.088960 -0.045729  
 C -2.658351 -0.097074 0.740677  
 C -1.911270 1.066922 0.115899  
 C -1.076528 0.038919 -0.737657  
 C 1.524623 0.016014 -0.195982  
 C 2.864888 -0.006455 0.096141  
 C 4.040071 -0.027848 0.351897  
 C 0.346455 0.036980 -0.451755  
 H -1.543364 -2.100461 0.188491  
 H -3.137497 -0.201364 1.705377  
 H -3.087983 -0.791223 -0.268740  
 H -2.490469 1.797263 -0.453239  
 H -1.276140 1.596684 0.829233  
 H -1.227730 0.115847 -1.818636  
 H 5.079023 -0.047736 0.576566

**Vibrational frequencies**

-1928.36 76.5081 87.8839  
 164.7053 229.3953 281.5001  
 431.166 476.1578 533.5785  
 580.5621 609.2155 643.6633  
 679.3571 696.7447 714.9108  
 842.8794 887.1222 927.2176  
 966.8043 1018.049 1058.75  
 1119.737 1181.925 1191.039  
 1221.523 1253.287 1272.046  
 1295.288 1356.803 1484.119  
 2200.564 2246.877 2395.574  
 3065.68 3075.293 3127.991  
 3206.091 3221.755 3485.888

**i46 - i45**

**Cartesian coordinates**

C -1.966253 -1.085173 0.010678  
 C -3.047312 -0.042653 0.200141  
 C -1.973176 1.069871 -0.010876  
 C -0.922023 -0.024674 -0.212793  
 C 1.680749 -0.004907 -0.036812  
 C 3.043544 0.004012 0.035591  
 C 4.247567 0.012116 0.100661

C 0.466265 -0.016358 -0.093409  
 H -1.853554 -2.122053 0.295810  
 H -3.461826 -0.035984 1.212168  
 H -3.877622 -0.058118 -0.510295  
 H -2.125315 1.754574 -0.846626  
 H -1.782534 1.648217 0.894186  
 H -1.384224 -0.679593 -1.163723  
 H 5.308913 0.019554 0.159396

**Vibrational frequencies**

-1879.36 82.3977 87.3492  
 178.985 229.3304 291.1093  
 428.2169 475.5199 488.9279  
 533.4122 561.1867 588.1562  
 631.4272 686.6479 792.5525  
 848.6059 918.4893 952.2841  
 1016.464 1035.074 1071.179  
 1101.146 1197.532 1204.253  
 1236.153 1267.342 1277.136  
 1441.653 1477.38 1506.838  
 2172.761 2229.574 2300.421  
 3062.892 3090.204 3105.3  
 3146.449 3240.31 3484.513

**i66 - p29**

**Cartesian coordinates**

C 4.036775 0.533566 -0.094516  
 C 3.042458 -0.159095 -0.001834  
 C 1.689156 -0.625784 -0.052229  
 C 0.637502 0.202350 0.042429  
 C -1.786277 0.576146 0.070911  
 C -3.138764 0.144867 0.007105  
 C -4.289275 -0.198964 -0.044606  
 C -0.734963 -0.253176 -0.022476  
 H 4.981048 1.023460 -0.118739  
 H 3.770202 -1.733729 0.730550  
 H 1.534735 -1.692712 -0.173460  
 H 0.809192 1.267053 0.176054  
 H -1.622361 1.642531 0.203861  
 H -5.305623 -0.508197 -0.091876  
 H -0.906866 -1.317871 -0.155092

**Vibrational frequencies**

-866.524 51.2691 72.0206  
 88.1433 182.2468 196.9411  
 237.0817 333.0234 397.3269  
 448.8619 510.8451 519.4001  
 545.8854 628.8831 658.8696  
 674.5711 698.8065 702.2804  
 854.6001 921.1387 983.823  
 1001.955 1037.931 1057.378  
 1185.497 1255.646 1333.246  
 1349.501 1357.687 1676.411  
 1723.125 2124.211 2237.816  
 3171.717 3179.849 3187.197  
 3195.604 3470.224 3484.974

**i46 - p21**

**Cartesian coordinates**

C -1.864690 1.046679 -0.056253  
 C -2.670005 0.151119 -0.655203  
 C -1.900586 -1.052474 -0.144078  
 C -1.031848 -0.009566 0.655035  
 C 1.581732 -0.000401 0.177879  
 C 2.929649 0.008518 -0.078217  
 C 4.111269 0.017009 -0.302350  
 C 0.397045 -0.008969 0.399900  
 H -1.807207 2.127346 -0.041798  
 H -3.455433 0.244307 -1.394286

H -4.215495 0.097928 0.660756  
H -2.446191 -1.770091 0.470748  
H -1.329680 -1.580859 -0.909595  
H -1.217378 -0.055058 1.733609  
H 5.155989 0.024938 -0.499710

**Vibrational frequencies**

-684.31 73.5267 86.0685  
176.9573 227.3403 269.9611  
341.85 385.2982 459.9177  
479.4357 543.8375 594.5414  
638.8393 681.2156 703.4319  
817.9492 865.5098 904.091  
941.8069 966.7432 1002.883  
1014.336 1101.102 1131.677  
1173.946 1207.54 1238.399  
1309.035 1351.915 1481.015  
1590.074 2201.439 2399.243  
3065.993 3088.493 3147.639  
3212.954 3242.296 3483.975

**i46 – p19**

**Cartesian coordinates**

C -1.895425 1.041853 -0.070011  
C -3.047462 0.076235 -0.164439  
C -1.979405 -1.058387 -0.064540  
C -0.964773 0.069124 0.133490  
C 1.656995 0.028327 0.033138  
C 3.024188 -0.005551 -0.039565  
C 4.225107 -0.035321 -0.105324  
C 0.451926 0.063563 0.095655  
H -1.823406 2.120183 -0.133600  
H -3.611555 0.103215 -1.100633  
H -3.751826 0.111205 0.672231  
H -2.088539 -1.762445 0.760272  
H -1.832529 -1.603602 -0.998913  
H -1.005474 0.015423 2.054908  
H 5.286423 -0.063040 -0.164690

**Vibrational frequencies**

-901.588 80.7872 88.14  
196.6402 222.9646 304.9324  
412.4624 438.642 458.9376  
491.5643 513.2756 556.0861  
569.7743 686.9842 689.0597  
757.883 851.3441 887.0419  
920.8673 944.9948 1033.598  
1037.681 1100 1181.184  
1210.486 1229.147 1280.454  
1293.716 1465.193 1490.765  
1588.727 2200.685 2379.693  
3063.312 3092.975 3111.476  
3154.869 3226.523 3484.756

**i70 – p30**

**Cartesian coordinates**

C -3.308890 0.762851 0.141450  
C -2.585135 -0.204368 0.003436  
C -1.460827 -1.094588 0.040010  
C -0.180435 -0.687589 0.016596  
C 1.545188 1.074655 -0.073881  
C 2.654308 0.186033 -0.001218  
C 3.604395 -0.547990 0.058595  
C 0.257321 0.690089 -0.065947  
H -4.053238 1.521911 0.188767  
H -3.733496 -1.384350 -0.896830  
H -1.681016 -2.153882 0.090214  
H 0.594112 -1.446977 0.060138  
H 1.782846 2.131291 -0.141499

H 4.444903 -1.197479 0.110303  
H -0.509656 1.454923 -0.125338

**Vibrational frequencies**

-880.299 33.4173 53.3474  
106.5151 154.1322 241.2858  
313.5155 326.8606 403.3064  
460.4368 522.7733 613.6058  
635.8291 667.5227 687.9223  
696.6765 710.6401 767.5838  
780.3751 827.0545 904.2922  
972.9882 1008.676 1030.186  
1125.21 1246.067 1289.835  
1387.348 1464.179 1651.023  
1712.381 2120.79 2233.085  
3188.129 3194.4 3210.079  
3218.128 3470.708 3482.832

**i1 – i46**

**Cartesian coordinates**

C -3.097219 -0.463399 0.221870  
C -1.841350 -0.994721 -0.019681  
C -1.026038 0.173498 -0.531277  
C -1.767773 1.191747 0.350586  
C 1.603449 0.021576 -0.151813  
C 2.957736 -0.055714 0.055271  
C 4.144895 -0.124812 0.235409  
C 0.413979 0.087485 -0.334351  
H -3.775034 -0.906001 0.949198  
H -3.593774 0.136813 -0.535686  
H -1.401551 -1.811752 0.537329  
H -1.223986 0.381937 -1.590546  
H -1.423525 1.243320 1.378292  
H -2.102405 2.129893 -0.089044  
H 5.194204 -0.188170 0.394371

**Vibrational frequencies**

-900.153 76.1029 83.9763  
182.9885 226.9251 285.4389  
424.9723 468.3385 486.5935  
535.7151 562.547 590.7307  
653.0241 690.649 706.9599  
736.599 821.3952 897.7132  
949.16 955.3695 971.7212  
1056.534 1096.673 1196.123  
1232.114 1237.734 1327.648  
1393.383 1446.505 1540.298  
2202.409 2401.164 3031.572  
3110.661 3123.731 3197.121  
3230.149 3235.936 3485.884

**i54 – i53**

**Cartesian coordinates**

C 0.196699 1.340302 -0.040223  
C -1.263115 1.153077 -0.037835  
C -1.520716 -0.250975 -0.019908  
C -2.780173 -0.858034 0.018617  
C 0.774282 0.038931 -0.036837  
C 2.170495 -0.225142 -0.002810  
C 3.351494 -0.445554 0.019773  
C -0.250999 -0.896946 -0.028537  
H -0.517528 1.448658 1.026646  
H 0.702550 2.278714 -0.213111  
H -1.981285 1.950222 -0.166358  
H -2.875810 -1.936110 0.013674  
H -3.686062 -0.265356 0.034535  
H 4.395840 -0.643027 0.040508  
H -0.105504 -1.967056 0.030671

**Vibrational frequencies**

-1371.05 130.6042 148.9406  
267.7742 338.8958 431.063  
481.564 530.8367 547.5564  
598.5206 623.53 637.6555  
666.6536 700.1672 730.2295  
759.6283 878.3795 948.56  
956.1125 967.5215 990.0657  
1052.883 1190.972 1225.629  
1247.383 1273.571 1401.561  
1430.729 1438.172 1507.47  
1546.557 2156.349 2243.128  
3167.984 3242.217 3246.771  
3260.586 3268.968 3484.139

**i54 – i56**

**Cartesian coordinates**

C 0.197095 1.350857 -0.063816  
C -1.179626 1.220149 -0.008376  
C -1.498591 -0.237317 0.077389  
C -2.783869 -0.838554 -0.120109  
C 0.774832 0.053727 -0.032528  
C 2.176096 -0.213020 -0.018513  
C 3.356469 -0.433429 -0.013758  
C -0.224645 -0.898321 0.053967  
H 0.746943 2.279823 -0.077314  
H -1.480841 0.450354 1.131856  
H -1.933925 1.991248 -0.070349  
H -2.876395 -1.914894 -0.160678  
H -3.679697 -0.233931 -0.172165  
H 4.401314 -0.629708 -0.009066  
H -0.083969 -1.967443 0.112171

**Vibrational frequencies**

-1246.21 132.1194 149.1841  
286.6024 306.5754 326.7103  
457.1025 529.0416 535.5388  
548.4675 652.4258 656.7656  
669.8128 706.7229 724.3415  
768.3656 838.4119 898.6425  
923.4566 969.5585 983.1296  
1093.551 1138.841 1189.435  
1241.816 1317.552 1355.166  
1436.416 1468.293 1499.105  
1578.573 2068.526 2248.412  
3175.767 3248.146 3258.462  
3266.734 3284.814 3483.952

**i56 – i58**

**Cartesian coordinates**

C 0.029294 1.365210 0.158957  
C 1.353639 1.230133 -0.041780  
C 1.656036 -0.176577 -0.450803  
C 1.920423 -1.077430 0.171541  
C -0.644350 0.106230 -0.133844  
C -2.031565 -0.130517 0.013666  
C -3.214523 -0.314404 0.137958  
C 0.304576 -0.802036 -0.558151  
H -0.481123 2.251181 0.512449  
H 2.111943 1.983739 0.118188  
H 2.346307 -0.308955 -1.284138  
H 1.598021 -0.777765 1.705100  
H 2.321492 -2.070739 0.562982  
H -4.258716 -0.480447 0.248283  
H 0.120899 -1.800670 -0.924128

**Vibrational frequencies**

-481.806 130.5912 162.8597





702.8441	723.5672	765.9844	726.9586	800.4871	870.0498	936.1066	979.8214	998.198
801.4628	886.2457	940.3369	929.3597	943.1564	950.2901	1070.132	1120.129	1195.081
977.1439	979.8192	1019.344	974.795	979.4939	1102.804	1258.184	1290.314	1326.006
1135.51	1187.633	1206.269	1188.156	1237.954	1340.624	1340.061	1484.7	1611.128
1232.61	1313.343	1341.238	1367.618	1451.488	1528.684	1723.636	2200.454	3159.114
1417.18	1436.192	1518.044	1637.6	1742.383	2242.759	3173.733	3181.83	3184.706
1611.054	2190.62	2219.101	3161.494	3238.138	3253.66	3194.155	3322.342	3482.843
3198.251	3208.635	3224.45	3258.085	3260.254	3482.525			
3230.119	3247.553	3482.493						
<b><i>i59 – p1</i></b>								
<b>Cartesian coordinates</b>			<b><i>i56 – p26</i></b>					
C -0.070612	1.210638	-0.046235	<b>Cartesian coordinates</b>			<b><i>i61 – i11</i></b>		
C -1.450839	1.211932	-0.079660	C 0.138204	1.355756	-0.050515	<b>Cartesian coordinates</b>		
C -2.161567	0.000000	-0.037619	C -1.196331	1.218352	-0.000249	C 2.270482	-1.212215	-0.649023
C -1.450839	-1.211932	-0.079660	C -1.508992	-0.225684	0.057812	C 1.990591	-0.898325	0.567134
C 0.636829	0.000000	-0.015719	C -2.707577	-0.793428	-0.213748	C 2.032168	0.546369	0.212176
C 2.065546	0.000000	0.023365	C 0.763335	0.021003	0.000573	C 0.951714	1.361046	-0.084160
C 3.266323	0.000000	0.058507	C 2.166353	-0.205785	-0.028002	C -1.051451	-0.143333	0.098674
C -0.070612	-1.210638	-0.046236	C 3.355231	-0.375971	-0.056400	C -2.456363	-0.304207	0.028341
H 0.479550	2.143902	-0.052986	C -0.208467	-0.917034	0.080070	C -3.648999	-0.462694	-0.027432
H -1.990731	2.150785	-0.109414	H 0.697192	2.278726	-0.114912	C -0.441745	1.054228	-0.118948
H -2.659162	0.000000	1.772954	H -1.941631	2.000046	-0.024746	H 2.413623	-1.909477	-1.455048
H -3.233040	-0.000001	-0.199661	H -1.481043	-0.162428	1.979237	H 1.770754	-1.400790	1.505077
H -1.990731	-2.150785	-0.109413	H -3.597863	-0.188141	-0.339487	H 3.008333	1.018782	0.238696
H 4.329186	0.000000	0.091052	H -2.816722	-1.869546	-0.282269	H 1.201338	2.387852	-0.334788
H 0.479551	-2.143901	-0.052986	H 4.406407	-0.534012	-0.080663	H -0.477057	-1.032494	0.327336
			H -0.076867	-1.987892	0.125603	H -4.702057	-0.598570	-0.080316
						H -1.093319	1.889484	-0.361529
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
-912.427	132.2223	154.7847	-917.469	119.6702	149.9934	-723.017	94.5131	107.5642
291.0104	368.6892	417.6328	214.9897	260.6096	343.1339	126.758	185.9656	222.6558
426.5386	476.6555	541.4233	425.6683	439.0534	528.9803	348.5301	383.5145	486.8464
555.4688	634.6199	665.5407	544.2953	596.9261	627.1786	522.9916	579.2296	623.006
703.586	731.4758	776.7239	661.5612	679.339	713.232	638.0833	716.5729	747.753
810.5909	854.2382	972.3484	727.1834	768.3884	852.1858	768.0097	854.8585	861.9031
998.4545	1011.814	1038.256	922.855	928.1665	941.7083	924.9819	946.5167	997.8308
1051.639	1104.38	1182.12	957.7674	968.6088	1106.965	1039.237	1099.512	1170.268
1207.25	1238.332	1309.613	1182.167	1237.157	1327.348	1267.867	1279.501	1333.248
1356.787	1488.309	1522.808	1368.102	1447.659	1577.256	1419.003	1466.488	1605.351
1610.132	1655.787	2236.224	1640.834	1662.293	2242.813	1722.738	2201.54	3157.113
3199.358	3208.469	3214.266	3165.116	3241.384	3260.913	3163.888	3180.063	3195.406
3224.162	3228.627	3482.768	3262.477	3265.85	3482.642	3214.39	3321.034	3483.574
<b><i>i54 – p26</i></b>			<b><i>i61 – i66</i></b>			<b><i>i62 – i66</i></b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C -0.128714	1.323137	-0.137472	C -3.150003	-0.652399	-0.681346	C 2.474142	1.082540	-0.401959
C 1.215756	1.165977	-0.098144	C -3.080367	-0.025594	0.440221	C 3.077658	-0.097959	-0.142351
C 1.499489	-0.282228	-0.025967	C -1.594485	-0.132128	0.432019	C 1.974939	-0.965779	0.070795
C 2.700080	-0.866314	-0.049051	C -0.763027	0.843212	-0.080697	C 0.887472	-0.116463	0.400156
C -0.766518	0.003499	-0.024327	C 1.442814	-0.300447	0.120530	C -1.527931	0.348604	0.420046
C -2.172390	-0.203526	0.005301	C 2.853713	-0.276574	0.018450	C -2.866135	0.133226	-0.003620
C -3.363495	-0.357917	0.027782	C 4.055316	-0.274622	-0.064290	C -4.006477	-0.034004	-0.346265
C 0.198328	-0.947414	0.042932	C 0.661968	0.776051	-0.163297	C -0.479174	-0.372132	-0.014571
H -0.673608	2.252478	-0.223010	H -3.679984	-1.064227	-1.521680	H 2.786725	2.109969	-0.562087
H 1.965177	1.928247	-0.254027	H -3.758248	0.417213	1.163894	H 4.139058	-0.325342	-0.111171
H 1.568348	1.548066	1.958234	H -1.165900	-1.012406	0.901750	H 1.886904	-2.011961	-0.202956
H 2.802797	-1.945163	-0.010153	H -1.230984	1.744593	-0.466038	H 1.007808	0.552470	1.245977
H 3.610653	-0.279849	-0.103325	H 0.998449	-1.242112	0.428596	H -1.367242	1.155314	1.131270
H -4.416754	-0.502035	0.050351	H 5.115604	-0.267687	-0.141387	H -5.013323	-0.186906	-0.652094
H 0.048172	-2.013029	0.135610	H 1.165493	1.679632	-0.494677	H -0.646890	-1.161751	-0.742327
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
-580.684	117.0261	149.141	-734.476	60.7401	85.7564	-653.813	81.2519	110.9354
206.3871	261.0125	298.0664	125.305	183.1751	230.8476	135.9565	246.2473	314.7643
344.6315	425.01	527.8592	301.7921	348.8253	464.6196	408.4743	432.3442	495.5799
545.3204	615.8785	663.0721	496.8492	587.8356	612.8095	546.4918	659.9478	663.4775
664.8032	701.0853	715.625	641.1596	678.5815	691.0921	708.2463	715.1266	759.2072
			798.9207	848.6695	851.4516	790.4114	885.7477	897.3574
						907.9853	1005.395	1029.524



1562.989	2131.943	3155.252	3136.638	3192.287	3193.948	3253.667	3262.841	3481.992			
3216.399	3217.738	3237.752	3216.907	3267.898	3483.258	<i>i42 – i44</i>					
3248.26	3263.923	3481.829	<i>i62 – i69</i>			<b>Cartesian coordinates</b>					
<i>i11 – i68</i>			<b>Cartesian coordinates</b>			C	3.267794	-0.404269	-0.000033		
<b>Cartesian coordinates</b>			C	0.950856	0.410481	0.952904	C	1.853292	-0.969160	0.000023	
C	1.053731	1.515136	0.071434	C	1.529358	1.268741	-0.056993	C	0.956576	0.263224	0.000014
C	2.236198	0.932284	0.082614	C	1.940704	0.235116	-0.830033	C	1.635054	1.407196	0.000006
C	2.313838	-0.529160	0.028170	C	1.376725	-0.823833	0.109635	C	-1.661828	0.040450	0.000007
C	1.182966	-1.217822	-0.161945	C	-0.867757	-0.498521	0.491826	C	-3.025692	-0.085056	-0.000004
C	-1.188622	-0.667204	0.395072	C	-2.106533	0.047758	0.035424	C	-4.223738	-0.195667	-0.000015
C	-2.435048	-0.058124	0.109250	C	-3.130793	0.541345	-0.356109	C	-0.459528	0.157811	0.000013
C	-3.496946	0.461871	-0.116960	C	0.002908	-1.216292	-0.351672	H	3.850433	-0.560576	-0.905505
C	-0.086514	-0.504384	-0.381495	H	0.940030	0.542173	2.028667	H	3.850534	-0.560619	0.905366
H	0.667339	2.523215	0.057664	H	1.544337	2.343983	-0.178711	H	1.647635	-1.586043	-0.879129
H	3.159313	1.511704	0.128510	H	2.399697	0.155178	-1.807731	H	1.647684	-1.585985	0.879228
H	3.269676	-1.024932	0.154325	H	2.059738	-1.578622	0.505227	H	1.315898	2.441517	0.000001
H	1.175936	-2.302980	-0.160706	H	-0.846511	-0.723461	1.555931	H	2.918719	0.857918	-0.000001
H	-1.122909	-1.250066	1.309096	H	-4.038599	0.972744	-0.702544	H	-5.282481	-0.293388	-0.000026
H	-4.435348	0.918723	-0.319175	H	-0.231500	-1.500767	-1.370739	<b>Vibrational frequencies</b>			
H	-0.191628	0.028752	-1.326557	<b>Vibrational frequencies</b>			-1767.23	75.7315	78.005		
<b>Vibrational frequencies</b>			-768.243	103.6151	152.5272	138.3293	223.1506	282.5142			
-353.767	92.0358	108.9412	269.3352	325.5673	428.8812	421.5888	448.8435	484.6226			
160.7607	256.5172	333.9277	502.9614	528.8932	585.4124	498.4578	579.0895	590.5147			
403.0922	469.1567	500.7374	668.9093	691.8217	702.34	646.2291	696.9397	697.703			
565.4008	657.5399	666.8391	711.1657	769.9943	842.9502	780.5006	804.0484	851.2295			
707.3072	712.3753	733.8844	896.0148	920.2336	931.0699	892.2457	1005.725	1056.807			
813.0219	861.7426	897.8979	965.9679	1017.865	1036.188	1087.397	1098.826	1235.113			
914.3781	997.5009	1009.13	1060.172	1140.317	1169.057	1260.598	1267.34	1328.951			
1038.6	1070.103	1188.73	1202.877	1225.594	1248.677	1456.875	1496.156	1659.135			
1243.089	1270.217	1296.574	1272.245	1343.787	1463.321	1725.9	2197.339	2375.809			
1411.641	1588.138	1624.478	1558.292	2219.625	3093.985	3063.553	3103.991	3114.142			
1700.058	2207.894	3115.34	3129.824	3197.211	3203.412	3198.561	3234.137	3486.911			
3136.068	3179.067	3190.359	3209.638	3237.733	3485.604	<i>i44 – p16</i>					
3213.773	3271.756	3484.182	<i>i68 – p28</i>			<b>Cartesian coordinates</b>					
<i>i70 – i68</i>			<b>Cartesian coordinates</b>			C	3.151073	-1.020371	0.000290		
<b>Cartesian coordinates</b>			C	0.504017	-1.069362	0.081797	C	1.665817	-1.141816	-0.000375	
C	-0.459080	0.882377	0.764079	C	1.838186	-1.158722	-0.072054	H	3.507568	-0.489125	-0.886197
C	-1.575166	1.163230	0.083178	C	2.411702	0.191724	-0.140595	H	3.624946	-2.010696	0.000177
C	-2.258371	0.065174	-0.602913	C	1.423424	1.098489	-0.028360	H	3.506813	-0.489681	0.887412
C	-1.689620	-1.124032	-0.637731	C	-1.085683	0.906332	-0.052740	H	1.179435	-1.464705	-0.915552
C	1.243243	-0.934294	0.496079	C	-2.280816	0.153044	-0.068481	H	1.178707	-1.465490	0.914138
C	2.168715	-0.118100	-0.197671	C	-3.309528	-0.471379	-0.080112	C	0.850781	0.947026	-0.000042
C	2.964856	0.571809	-0.780908	C	0.152737	0.362442	0.095688	C	1.749824	1.786981	-0.000009
C	0.005935	-0.509594	0.869198	H	-0.215320	-1.871089	0.155868	C	-1.639025	0.231807	0.000011
H	0.131477	1.661184	1.234990	H	2.412891	-2.072744	-0.135592	C	-2.950590	-0.155972	0.000047
H	-1.965965	2.171963	0.014255	H	3.464905	0.406250	-0.260950	C	-4.104155	-0.498702	0.000079
H	-3.225302	0.248552	-1.073076	H	1.505469	2.175610	-0.047097	C	-0.484817	0.590621	-0.000013
H	-1.946863	-2.105003	-1.009346	H	-1.183488	1.984303	-0.140513	H	2.693239	2.281563	0.000005
H	1.544514	-1.955602	0.703462	H	-4.216973	-1.025902	-0.091125	H	-5.124156	-0.799315	0.000098
H	3.662688	1.181265	-1.302292	H	0.308280	0.328165	2.108549	<b>Vibrational frequencies</b>			
H	-0.603612	-1.181786	1.472142	<b>Vibrational frequencies</b>			-569.941	49.9176	67.8027		
<b>Vibrational frequencies</b>			-802.989	111.9245	123.3515	111.9758	156.4978	175.508			
-370.361	68.9066	115.981	181.5188	253.2808	331.0809	205.1872	275.3521	292.2551			
192.4003	264.3507	338.6503	395.9534	446.8238	487.2113	434.7365	468.1595	490.7433			
420.8326	469.6823	537.432	574.4258	623.6082	682.7167	549.8445	552.9445	589.0616			
631.1806	640.6582	678.8359	706.5383	740.4376	745.0981	643.3161	680.7736	690.0314			
701.8399	724.5976	759.0812	783.3455	817.7409	877.1678	692.4452	816.9178	840.1275			
804.1265	865.5863	896.6757	911.5231	954.4349	966.4168	1022.091	1086.966	1177.551			
912.9991	948.1183	989.9062	1004.944	1049.242	1110.192	1220.165	1403.084	1478.007			
1013.542	1055.909	1180.319	1112.127	1188.355	1309.262	1482.966	1496.631	1983.2			
1221.178	1251.097	1371.449	1359.022	1408.481	1557.707	2211.607	2373.028	3024.681			
1433.965	1556.07	1624.278	1624.761	1648.24	2206.787	3090.654	3125.509	3141.634			
1699.624	2201.889	3115.523	3180.169	3223.907	3234.585	3239.451	3451.012	3486.498			

**i63 – i68**

**Cartesian coordinates**

C	-2.100224	-0.625820	-0.540826
C	-2.057748	0.710748	-0.517764
C	-1.087454	1.020610	0.575328
C	-1.154910	-1.033851	0.543776
C	0.974162	-0.060501	-0.490869
C	2.327591	-0.009176	-0.273534
C	3.526414	0.033519	-0.058699
C	-0.019000	-0.043576	0.629125
H	-2.661403	-1.291356	-1.183981
H	-2.576148	1.432221	-1.136199
H	-1.377006	1.553787	1.475657
H	-1.493672	-1.548637	1.437891
H	0.597997	-0.097598	-1.507624
H	4.573667	0.070778	0.120035
H	0.483584	-0.070911	1.594993

**Vibrational frequencies**

-742.323	37.3419	131.4538
198.9021	222.6083	292.6744
397.0237	445.1763	495.9389
513.4285	574.9336	621.9639
672.5618	686.3382	743.1948
777.7646	882.1634	925.094
960.0279	1003.645	1027.306
1094.84	1112.191	1159.214
1186.575	1253.97	1265.179
1301.317	1343.748	1435.956
1566.146	2026.705	3134.613
3182.127	3186.016	3191.744
3206.088	3230.617	3476.411

**i71 – i13**

**Cartesian coordinates**

C	0.172393	-0.940570	0.453970
C	1.560689	-1.151722	0.044553
C	2.236307	-0.022509	-0.276572
C	1.504763	1.177209	0.053785
C	-0.630824	-0.074128	-0.427281
C	-2.062055	-0.040105	-0.202811
C	-3.245079	-0.008680	-0.010780
C	0.149565	1.036129	0.276011
H	-0.272094	-1.397953	1.330017
H	1.987842	-2.147346	0.012685
H	3.257355	-0.011118	-0.634696
H	2.016129	2.099822	0.303487
H	-0.383395	-0.159234	-1.489498
H	-4.295244	0.016878	0.153411
H	-0.425144	1.745205	0.859340

**Vibrational frequencies**

-751.902	143.4879	148.7387
313.4333	401.3838	498.0015
504.4715	518.1802	600.1821
669.2661	697.6141	702.9748
712.5876	741.6587	825.9607
869.0862	929.5964	985.0641
1021.719	1033.035	1060.695
1119.222	1146.427	1180.423
1185.077	1283.035	1315.41
1409.604	1434.027	1458.977
1596.137	2254.55	3062.218
3193.257	3197.537	3209.577
3211.763	3229.227	3487.081

**i13 – i69**

**Cartesian coordinates**

C	-0.503544	-0.214481	1.115235
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C	-0.809016	-1.405564	0.281955
C	-1.512695	-0.853293	-0.694536
C	-1.574758	0.620054	-0.351394
C	0.567846	0.730679	0.525244
C	1.757818	0.090330	-0.031261
C	2.737393	-0.433671	-0.483571
C	-0.410227	1.415277	-0.408561
H	-0.743273	-0.145272	2.172135
H	-0.425516	-2.413462	0.388756
H	-1.890362	-1.279205	-1.619691
H	-2.548384	1.105189	-0.449700
H	0.883709	1.453002	1.285412
H	3.603062	-0.896680	-0.891489
H	-0.396133	2.480444	-0.604089

**Vibrational frequencies**

-939.582	106.1344	152.9807
277.1198	357.5956	380.7923
454.6821	528.2091	584.3391
660.01	698.4563	707.5044
712.9203	788.5782	828.392
889.095	918.922	961.1093
978.8911	1003.985	1059.834
1093.332	1114.946	1129.629
1198.55	1278.895	1305.69
1355.971	1366.649	1400.961
1704.558	2245.214	3061.123
3106.929	3171.834	3183.266
3212.551	3215.468	3484.595

**i66 – p35**

**Cartesian coordinates**

C	-3.948682	-0.797719	0.382826
C	-3.683948	0.134998	-0.345310
C	-1.574675	0.903793	0.125726
C	-0.590699	0.069614	-0.154248
C	1.806052	-0.494055	-0.236378
C	3.184742	-0.221272	-0.018767
C	4.355284	-0.011227	0.156556
C	0.821257	0.362948	0.070766
H	-4.039956	-1.587483	1.090675
H	-3.787139	0.871130	-1.110279
H	-1.586267	1.892774	0.568661
H	-0.827198	-0.904191	-0.583330
H	1.565525	-1.458069	-0.677606
H	5.389361	0.178651	0.314444
H	1.069687	1.324710	0.510412

**Vibrational frequencies**

-419.52	44.1609	59.3313
85.4234	137.6693	155.7331
203.9932	250.8701	336.6561
435.0392	468.0379	563.8328
586.7202	690.6372	692.7225
724.1382	729.1664	762.8397
787.8735	883.6019	917.0836
949.7589	1011.711	1037.329
1148.022	1248.831	1312.143
1332.633	1645.291	1701.613
1958.583	2234.356	3137.318
3173.851	3191.175	3225.477
3399.147	3483.499	3491.046

**i11 – p35**

**Cartesian coordinates**

C	2.651749	1.643216	0.469735
C	2.704561	0.940595	-0.518297
C	1.972341	-1.178794	-0.045688
C	0.681722	-1.416986	0.100712

C	-1.674895	-0.713830	0.119375
C	-2.714912	0.248019	-0.007714
C	-3.608340	1.045618	-0.111042
C	-0.374577	-0.423291	-0.033295
H	2.542295	2.122140	1.414201
H	2.883864	0.654731	-1.530661
H	2.832582	-1.828108	0.050404
H	0.360178	-2.435959	0.337350
H	-1.979632	-1.731324	0.352214
H	-4.392237	1.757818	-0.203410
H	-0.072947	0.593416	-0.262806

**Vibrational frequencies**

-443.75	57.9309	87.589
93.8627	144.2517	159.3794
206.7414	284.6824	331.9246
465.5941	484.9422	571.5307
589.5987	671.9032	682.7086
695.6064	721.5849	758.7239
792.7219	879.4105	893.8965
925.3716	1016.039	1036.408
1166.259	1234.141	1311.121
1328.475	1648.169	1708.122
1950.033	2235.072	3080.166
3167.079	3205.56	3241.174
3397.652	3484.8	3488.736

**i69 – p36**

**Cartesian coordinates**

C	0.532699	0.337095	0.834706
C	1.302075	1.321267	-0.031776
C	2.079092	0.386985	-0.580017
C	1.428148	-0.768604	0.177855
C	-0.648338	-0.379664	0.162470
C	-1.979002	0.060134	-0.073980
C	-3.088790	0.474219	-0.272151
C	0.149552	-1.300484	-0.439992
H	0.497913	0.488827	1.911320
H	1.195734	2.389073	-0.173979
H	2.849562	0.401857	-1.340917
H	2.052039	-1.435463	0.772727
H	-1.124896	-1.377560	1.771713
H	-4.073509	0.834893	-0.447781
H	-0.049460	-2.087312	-1.155770

**Vibrational frequencies**

-876.85	120.0998	161.5871
312.5481	356.1458	405.3731
414.5321	455.7607	533.6387
585.9377	636.7113	685.9633
701.9289	797.3018	833.1826
843.5357	886.4206	925.8982
953.3462	978.5257	988.3443
1008.959	1069.469	1138.28
1164.324	1197.971	1218.945
1222.825	1259.484	1308.024
1569.898	1649.499	2241.729
3129.284	3159.047	3212.154
3231.131	3244.562	3485.052

**i70 – p34**

**Cartesian coordinates**

C	-3.345434	-0.712449	0.598674
C	-3.095313	-0.062285	-0.395319
C	-1.309908	1.326196	-0.035223
C	-0.081139	0.843065	-0.012386
C	1.515909	-1.042370	-0.215609
C	2.681844	-0.264981	0.037839
C	3.679111	0.372507	0.249461

C 0.265866 -0.552764 -0.240251  
H -3.432219 -1.198057 1.542086  
H -3.182471 0.307166 -1.392707  
H -1.685929 2.326104 0.137916  
H 0.750841 1.523417 0.187143  
H 1.676584 -2.100146 -0.396228  
H 4.562593 0.933546 0.437124  
H -0.555008 -1.233536 -0.438452

**Vibrational frequencies**

-444.419 33.3385 51.6402  
101.6033 128.9742 167.0667  
262.154 290.0367 331.9452  
465.6364 500.8198 581.4609  
671.7662 678.5284 702.9095  
712.5728 721.351 765.3174  
782.2178 815.3938 868.2532  
923.5299 960.6481 1019.708  
1140.37 1256.16 1275.74  
1428.237 1642.183 1701.286  
1947.684 2231.709 3100  
3188.061 3213.554 3236.831  
3394.651 3484.051 3487.504

**i62 – i65**

**Cartesian coordinates**

C 2.222150 -0.729202 -0.206075  
C 2.667667 0.494269 0.287236  
C 1.503845 1.166757 -0.087404  
C 0.870196 -0.128680 -0.585196  
C -1.493025 -0.952511 0.113510  
C -2.533594 -0.051866 0.026933  
C -3.446155 0.750367 -0.048671  
C -0.121392 -0.540079 0.426436  
H 2.561214 -1.753599 -0.135144  
H 3.561875 0.798815 0.817030  
H 1.083480 2.144630 0.101448  
H 0.530418 -0.189538 -1.618977  
H -1.715029 -2.002797 -0.074827  
H -4.244061 1.449933 -0.113710  
H 0.203951 -0.501779 1.463566

**Vibrational frequencies**

-628.989 45.9457 124.9687  
158.0014 199.0543 329.6399  
395.59 453.4163 485.6649  
520.4204 579.528 619.3326  
635.0691 653.1449 672.4114  
908.0737 919.4552 936.1857  
959.1507 981.0326 985.8453  
1105.952 1164.131 1168.952  
1190.548 1208.098 1231.651  
1336.526 1348.912 1401.448  
1460.642 2030.932 3117.459  
3125.114 3156.789 3209.186  
3238.924 3253.106 3475.959

**i65 – p40**

**Cartesian coordinates**

C -2.263218 0.463659 0.080636  
C -2.325140 -0.966992 0.081990  
C -0.924858 -1.077301 0.022295  
C -0.813664 0.400761 0.026024  
C 1.556798 1.119589 0.085483  
C 2.161463 -0.151953 0.030227  
C 2.712148 -1.223867 -0.019328  
C 0.199502 1.355311 0.075337  
H -2.986237 1.265385 0.114850  
H -3.134124 -1.682903 0.113749

H -0.212818 -1.886224 -0.009149  
H -0.792217 0.596280 -2.699126  
H 2.230547 1.968416 0.133441  
H 3.197825 -2.168637 -0.062938  
H -0.121172 2.392439 0.113191

**Vibrational frequencies**

-251.311 79.9729 120.2007  
144.3201 182.3074 185.7975  
234.265 336.6013 376.6628  
467.8987 513.4806 544.7047  
594.5919 629.1613 643.0115  
660.0194 701.0523 742.626  
789.5647 816.1838 928.8187  
951.5466 963.5158 1026.429  
1112.909 1159.758 1203.93  
1302.002 1369.438 1389.432  
1481.425 1524.501 2173.57  
3173.453 3192.761 3236.834  
3255.768 3280.482 3482.383

**i70 – i65**

**Cartesian coordinates**

C 1.896015 0.418161 1.129347  
C 2.667658 -0.000459 0.102642  
C 1.815448 -0.906592 -0.578298  
C 0.486444 -0.563279 -0.218322  
C -1.453723 0.972048 -0.432274  
C -2.414029 0.049109 0.066039  
C -3.235165 -0.723808 0.485299  
C -0.136468 0.713344 -0.536951  
H 1.960599 1.159659 1.919836  
H 3.695946 0.268157 -0.121769  
H 2.097062 -1.844732 -1.044459  
H -0.234237 -1.367430 -0.058463  
H -1.826989 1.943650 -0.736743  
H -3.963062 -1.403317 0.857412  
H 0.513596 1.492870 -0.920710

**Vibrational frequencies**

-678.379 70.4377 122.9451  
187.6293 241.4997 343.9502  
368.1529 464.4627 548.3138  
646.1109 649.772 682.8035  
709.5002 746.9417 767.2908  
786.5917 875.7955 911.8948  
935.0167 976.2897 1004.429  
1060.386 1069.817 1181.849  
1250.765 1261.362 1374.553  
1419.195 1463.501 1504.116  
1655.972 2223.078 3122.875  
3164.133 3182.846 3190.819  
3200.999 3201.513 3486.034

**i65 – i67**

**Cartesian coordinates**

C -1.760176 1.180778 0.665520  
C -2.656143 0.518571 -0.098709  
C -1.943329 -0.654043 -0.462456  
C -0.574748 -0.326172 -0.292723  
C 1.727885 -1.000885 0.320894  
C 2.320052 0.244406 -0.023351  
C 2.830457 1.294956 -0.309481  
C 0.414436 -1.268254 0.192191  
H -1.694284 2.151680 1.146470  
H -3.668696 0.808726 -0.362938  
H -2.335365 -1.657895 -0.589172  
H -0.187686 0.538766 -0.819719  
H 2.393889 -1.757360 0.722800

H 3.283515 2.222822 -0.563124  
H 0.058021 -2.242881 0.514374

**Vibrational frequencies**

-652.619 56.7409 107.0208  
178.5968 243.5599 336.8997  
395.4854 460.2447 568.6546  
633.5431 676.8702 678.2165  
706.2225 708.2733 759.0178  
790.4988 809.1141 904.1171  
910.3557 958.3866 1006.579  
1060.503 1138.725 1170.352  
1243.16 1270.795 1332.515  
1412.585 1469.47 1516.898  
1651.762 2226.166 3165.524  
3169.387 3188.227 3189.369  
3193.313 3202.604 3485.694

**i61 – p37**

**Cartesian coordinates**

C 1.414004 1.040761 -0.502409  
C 2.498247 0.478592 -0.013887  
C 1.271866 -0.242110 0.109763  
C 0.599959 -1.422911 0.214717  
C -1.773084 -0.697337 -0.248175  
C -1.686807 0.690587 0.028614  
C -1.684221 1.869970 0.277101  
C -0.783445 -1.611803 -0.113952  
H 0.926049 1.864151 -0.993024  
H 3.556080 0.527329 0.181868  
H 1.151740 -2.278400 0.587387  
H -2.756004 -1.048320 -0.545454  
H -1.686994 2.902093 0.531340  
H -1.076570 -2.648267 -0.259920  
H 0.746583 0.046917 1.987164

**Vibrational frequencies**

-807.203 84.7755 140.7205  
172.4804 200.3308 284.243  
332.065 361.0209 489.6688  
509.2612 533.9775 596.7434  
628.0494 692.8826 728.5778  
736.947 752.2589 819.5116  
857.6941 933.3963 936.6238  
981.439 988.345 1007.31  
1103.188 1140.867 1268.381  
1386.632 1454.125 1552.64  
1635.545 1764.724 2202.984  
3161.865 3184.082 3195.429  
3279.793 3326.698 3484.714

**i64 – p37**

**Cartesian coordinates**

C 2.930696 0.454826 -0.115169  
C 2.954843 -0.858443 -0.147841  
C 1.687774 -0.235491 0.081341  
C 0.328781 -0.240743 0.022309  
C -1.787350 1.044598 -0.017413  
C -2.644356 -0.087422 -0.040032  
C -3.377823 -1.041608 -0.059329  
C -0.438150 0.968361 0.016494  
H 3.468041 1.385477 -0.176731  
H 3.521301 -1.767728 -0.253971  
H -0.186996 -1.193971 0.034405  
H -2.266224 2.017388 -0.033308  
H -4.028735 -1.881784 -0.074102  
H 0.117498 1.902280 0.037005  
H 1.448634 -0.486118 2.024542

**Vibrational frequencies**

-797.886	74.6613	97.1106	146.8507	224.3057	262.54	233.2137	284.1313	343.3281
160.0098	191.2242	267.9566	349.5732	394.8228	518.7872	413.4073	508.5492	581.9218
333.1472	357.0678	472.2777	560.5497	603.947	636.1411	672.0894	678.585	708.0453
508.0596	545.9452	560.5762	651.1869	701.1697	716.2084	708.6939	725.5509	764.1553
643.7418	678.6304	707.3831	793.2974	826.3314	861.2073	774.5564	806.5269	906.7954
726.7835	762.7353	846.6288	872.4578	927.7766	980.6314	955.4498	957.1707	1011.44
864.9357	933.2331	946.8316	987.3641	1077.753	1151.334	1121.528	1254.016	1282.399
969.9573	991.377	1040.267	1266.045	1280.729	1411.133	1420.309	1638.487	1690.693
1126.048	1155.227	1254.845	1441.42	1480.157	1611.132	1958.101	2231.001	3147.047
1327.921	1451.731	1577.186	1724.181	2203.077	3146.786	3174.819	3194.723	3207.979
1628.775	1760.729	2217.664	3159.85	3176.523	3180.74	3401.572	3485.916	3493.405
3167.582	3195.284	3202.366	3195.286	3327.782	3484.013			
3277.98	3319.747	3487.622						

**i61 – i67****Cartesian coordinates**

C	2.598015	0.656425	-0.756135
C	2.499570	0.405438	0.501386
C	1.045614	0.118550	0.344321
C	0.555183	-1.152822	0.113457
C	-1.941693	-0.789498	-0.133586
C	-2.047593	0.616963	-0.031114
C	-2.196654	1.809988	0.051228
C	-0.805559	-1.539883	-0.072923
H	3.133328	0.918177	-1.650888
H	3.138871	0.394278	1.379108
H	0.360172	0.948886	0.460714
H	1.285161	-1.956272	0.059335
H	-2.882245	-1.310136	-0.283813
H	-2.318640	2.863807	0.120943
H	-0.957948	-2.609711	-0.185202

**Vibrational frequencies**

-719.161	52.0081	122.561	134.008	139.5371	185.0601	317.4484	407.8456	483.7623
143.5158	213.473	225.209	296.2385	339.3478	392.1173	522.8199	593.0159	650.4315
344.1414	359.5881	496.9256	450.9728	537.3397	570.5434	685.5736	725.3557	743.4346
539.3445	596.0274	613.4252	579.0436	671.0304	682.9611	856.9664	869.0389	918.733
646.1905	698.6086	732.2533	684.4212	711.7607	712.4992	987.4408	1007.617	1017.187
766.3225	839.4771	848.3606	786.7231	898.794	950.2014	1060.876	1064.836	1108.25
938.6681	944.6996	994.4331	994.075	1030.543	1031.221	1150.05	1265.549	1302.639
1043.053	1096.358	1187.586	1146.57	1250.067	1298.361	1328.417	1419.695	1708.269
1258.602	1283.722	1321.388	1339.556	1435.252	1660.505	1749.124	2240.143	3098.923
1442.296	1478.115	1601.699	1713.131	2122.213	2232.604	3107.776	3167.154	3170.887
1724.532	2194.306	3156.915	3174.187	3188.908	3193.418	3265.873	3316.988	3486.655
3158.46	3171.831	3187.389	3196.545	3472.111	3484.927			
3216.503	3321.969	3484.225						

**i61 – i70****Cartesian coordinates**

C	-2.011122	-0.952454	0.869009
C	-1.116553	-1.245168	-0.006664
C	-1.453577	0.016171	-0.722893
C	-0.857733	1.258404	-0.566865
C	1.403828	0.923537	0.529983
C	1.793675	-0.346798	0.041869
C	2.219344	-1.394661	-0.372678
C	0.287941	1.626937	0.208923
H	-2.557498	-1.091701	1.783726
H	-0.380235	-2.016142	-0.196553
H	-2.269444	-0.042057	-1.436552
H	-1.389904	2.090709	-1.020188
H	2.138875	1.408788	1.165197
H	2.586709	-2.319250	-0.747609
H	0.276686	2.653839	0.567879

**Vibrational frequencies**

-705.22	56.4615	127.7127	77.7564	131.5827	148.4996	286.4812	312.0615	360.5863
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**i67 – p31****Cartesian coordinates**

C	-3.336999	1.214869	0.035526
C	-2.681677	0.192040	-0.006450
C	-1.585244	-0.729921	0.003868
C	-0.305936	-0.323639	-0.000106
C	2.101615	-0.891838	0.012799
C	2.563570	0.453462	-0.005521
C	2.973186	1.583446	-0.020924
C	0.806308	-1.250103	0.015252
H	-4.028058	2.023714	0.051047
H	-4.050060	-1.075319	-0.277908
H	-1.823113	-1.788189	0.015499
H	-0.077912	0.737876	-0.015947
H	2.866610	-1.661223	0.025410
H	3.335771	2.583020	-0.034651
H	0.567827	-2.309775	0.029888

**Vibrational frequencies**

-854.723	16.5316	82.9641	134.008	139.5371	185.0601	317.4484	407.8456	483.7623
296.2385	339.3478	392.1173	450.9728	537.3397	570.5434	685.5736	725.3557	743.4346
579.0436	671.0304	682.9611	684.4212	711.7607	712.4992	987.4408	1007.617	1017.187
786.7231	898.794	950.2014	994.075	1030.543	1031.221	1150.05	1265.549	1302.639
1146.57	1250.067	1298.361	1339.556	1435.252	1660.505	1749.124	2240.143	3098.923
1713.131	2122.213	2232.604	3174.187	3188.908	3193.418	3265.873	3316.988	3486.655
3196.545	3472.111	3484.927						

**i67 – p34****Cartesian coordinates**

C	-3.162637	1.246549	0.430514
C	-3.211819	0.358286	-0.393152
C	-1.471246	-1.104340	-0.060479
C	-0.268274	-0.561320	-0.049116
C	2.197897	-0.797622	0.131257
C	2.481485	0.587759	-0.032614
C	2.742644	1.753230	-0.169600
C	0.962927	-1.325019	0.124949
H	-2.996293	1.949635	1.212126
H	-3.544824	-0.219424	-1.225546
H	-1.809255	-2.127051	0.064304
H	-0.166517	0.515217	-0.177740
H	3.054476	-1.449350	0.269234
H	2.973244	2.783889	-0.291940
H	0.863304	-2.398059	0.259016

**Vibrational frequencies**

-418.276	31.8182	63.7133	77.7564	131.5827	148.4996	286.4812	312.0615	360.5863
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**i61 – i64****Cartesian coordinates**

C	3.209258	-0.524277	-0.248809
C	3.074979	0.744520	-0.095541
C	1.785715	0.001561	-0.418812
C	0.779270	-0.222014	0.619019
C	-1.584672	0.437756	0.247491
C	-2.945535	0.155440	-0.074623
C	-4.097061	-0.057636	-0.343578
C	-0.627279	-0.494447	0.295945
H	3.812208	-1.415657	-0.217942
H	3.485125	1.707327	0.157518
H	1.386626	0.084555	-1.429999
H	1.113786	-0.318530	1.649302
H	-1.341987	1.474861	0.462703
H	-5.115423	-0.251967	-0.579028
H	-0.908380	-1.526001	0.070888

**Vibrational frequencies**

-231.863	52.5867	89.8694	134.008	139.5371	185.0601	317.4484	407.8456	483.7623
175.2258	266.694	305.1562	296.2385	339.3478	392.1173	522.8199	593.0159	650.4315
450.9728	537.3397	570.5434	450.9728	537.3397	570.5434	685.5736	725.3557	743.4346
579.0436	671.0304	682.9611	579.0436	671.0304	682.9611	856.9664	869.0389	918.733
684.4212	711.7607	712.4992	684.4212	711.7607	712.4992	987.4408	1007.617	1017.187
786.7231	898.794	950.2014	786.7231	898.794	950.2014	1060.876	1064.836	1108.25
994.075	1030.543	1031.221	994.075	1030.543	1031.221	1150.05	1265.549	1302.639
1146.57	1250.067	1298.361	1146.57	1250.067	1298.361	1328.417	1419.695	1708.269
1339.556	1435.252	1660.505	1339.556	1435.252	1660.505	1749.124	2240.143	3098.923
1713.131	2122.213	2232.604	1713.131	2122.213	2232.604	3107.776	3167.154	3170.887
3174.187	3188.908	3193.418	3174.187	3188.908	3193.418	3265.873	3316.988	3486.655
3196.545	3472.111	3484.927						

**i5 – p5****Cartesian coordinates**

C	1.521286	1.735946	0.219330
C	2.387642	0.798164	-0.180532
C	2.196951	-0.640260	-0.164823
C	1.046272	-1.352904	-0.017601
C	-1.408031	-0.417347	-0.034454
C	-2.689900	0.063215	-0.048535
C	-3.815111	0.489317	-0.059632
C	-0.269713	-0.821461	-0.015978
H	1.789587	2.784684	0.166187
H	0.543914	1.495448	0.617711
H	3.362838	1.120888	-0.535761
H	3.101871	-1.230697	-0.271813
H	1.105040	-2.434076	-0.095345
H	-4.810217	0.863849	-0.069737
H	1.090594	-1.728111	2.002106

**Vibrational frequencies**

-734.302	67.5157	72.3511	77.7564	131.5827	148.4996	286.4812	312.0615	360.5863
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435.5908	488.5347	547.6835	570.5049	636.0338	694.4562	780.5454	858.6677	860.4646			
555.8242	644.71	663.8787	698.3797	746.4102	786.9316	923.9367	973.5905	997.4944			
695.336	699.5698	803.6768	859.6402	935.6815	998.9137	1046.487	1137.763	1175.163			
825.5585	951.0134	975.5295	1148.555	1196.183	1231.144	1234.535	1281.417	1324.795			
996.8839	1037.617	1104.689	1273.001	1278.904	1295.826	1421.755	1479.331	1581.619			
1173.036	1267.489	1350.408	1431.857	1527.824	1601.432	1725.4	2202.27	3164.86			
1440.455	1475.233	1580.618	1870.092	2167.687	2277.48	3170.989	3172.368	3188.105			
1690.27	2195.8	2368.162	3160.772	3172.579	3174.581	3199.919	3316.699	3484.664			
3159.336	3171.208	3176.763	3181.285	3277.233	3487.153						
3191.101	3266.941	3486.244									
<b><i>i10 – p5</i></b>			<b><i>i64 – i66</i></b>			<b><i>i64 – i67</i></b>					
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>					
C	3.174701	-1.187874	-0.179090	C	-3.341851	-0.132662	-0.847471	C	2.969222	0.610996	0.759402
C	1.973678	-0.593436	-0.122170	C	-3.216090	0.086063	0.414420	C	2.773310	0.542204	-0.510331
C	1.806418	0.841292	-0.029018	C	-1.824122	-0.439291	0.366809	C	1.716765	-0.483287	-0.290121
C	0.622658	1.480057	0.035244	C	-0.705592	0.351123	0.182866	C	0.372148	-0.190973	-0.167403
C	-1.719954	0.295593	0.015755	C	1.726057	0.597999	-0.030208	C	-1.956021	-0.960408	0.146781
C	-2.945030	-0.315665	0.008645	C	3.037593	0.071258	-0.080614	C	-2.554884	0.319110	0.043659
C	-4.021115	-0.854242	0.003166	C	4.160627	-0.361661	-0.128057	C	-3.075057	1.401873	-0.041743
C	-0.636063	0.830587	0.022912	C	0.613729	-0.169246	0.125769	C	-0.616842	-1.186345	0.051644
H	3.269285	-2.261494	-0.286177	H	-3.881035	-0.097489	-1.777753	H	3.433899	1.020666	1.638773
H	3.694577	-1.587412	1.996075	H	-3.807053	0.476875	1.237181	H	3.154981	0.995298	-1.420125
H	4.092140	-0.607778	-0.199733	H	-1.684292	-1.504048	0.536132	H	2.027124	-1.525378	-0.276067
H	1.070438	-1.197140	-0.134527	H	-0.841641	1.423190	0.060999	H	0.051917	0.845419	-0.232140
H	2.711468	1.442274	-0.009827	H	1.625097	1.675790	-0.126589	H	-2.626899	-1.796878	0.310469
H	0.602671	2.563127	0.102931	H	5.149169	-0.750380	-0.171567	H	-3.537583	2.356031	-0.118285
H	-4.972340	-1.329444	-0.001405	H	0.737652	-1.245437	0.220522	H	-0.275280	-2.214184	0.146041
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>					
			-733.111	73.45	100.8973	-726.537	78.195	106.6546			
-435.553	63.6984	101.338	142.4047	230.5965	243.4463	313.7755	398.2135	447.2826			
130.1541	181.0039	187.9938	274.2328	400.3183	432.1549	519.8768	606.8821	637.1708			
260.5998	296.4553	312.3643	469.6645	567.9395	620.9164	649.8013	709.87	725.1509			
415.2959	466.3222	540.5519	631.0834	639.115	701.2992	758.3276	844.2528	859.7757			
555.0721	633.2619	676.4384	817.2007	852.6392	872.3269	929.619	953.6005	996.6798			
714.4709	718.5112	776.3761	931.6872	1004.15	1017.802	1066.725	1159.304	1184.767			
817.0082	945.9742	968.0122	1074.636	1174.166	1187.799	1209.99	1260.088	1300.027			
1001.501	1047.901	1136.054	1246.06	1275.389	1320.034	1420.289	1502.838	1554.981			
1202.213	1266.147	1314.961	1349.241	1505.893	1581.378	1724.483	2204.076	3156.063			
1393.725	1473.374	1642.723	1724.203	2199.162	3162.868	3166.034	3171.995	3184.185			
1674.185	2197.831	2372.579	3165.955	3168.44	3168.599	3201.383	3318.523	3484.554			
3155.979	3170.921	3179.745	3175.229	3315.568	3482.001						
3194.858	3253.077	3485.155									
<b><i>i6 – i49</i></b>			<b><i>i64 – i11</i></b>			<b><i>i64 – i70</i></b>					
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>					
C	-3.989446	-0.708288	-0.106563	C	2.765014	-0.991869	-0.655248	C	2.951450	0.047849	0.829426
C	-2.955668	0.202047	0.054296	C	-2.478239	-0.736040	0.572840	C	2.711639	0.164566	-0.429373
C	-1.517715	-0.116727	0.036200	C	2.092083	0.649857	0.188039	C	1.627591	-0.850030	-0.308696
C	-0.495363	0.817059	-0.078220	C	0.791387	1.069038	-0.039218	C	0.280686	-0.555182	-0.175351
C	2.029212	0.159078	-0.026389	C	-1.627145	0.690996	-0.142052	C	-1.583253	1.058350	-0.033471
C	3.350658	-0.181563	-0.002156	C	-2.774125	-0.130019	-0.034581	C	-2.611901	0.090804	0.082019
C	4.517661	-0.483488	0.020499	C	-3.761711	-0.813771	0.053665	C	-3.494328	-0.722287	0.182646
C	0.851383	0.461473	-0.042377	C	-0.360181	0.243982	0.066176	C	-0.260860	0.758640	-0.150559
H	-5.017079	-0.376099	-0.063599	H	3.046092	-1.650157	-1.458376	H	3.440792	0.326633	1.745852
H	-3.796596	-1.769494	-0.209082	H	2.452412	-1.251366	1.528441	H	3.064339	0.746612	-1.275767
H	-3.188792	1.264684	0.064639	H	2.881790	1.392007	0.150205	H	1.914833	-1.892213	-0.395227
H	-2.285071	0.033179	1.168220	H	0.641281	2.106423	-0.326900	H	-0.412862	-1.384989	-0.076628
H	-1.265317	-1.173714	0.048131	H	-1.794227	1.733279	-0.401409	H	-1.894120	2.097632	-0.026791
H	-0.738778	1.870822	-0.180590	H	-4.631543	-1.420050	0.131656	H	-4.273750	-1.439912	0.270951
H	5.547305	-0.746923	0.040547	H	-0.217175	-0.803171	0.318658	H	0.434626	1.589975	-0.222239
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>					
			-737.353	86.8911	113.6525	-732.034	60.2848	115.2008			
-1878.75	63.4957	71.4335	139.8885	199.6019	229.8662	341.309	356.0207	520.9361			
174.9627	191.5133	240.0233	345.3551	359.7432	482.7412	532.2185	618.9117	632.3363			
296.205	411.3692	420.2747	516.844	573.7465	629.1923	652.0944	720.2132	750.2703			
503.9489	523.8127	549.1238	637.9184	686.9516	694.0901	761.1127	813.793	855.7661			





1719.32	2200.44	2397.259	491.7163	503.3421	515.3134
2988.205	3044.368	3077.969	558.3789	569.7263	675.8781
3084.104	3096.089	3127.141	706.5117	712.1329	789.761
3153.09	3242.774	3487.162	870.8748	896.399	943.4659

H	-0.398989	1.502832	1.961801
H	5.697066	-0.594665	-0.112039
H	-1.684730	-1.803225	1.053603
H	-0.128440	-1.679744	0.215390
H	-1.616195	-1.982243	-0.699760

**i17 - i18**

**Cartesian coordinates**

C	1.400411	1.664842	0.222514
C	2.010502	0.483132	0.160146
C	1.386368	-0.738691	0.708342
C	0.424927	-1.543792	-0.121947
C	-1.983790	-0.393338	-0.108006
C	-3.211205	0.219739	-0.082469
C	-4.286444	0.758250	-0.058042
C	-0.906292	-0.932364	-0.131055
C	3.362758	0.297430	-0.484650
H	1.858254	2.556537	-0.194790
H	0.426533	1.773880	0.686429
H	1.508863	-0.990525	1.756398
H	0.781077	-1.614635	-1.157133
H	0.340992	-2.565207	0.262136
H	-5.236673	1.234566	-0.035800
H	3.308803	-0.439858	-1.292639
H	4.087423	-0.081036	0.243424
H	3.741320	1.235024	-0.897018

**Vibrational frequencies**

-153.728	39.4073	66.4388
136.4848	169.8042	219.6044
226.956	256.7065	330.5486
395.0492	437.25	518.6121
543.7133	551.6805	589.3006
679.2632	710.3497	711.7543
737.401	794.3414	935.833
964.0337	1002.077	1024.965
1077.729	1086.271	1164.84
1221.229	1271.472	1311.257
1376.902	1415.807	1453.737
1459.253	1487.159	1500.889
1724.862	2201.388	2400.35
3035.316	3036.809	3090.273
3097.451	3128.994	3149.161
3196.619	3240.405	3486.431

**i17 - p9**

**Cartesian coordinates**

C	3.338596	-1.331231	-0.013801
C	2.536374	-0.257908	0.034117
C	1.097669	-0.444343	-0.047612
C	0.183016	0.561178	-0.030345
C	-2.407661	0.120410	0.009983
C	-3.758185	-0.104334	0.044948
C	-4.944598	-0.302080	0.078041
C	-1.216489	0.316067	-0.019201
C	3.081728	1.138173	0.161792
H	4.416901	-1.235775	0.045765
H	2.933537	-2.332679	-0.112347
H	0.738925	-1.462777	-0.163793
H	0.491020	1.581740	0.174381
H	0.294952	1.242647	-1.942367
H	-5.993192	-0.475614	0.108343
H	2.715859	1.620788	1.073252
H	2.767739	1.755528	-0.685963
H	4.171560	1.130555	0.195197

**Vibrational frequencies**

-769.884	63.323	63.9795
138.6305	171.4405	190.2945
200.6404	254.3264	293.7768
373.6458	385.711	438.0585

994.0324	1001.329	1043.115
1071.065	1214.89	1291.698
1309.043	1351.136	1415.572
1451.293	1483.787	1502.55
1607.599	1683.504	2198.369
2375.183	3045.314	3107.779
3149.117	3156.615	3187.275
3194.087	3248.218	3483.207

**i17 - p22**

**Cartesian coordinates**

C	3.636627	0.252592	0.030828
C	2.386999	-0.069115	0.258805
C	1.377257	-0.872453	0.592300
C	0.400452	-1.419207	-0.423038
C	-2.031205	-0.370806	-0.113649
C	-3.277251	0.178664	0.057464
C	-4.368379	0.661439	0.207731
C	-0.937641	-0.852376	-0.267828
C	1.316888	1.927740	-0.226681
H	3.955965	1.267621	-0.167676
H	4.395186	-0.524767	0.034027
H	1.134735	-1.012816	1.641778
H	0.763758	-1.218163	-1.434546
H	0.331573	-2.508328	-0.317759
H	-5.333026	1.088220	0.340512
H	0.262209	1.713392	-0.104091
H	1.675519	2.063500	-1.240112
H	1.791597	2.512468	0.552277

**Vibrational frequencies**

-554.249	24.5635	45.7609
76.4453	103.4015	141.4572
194.4453	223.4528	250.6783
323.7801	341.7918	427.1024
460.3633	533.9633	548.8048
552.7707	567.7968	591.3645
695.0189	699.2614	744.4172
814.7103	848.6205	888.3836

912.6323	1015.96	1025.847
1129.262	1170.051	1222.307
1305.688	1380.735	1417.287
1429.9	1461.963	1478.899
1939.608	2200.385	2400.461
3042.252	3096.052	3098.586
3145.988	3171.972	3239.184
3265.412	3266.64	3487.113

**i32 - p11**

**Cartesian coordinates**

C	-3.874533	-0.195599	-0.129005
C	-2.765071	0.547724	-0.132047
C	-1.407771	0.033684	-0.007765
C	-0.377072	0.929210	0.006110
C	2.168415	0.278217	-0.029399
C	3.497305	-0.051003	-0.059467
C	4.664702	-0.341338	-0.087234
C	0.995429	0.565579	-0.001385
C	-1.188741	-1.439007	0.148226
H	-4.851244	0.262234	-0.228800
H	-3.846743	-1.275061	-0.028232
H	-2.857208	1.626497	-0.232964
H	-0.589507	1.978570	-0.177202

**Vibrational frequencies**

-737.001	62.2127	66.3303
134.4818	168.1344	202.1962
214.4999	275.2348	289.1622
327.8714	378.7828	416.6903
423.4099	505.7779	547.417
581.4976	600.6579	678.7045
700.3712	701.0547	797.317
832.4761	930.3285	962.8803
994.5975	1035.039	1057.287
1090.976	1218.889	1243.418
1341.378	1384.413	1431.861
1458.986	1488.568	1495.302
1601.98	1688.078	2198.365
2372.362	3050.985	3111.594
3159.647	3162.132	3170.938
3176.096	3253.944	3486.45

**i32 - p49**

**Cartesian coordinates**

C	3.849551	0.212550	-0.458281
C	2.821039	-0.405615	0.116566
C	1.422850	0.055871	0.090963
C	0.402400	-1.067191	0.131096
C	-2.145390	-0.323806	-0.023613
C	-3.462713	0.053034	-0.105132
C	-4.616813	0.382797	-0.177112
C	-0.990472	-0.656998	0.047617
C	1.081401	1.351115	0.091662
H	4.854171	-0.186760	-0.383562
H	3.719795	1.127963	-1.026365
H	2.999649	-1.348398	0.631836
H	0.614682	-1.772034	-0.681893
H	0.548329	-1.631969	1.061330
H	-5.637745	0.672823	-0.241599
H	1.840186	2.124523	0.095112
H	0.843260	1.741111	2.249305
H	0.046565	1.662195	0.013240

**Vibrational frequencies**

-465.579	36.873	63.1452
101.9341	151.6054	171.1726
205.0346	223.5393	265.4478
334.5551	355.567	392.4776
438.3664	544.4609	549.6457
591.2811	671.428	688.2164
692.1541	758.2838	805.9029
853.3473	948.4479	955.4738
965.4922	969.5646	1039.969
1097.242	1178.105	1211.874
1244.567	1341.639	1372.336
1430.375	1462.939	1463.555
1673.749	1720.046	2206.568
2410.176	3033.769	3067.408
3147.143	3164.386	3172.46
3252.668	3265.953	3486.603

**i33 – p59**

**Cartesian coordinates**

C	3.377755	-1.196077	-0.695429
C	2.501875	-0.364946	-0.200045
C	1.438030	0.363772	0.082608
C	0.472196	-0.105437	1.156760
C	-2.037407	-0.196245	0.268790
C	-3.328093	-0.240636	-0.195901
C	-4.458753	-0.279599	-0.603509
C	-0.905449	-0.158916	0.678522
C	1.215956	1.727049	-0.506199
H	4.380386	-1.283763	-0.295777
H	3.104410	-1.828208	-1.535227
H	3.572307	0.406160	1.295130
H	0.770722	-1.090414	1.523415
H	0.523606	0.584479	2.009437
H	-5.458029	-0.315691	-0.965097
H	1.965137	1.958290	-1.262553
H	1.262456	2.491531	0.277618
H	0.222341	1.783821	-0.960525

**Vibrational frequencies**

-720.432	30.8804	67.8585
96.602	138.7941	172.546
190.4486	204.2365	286.5832
333.6413	336.6281	430.9546
471.8744	540.9532	546.6842
557.8128	596.8997	660.0129
680.445	691.5998	752.3048
784.1971	910.2183	915.3127
1009.748	1024.6	1060.792
1170.214	1191.095	1231.989
1301.202	1356.135	1417.863
1456.849	1473.218	1492.668
1507.947	2022.446	2203.454
2405.225	3034.295	3040.31
3105.097	3111.373	3146.867
3159.576	3239.705	3483.869

**i29 – p51**

**Cartesian coordinates**

C	-2.549717	-1.836145	0.123121
C	-1.532839	-1.300015	-0.502840
C	-0.849726	0.836084	-0.059807
C	-1.345003	1.463425	-1.169059
C	1.699662	0.144439	0.007948
C	3.022884	-0.209939	0.051423
C	4.184374	-0.521312	0.089200
C	0.534966	0.457832	-0.035537
C	-1.519303	0.985878	1.290579
H	-2.918242	-2.828880	-0.138234
H	-3.068008	-1.327953	0.932951
H	-0.913342	-1.642184	-1.321553
H	-0.780551	1.502151	-2.091810
H	-2.350454	1.867206	-1.164170
H	5.210761	-0.796373	0.123252
H	-1.141070	1.884927	1.784815
H	-1.311372	0.131699	1.935150
H	-2.599514	1.087926	1.169429

**Vibrational frequencies**

-482.292	45.7181	78.1429
92.8613	159.1697	186.5174
229.4672	238.9461	254.4415
303.4	354.5996	360.3563
452.302	502.0723	551.2209
597.4219	627.5523	643.5607
687.1561	699.7707	826.3801
843.1268	903.3373	917.5534
941.0671	1017.169	1051.298

1087.839	1104.746	1321.851	105.94	138.3622	155.2573
1395.738	1406.429	1420.257	171.3319	222.5627	267.8382
1490.66	1505.172	1549.305	320.2132	326.844	390.7242
1667.271	2196.708	2379.5	492.0627	531.5439	551.8951
3054.701	3093.342	3128.801	566.6046	612.8492	685.8238
3154.535	3162.406	3179.166	692.2614	698.3171	852.5593
3232.662	3266.098	3487.208	900.9394	910.7525	937.8164

**i29 – p6**

**Cartesian coordinates**

C	1.422803	2.110091	0.072421
C	1.908303	0.910315	-0.222942
C	1.104758	-0.324963	-0.412116
C	1.616478	-1.350105	-1.178869
C	-1.519060	-0.104772	-0.173057
C	-2.878481	0.017843	-0.045583
C	-4.070915	0.127860	0.068907
C	-0.322964	-0.214819	-0.283819
H	2.080546	2.964558	0.175801
H	0.359665	2.274307	0.214452
H	2.977342	0.773696	-0.364054
H	2.671675	-1.372693	-1.424155
H	0.998467	-2.184369	-1.482942
H	-5.124479	0.227219	0.171598
C	1.378040	-1.058268	1.687421
H	0.833839	-1.995078	1.659378
H	0.911230	-0.238191	2.219909
H	2.457952	-1.128541	1.755844

**Vibrational frequencies**

-569.366	72.7754	83.7582
122.2116	152.6512	179.8223
198.436	225.4943	282.9286
308.6707	432.8885	457.4253
525.9268	538.8643	557.643
579.7266	604.5286	606.7096
646.8738	697.0288	704.8017
711.2763	801.4881	887.2603
945.3737	966.5718	1039.734
1045.23	1100.078	1310.224
1335.513	1391.147	1420.386
1422.91	1454.159	1513.881
1723.118	2202.112	2388.17
3094.628	3160.92	3164.542
3177.202	3257.067	3260.137
3268.68	3270.959	3489.193

**i14 – p17**

**Cartesian coordinates**

C	2.555989	-1.132169	-1.075573
C	1.793237	-0.760971	-0.077363
C	0.754609	1.250619	-0.395677
C	1.256013	2.098595	0.545984
C	-1.691245	0.285483	-0.212558
C	-2.960934	-0.220166	-0.111703
C	-4.074953	-0.665594	-0.021141
C	-0.572798	0.730971	-0.300189
C	1.448747	-1.280085	1.255489
H	3.129176	-2.059944	-1.029167
H	2.650197	-0.549835	-1.987933
H	1.203555	1.223099	-1.383352
H	0.741941	2.261096	1.485304
H	2.213229	2.581069	0.394625
H	-5.059783	-1.058339	0.057263
H	1.721530	-0.557081	2.029845
H	1.975453	-2.220663	1.456764
H	0.372708	-1.459494	1.333042

**Vibrational frequencies**

-424.244	20.1892	56.8776
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105.94	138.3622	155.2573
171.3319	222.5627	267.8382
320.2132	326.844	390.7242
492.0627	531.5439	551.8951
566.6046	612.8492	685.8238
692.2614	698.3171	852.5593
900.9394	910.7525	937.8164
977.2813	1035.905	1060.918
1115.554	1193.992	1270.9
1395.369	1427.162	1430.087
1463.8	1480.805	1555.234
1763.044	2196.36	2378.707
3021.562	3088.1	3096.702
3113.357	3164.39	3176.712
3181.764	3267.94	3486.671

**i14 – p42**

**Cartesian coordinates**

C	-1.228905	-1.792708	-0.158016
C	-1.706911	-0.558329	-0.014273
C	-0.788411	0.621814	0.042830
C	-1.210472	1.890252	-0.229466
C	1.814224	0.159861	0.026847
C	3.163607	-0.080249	0.010312
C	4.347248	-0.293348	-0.005283
C	0.627178	0.370044	0.044286
C	-3.179805	-0.278420	0.087967
H	-1.900215	-2.642422	-0.207461
H	-0.166291	-1.991110	-0.231053
H	-2.261892	2.123862	-0.330403
H	-0.500015	2.703643	-0.292762
H	5.393846	-0.480884	-0.018939
H	-3.403110	0.310863	0.982965
H	-3.742148	-1.210942	0.140085
H	-3.540806	0.284178	-0.778664
H	-0.905887	0.669294	1.905009

**Vibrational frequencies**

-1042.39	54.5017	71.2028
119.0103	220.222	226.1677
279.2346	323.4486	359.7076
387.3068	444.8591	446.0736
475.9961	521.7292	540.8361
590.695	612.0162	659.8192
678.7772	686.8994	714.1325
773.2121	833.9675	899.9494
954.7694	971.4607	1032.003
1071.991	1076.594	1225.746
1372.445	1412.63	1418.622
1450.916	1490.418	1504.636
1571.16	1730.23	2200.929
2389.135	3044.051	3106.121
3148.12	3167.767	3184.438
3258.897	3286.171	3482.86

**i14 – i74**

**Cartesian coordinates**

C	2.977188	-0.299225	0.594409
C	1.772016	-0.495175	0.051970
C	0.832445	0.629232	-0.187014
C	1.286698	2.045335	-0.158569
C	-1.750316	0.167319	0.007797
C	-3.093233	-0.073159	0.107793
C	-4.275491	-0.284685	0.196533



H 3.459923 -1.077233 0.274837  
H 2.665966 -1.589581 -1.221768  
H 2.286867 -2.399746 0.305746

**Vibrational frequencies**

-984.655 130.5352 139.8347  
197.0195 217.2463 323.6124  
367.6076 441.4972 463.3079  
472.3093 488.9548 554.7163  
579.3956 613.7069 670.7381  
696.1634 702.5921 728.8786  
803.6344 899.0011 923.9986  
928.4007 1001.305 1012.56  
1025.348 1075.279 1127.445  
1177.344 1198.117 1272.555  
1302.159 1341.919 1425.337  
1447.65 1497.335 1504.823  
1525.873 1624.432 1652.81  
2245.462 3053.752 3126.647  
3150.305 3192.301 3205.26  
3210.209 3229.231 3484.11

**i96 – p1**

**Cartesian coordinates**

C -0.023853 -0.756537 0.706345  
C 1.353013 -0.437543 0.763257  
C 1.753666 0.872603 0.399895  
C 0.855619 1.728164 -0.207478  
C -0.920481 0.109014 0.092649  
C -2.302314 -0.251182 -0.027285  
C -3.460229 -0.552188 -0.130523  
C -0.472742 1.349983 -0.391443  
C 2.128877 -1.599644 -0.905905  
H -0.376652 -1.704265 1.094860  
H 1.990215 -1.016726 1.421445  
H 2.782612 1.176934 0.553323  
H 1.179464 2.711013 -0.531251  
H -4.485898 -0.816776 -0.222439  
H -1.177445 2.019597 -0.868613  
H 3.194011 -1.395549 -0.860858  
H 1.591601 -1.136273 -1.725508  
H 1.832766 -2.613970 -0.658034

**Vibrational frequencies**

-576.012 90.7075 120.2586  
143.9141 160.8463 194.6872  
366.7872 398.9726 470.5076  
539.6141 550.7112 569.9253  
588.5261 648.5182 675.1869  
680.6475 710.2265 779.0543  
787.7206 868.0092 906.2574  
907.8993 989.3116 1001.093  
1013.166 1051.449 1094.691  
1181.033 1193.297 1220.262  
1307.09 1345.35 1425.64  
1429.463 1460.1 1519.307  
1600.718 1628.495 2243.717  
3086.926 3188.498 3197.596  
3210.682 3216.141 3226.029  
3244.555 3254.422 3485.041

**i40 – i103**

**Cartesian coordinates**

C -0.424515 1.184777 -0.037348  
C 1.018811 1.182012 -0.035701  
C 1.747064 -0.014530 -0.058984  
C 0.985113 -1.224554 0.008079  
C -1.145275 -0.016044 -0.033747  
C -2.558371 -0.015573 -0.013373  
C -3.764467 -0.023802 -0.004137  
C -0.376783 -1.238899 0.022708  
C 3.245519 -0.032997 -0.004760  
H -0.935235 2.134718 -0.150485  
H 0.332946 1.428492 1.145005  
H 1.517322 2.137377 -0.172602  
H 1.519920 -2.169227 0.035420  
H -4.827194 -0.031032 0.000757  
H -0.911971 -2.180142 0.059836  
H 3.667648 0.943591 -0.255030  
H 3.656996 -0.760759 -0.711144  
H 3.616987 -0.305363 0.991816

**Vibrational frequencies**

-2091.01 82.2635 105.8846  
141.3434 204.8408 310.5317  
327.5568 401.6481 433.1602  
483.534 538.571 539.7581  
647.3061 666.0891 692.289  
708.0053 776.9464 788.0233  
798.7656 974.897 986.109  
1007.916 1034.443 1043.882  
1088.851 1129.387 1211.858  
1225.695 1246.253 1305.251  
1338.142 1402.325 1426.415  
1459.138 1483.656 1484.657  
1503.397 1526.815 1678.325  
2193.724 3017.172 3076.711  
3120.706 3181.568 3185.245  
3210.538 3219.946 3482.637

**Vibrational frequencies**

-2754.09 81.8055 142.3957  
180.0272 206.4468 308.8207  
320.2965 391.5077 402.2313  
481.0076 538.2846 589.3002  
627.4117 642.1769 677.4016  
703.759 733.5608 766.4398  
774.1296 927.1064 945.8361  
970.8549 981.1055 1055.558  
1100.444 1170.647 1193.314  
1218.967 1248.196 1286.974

1334.047 1416.611 1431.015  
1442.716 1487.362 1501.641  
1525.137 1616.695 2184.999  
2211.926 3013.187 3081.164  
3125.532 3185.636 3206.923  
3223.319 3226.202 3483.623

**i106 – p3**

**Cartesian coordinates**

C -0.416273 1.207560 -0.017281  
C 0.962946 1.206402 -0.004428  
C 1.692187 0.000000 0.066788  
C 0.962945 -1.206401 -0.004428  
C -1.128391 0.000001 -0.009108  
C -2.557140 0.000001 -0.016116  
C -3.758603 -0.000002 -0.020585  
C -0.416274 -1.207558 -0.017281  
C 3.186292 -0.000002 -0.159127  
H -0.961817 2.143357 -0.040899  
H 1.502152 2.147551 -0.014920  
H 1.873473 0.000004 1.904270  
H 1.502151 -2.147550 -0.014916  
H -4.821903 -0.000004 -0.024196  
H -0.961819 -2.143355 -0.040898  
H 3.653220 0.884390 0.277283  
H 3.395199 0.000004 -1.233594  
H 3.653213 -0.884405 0.277268

**Vibrational frequencies**

-964.803 94.5824 143.5977  
175.6476 232.8464 326.9628  
398.4055 406.269 437.6301  
439.153 524.4393 542.7126  
557.2672 656.3216 657.1077  
700.5554 703.9229 738.9405  
829.5372 847.588 847.7442  
984.5876 994.4844 1016.292  
1033.882 1071.06 1152.849  
1204.792 1237.73 1242.686  
1301.854 1341.219 1427.922  
1455.701 1497.748 1499.731  
1540.574 1598.88 1663.612  
2234.951 3053.651 3126.657  
3151.824 3197.02 3197.248  
3219.766 3221.606 3482.5

**i106 – p1**

**Cartesian coordinates**

C 0.339633 1.211856 -0.281943  
C -1.003444 1.214236 -0.585846  
C -1.729191 -0.000012 -0.640679  
C -1.003467 -1.214267 -0.585795  
C 1.029426 -0.000022 -0.100146  
C 2.419152 -0.000009 0.222717  
C 3.589590 0.000031 0.497485  
C 0.339612 -1.211896 -0.281882  
C -2.695236 0.000058 1.350577  
H 0.883686 2.145080 -0.195698  
H -1.521769 2.153989 -0.737674  
H -2.721748 -0.000014 -1.075359  
H -1.521782 -2.154025 -0.737629  
H 4.625304 0.000066 0.737388  
H 0.883641 -2.145128 -0.195581  
H -3.268672 0.920951 1.333414  
H -1.806515 0.000113 1.970765  
H -3.268598 -0.920885 1.333444

**Vibrational frequencies**

-555.15 69.5751 140.7768  
154.7031 165.2979 172.2326



731.3796	770.0826	851.3611
907.5869	942.8158	963.7346
971.3236	1014.801	1063.554
1135.711	1193.925	1210.574
1331.99	1365.057	1423.978
1452.69	1489.849	1496.09
1603.979	1658.422	1725.407
2243.193	3044.706	3103.66
3143.608	3162.132	3242.377
3253.661	3255.887	3484.076

**i85 - p63**

**Cartesian coordinates**

C	0.239685	-1.194545	-0.075209
C	-1.177840	-0.658279	-0.099444
C	-1.105117	0.823031	-0.024129
C	-2.119173	1.693452	0.006209
C	1.082714	0.059968	-0.009124
C	2.501458	0.017116	0.021898
C	3.700728	-0.056053	0.047078
C	0.317703	1.162661	0.019308
C	-2.282221	-1.405311	-0.163841
H	0.473556	-1.784063	-0.967400
H	0.418802	-1.836183	0.793758
H	-1.937156	2.760063	0.065844
H	-3.152627	1.368317	-0.024185
H	4.762397	-0.111646	0.071260
H	0.691960	2.176865	0.071340
H	-3.269491	-0.959537	-0.203446
H	-2.709398	-1.781108	2.100306
H	-2.225665	-2.484942	-0.243948

**Vibrational frequencies**

-336.914	46.5164	111.4243
131.9213	143.7328	181.4897
294.2268	300.5225	389.3574
395.8414	497.4741	530.0111
564.4589	616.4877	622.7581
670.5294	695.6744	705.911
772.2376	776.4827	904.2254
908.2507	922.3427	928.3531
938.4482	968.4043	976.3789
1161.397	1182.638	1213.154
1262.646	1311.263	1348.966
1438.193	1453.993	1463.809
1676.525	1696.013	1732.501
2239.412	3056.645	3094.118
3161.868	3165.994	3235.184
3250.535	3254.804	3483.445

**i86 - p61**

**Cartesian coordinates**

C	0.195490	-1.094782	-0.023490
C	-1.090344	-0.659149	0.041375
C	-1.042102	0.827629	0.008744
C	-2.086879	1.656247	-0.050266
C	1.105355	0.056793	-0.015827
C	2.522852	-0.047987	-0.023656
C	3.719048	-0.158828	-0.032168
C	0.373357	1.197512	0.006012
C	-2.339052	-1.465840	-0.132611
H	0.523103	-2.124896	-0.060043
H	-1.155546	-0.685986	2.102058
H	-1.950162	2.730705	-0.100096
H	-3.105228	1.282822	-0.050766
H	4.778257	-0.251559	-0.037944
H	0.753472	2.208391	0.026770
H	-3.126270	-1.142771	0.552178
H	-2.144032	-2.523093	0.053082

H -2.719945 -1.363173 -1.153915

**Vibrational frequencies**

-688.704	108.034	136.6865
160.5645	204.966	259.3732
292.0604	315.5778	386.6993
403.3933	437.384	509.486
564.1729	617.0707	628.7653
661.6573	663.3825	717.4644
725.9355	763.8185	837.4688
865.5012	949.4422	968.8875
970.8784	1017.331	1059.081
1138.527	1189.407	1214.457
1339.268	1359.465	1422.81
1450.978	1492.623	1498.425
1566.846	1644.571	1737.279
2242.719	3049.598	3116.935
3144.634	3163.064	3239.124
3254.473	3257.727	3483.829

**i86 - p26**

**Cartesian coordinates**

C	0.270843	-0.804379	0.933279
C	-1.051167	-0.467793	0.874552
C	-1.155418	0.801245	0.115219
C	-2.246383	1.558247	-0.035225
C	1.031456	0.135960	0.114858
C	2.433056	0.047738	-0.109105
C	3.617826	-0.043818	-0.286460
C	0.189699	1.086069	-0.378711
C	-1.885207	-1.851807	-0.921496
H	0.707216	-1.642168	1.457731
H	-1.842272	-0.862849	1.494972
H	-2.212121	2.493652	-0.582569
H	-3.199249	1.262165	0.389817
H	4.665996	-0.122072	-0.446642
H	0.458431	1.917420	-1.013868
H	-2.900125	-1.478417	-0.980536
H	-1.730997	-2.837859	-0.502180
H	-1.175105	-1.498648	-1.658183

**Vibrational frequencies**

-424.425	79.6476	126.4141
131.4716	136.9067	151.3365
249.324	338.9559	419.9633
451.8848	491.5245	527.3439
544.7735	622.9255	644.5928
689.1228	693.8459	709.613
717.8229	737.8371	803.9369
844.1138	893.495	929.5727
942.9907	962.6729	972.3775
1087.476	1182.58	1224.791
1337.31	1348.943	1411.857
1422.787	1425.082	1474.432
1604.37	1731.317	2241.819
3102.869	3162.16	3243.263
3252.784	3254.319	3261.958
3276.248	3278.056	3485.233

**i86 - i88**

**Cartesian coordinates**

C	0.253355	-1.119751	-0.006044
C	-1.067889	-0.697182	0.060272

C	-1.044281	0.800160	0.091046
C	-2.169264	1.660653	-0.108819
C	1.105100	0.015073	-0.027725
C	2.530589	-0.037889	-0.027997
C	3.730389	-0.089128	-0.036905
C	0.343163	1.167103	0.028588
C	-2.318090	-1.511137	-0.063250
H	0.582569	-2.148927	-0.000708
H	-1.136259	0.149457	1.173455
H	-2.024799	2.730013	-0.174633
H	-3.175140	1.265456	-0.161740
H	4.792543	-0.133614	-0.044395
H	0.716404	2.180056	0.057673
H	-3.102616	-1.160383	0.611873
H	-2.120826	-2.559266	0.166697
H	-2.710310	-1.450207	-1.083224

**Vibrational frequencies**

-1247.21	114.5909	136.7622
153.8585	230.6234	250.5709
306.3645	323.3283	375.9641
473.1284	518.9944	536.1751
560.5761	614.3525	653.5893
665.9922	702.764	705.0421
759.3191	800.2131	829.084
971.105	988.0961	1015.496
1065.253	1124.685	1159.724
1193.062	1206.326	1323.557
1365.645	1424.589	1432.353
1482.404	1493.072	1497.435
1527.903	1589.486	2047.594
2247.996	3049.078	3114.848
3140.608	3179.154	3245.927
3257.574	3286.652	3484.912

**i88 - i90**

**Cartesian coordinates**

C	0.015465	-1.104240	0.097437
C	1.250487	-0.603734	-0.112060
C	1.125778	0.848276	-0.473267
C	1.153692	1.735734	0.731909
C	-0.990366	-0.078850	-0.141911
C	-2.385158	-0.246828	0.026070
C	-3.570395	-0.404440	0.165500
C	-0.346960	1.076086	-0.540319
C	2.570062	-1.276496	0.053557
H	-0.215326	-2.109023	0.428126
H	1.737524	1.196969	-1.306291
H	1.261388	2.806990	0.622481
H	0.944633	1.315537	1.706102
H	-4.617495	-0.540174	0.288483
H	-0.811661	1.993317	-0.867930
H	3.195809	-0.726423	0.764978
H	3.117057	-1.311353	-0.894510
H	2.452449	-2.298896	0.417066

**Vibrational frequencies**

-489	111.1732	128.5618
144.8463	204.4002	270.3258
330.0793	396.6963	484.7497
509.1225	532.4003	581.6916
605.4191	643.5732	650.9284
663.5532	727.4191	788.9346
837.384	880.046	942.7023
989.0695	1011.387	1034
1076.085	1097.965	1152.869
1198.332	1226.801	1251.884
1329.823	1375.548	1423.628





3217.706	3250.085	3482.62	915.8495	955.6712	970.3304	<b>Vibrational frequencies</b>		
						-2536.93	109.4618	137.3168
<b>i96 – i99</b>			974.6172	1007.811	1033.85	145.6565	186.893	290.5966
<b>Cartesian coordinates</b>			1176.517	1211.068	1237.153	332.4661	429.7851	446.9659
C 0.093618 -0.975682 -0.441893			1315.696	1351.422	1373.157	512.077	524.9258	555.0842
C -1.387774 -0.781224 -0.494793			1440.119	1451.718	1459.772	590.504	598.7879	646.0346
C -1.854616 0.674843 -0.309964			1643.277	1668.965	1739.149	676.075	699.7281	794.7068
C -0.867155 1.677428 0.032170			2238.27	3012.205	3083.171	811.605	880.2622	934.3476
C 0.931474 0.012694 -0.070080			3161.867	3192.105	3200.277	942.4979	998.4996	1018.054
C 2.341629 -0.218471 0.029781			3220.261	3252.281	3486.85	1058.904	1137.095	1154.98
C 3.527143 -0.387221 0.125010						1217.98	1244.741	1302.264
C 0.434344 1.362930 0.198367						1343.746	1381.812	1411.713
C -2.131525 -1.214653 0.766977						1426.198	1481.974	1495.143
H 0.487790 -1.955418 -0.688393						1529.288	1634.497	2193.747
H -1.798954 -1.252654 -1.389905						2223.031	3045.446	3108.05
H -2.693569 0.982272 -0.931151						3145.23	3205.134	3208.536
H -1.206767 2.694058 0.198143						3222.97	3235.32	3482.28
H 4.575347 -0.543856 0.208137								
H 1.154765 2.117924 0.488370								
H -2.468806 0.226280 0.771750								
H -1.535928 -1.364825 1.663106								
H -3.036712 -1.807645 0.666498								
<b>Vibrational frequencies</b>								
-2037.59	103.1251	115.5009						
155.1915	267.3439	348.2402						
431.9098	462.6545	480.9137						
530.6646	592.1467	609.0693						
641.634	672.8229	711.4344						
729.6931	778.5016	852.2776						
865.8946	897.4518	928.0391						
939.2543	980.9754	991.0038						
1056.61	1068.314	1145.72						
1189.137	1197.009	1262.635						
1313.143	1332.864	1350.422						
1378.604	1417.969	1456.804						
1579.478	1692.917	1813.297						
2241.512	3093.766	3123.265						
3148.701	3197.07	3207.471						
3225.13	3244.036	3486.321						
<b>i99 – p62</b>								
<b>Cartesian coordinates</b>								
C 0.012847 -0.949611 -0.044163								
C 1.432448 -0.599329 0.013229								
C 1.773337 0.836974 -0.332099								
C 0.691707 1.804097 0.053904								
C -0.945728 0.000375 0.002318								
C -2.331638 -0.343679 -0.039819								
C -3.503860 -0.604316 -0.075170								
C -0.578308 1.412073 0.169395								
C 2.387547 -1.564690 0.058664								
H -0.258561 -1.998579 -0.084161								
H 1.380537 -0.168717 1.885620								
H 2.731018 1.117995 0.109663								
H 1.904656 0.896873 -1.423625								
H 0.956305 2.848685 0.175450								
H -4.539796 -0.841752 -0.107262								
H -1.367465 2.118131 0.398192								
H 1.212288 -2.609937 0.165304								
H 3.441913 -1.314056 0.043269								
<b>Vibrational frequencies</b>								
-874.602	115.5272	141.1957						
149.941	286.266	356.8106						
399.3461	419.0582	464.427						
475.3979	530.9931	543.2691						
559.5888	611.5029	633.2996						
665.5518	684.4467	719.7839						
769.395	860.5069	872.5247						
899.3444	944.8496	971.5546						
981.6046	1006.651	1033.51						
1175.346	1206.549	1220.368						
1307.808	1333.39	1362.053						
1437.856	1446.162	1467.6						
1589.07	1629.337	1728.048						
2238.092	3000.474	3116.787						
3159.851	3200.035	3203.877						
3223.974	3256.238	3485.087						
<b>i95 – p62</b>								
<b>Cartesian coordinates</b>								
C -0.018306 -0.918165 -0.018183								
C -1.420367 -0.536694 -0.083794								
C -1.761017 0.925426 0.122810								
C -0.598295 1.863373 -0.024415								
C 0.973089 -0.001329 -0.007095								
C 2.344884 -0.397535 0.027045								
C 3.506500 -0.703213 0.055968								
C 0.661808 1.434976 -0.064643								
C -2.372054 -1.459537 -0.292508								
H 0.223200 -1.975471 -0.020131								
H -2.167476 1.048902 1.137230								
H -2.569960 1.221061 -0.552268								
H -0.814808 2.925768 -0.061976								
H 4.532434 -0.981256 0.082619								
H 1.489425 2.129891 -0.141853								
H -3.416445 -1.185958 -0.395042								
H -3.051329 -1.918155 2.065318								
H -2.122497 -2.508597 -0.405017								
<b>Vibrational frequencies</b>								
-326.4	51.0468	101.2508						
117.7436	144.0862	159.9946						
274.0468	376.0694	400.7913						
432.4242	514.695	548.291						
554.3863	601.7052	665.4283						
684.8104	710.0879	727.2932						
765.9044	861.2522	908.0017						
<b>i93 – i95</b>								
<b>Cartesian coordinates</b>								
C 0.091955 -0.903789 0.038070								
C 1.393121 -0.521594 0.008952								
C 1.741702 0.873967 0.008941								
C 0.624212 1.886049 -0.020754								
C -1.005410 0.075116 0.002784								
C -2.348439 -0.385861 0.001383								
C -3.477497 -0.805434 0.002188								
C -0.714011 1.412325 -0.061437								
C 2.512486 -1.521897 -0.042674								
H -0.167080 -1.955715 0.054833								
H 2.754563 1.212622 -0.160825								
H 1.211612 1.530112 1.038122								
H 0.862968 2.917444 -0.240829								
H -4.476213 -1.169186 0.000311								
H -1.519385 2.133586 -0.137909								
H 3.222032 -1.352867 0.772857								
H 3.066586 -1.426165 -0.981875								
H 2.136201 -2.543122 0.030602								
<b>i96 – i95</b>								
<b>Cartesian coordinates</b>								
C 0.039745 -0.891420 0.057408								
C 1.409444 -0.505749 0.120950								
C 1.704862 0.975450 0.062882								
C 0.601083 1.879153 -0.062344								
C -0.990371 0.012017 0.013583								
C -2.342696 -0.417785 0.000234								
C -3.498367 -0.757520 -0.013517								
C -0.681496 1.450600 -0.061880								
C 2.525077 -1.476370 -0.141934								
H -0.187111 -1.952901 0.045625								
H 1.595672 0.213160 1.147149								
H 2.732001 1.287736 -0.063713								
H 0.815606 2.937481 -0.163632								
H -4.515903 -1.064384 -0.026733								
H -1.502653 2.150524 -0.146597								
H 3.450665 -1.160518 0.347570								
H 2.731825 -1.546573 -1.216321								
H 2.276219 -2.474792 0.224361								
<b>Vibrational frequencies</b>								
-2779.92	113.1316	139.6301						
162.1792	182.9639	306.3297						
325.6907	407.3901	442.4281						
495.4593	536.7635	548.0749						
592.1565	611.8824	674.1142						
687.561	704.6131	768.9415						



H	2.375767	0.560542	1.779323
H	-5.373657	-0.416232	-0.260372
H	0.811060	2.458139	-0.134632
H	1.138682	1.527168	-1.612917
H	2.407389	1.743045	-0.390562

**Vibrational frequencies**

-590.072	77.3313	80.3947
193.3155	218.1815	231.0319
280.4906	329.7225	342.4378
443.7569	472.5371	491.3627
534.406	564.055	575.376
589.3491	648.4456	687.7279
694.3481	712.8032	781.4265
856.981	929.1813	964.1136
985.416	1070.58	1081.168
1139.774	1269.922	1297.855
1310.811	1411.762	1425.247
1455.746	1500.301	1510.269
1552.334	2204.75	2404.283
3064.237	3146.339	3151.751
3171.651	3181.055	3203.495
3266.943	3307.631	3488.077

**i93 - p2**

**Cartesian coordinates**

C	0.071018	-0.897912	0.039214
C	1.407949	-0.497528	-0.016053
C	1.693214	0.857127	-0.096300
C	0.663611	1.815472	-0.067132
C	-0.969403	0.036507	-0.014265
C	-2.331877	-0.406795	-0.000364
C	-3.472837	-0.780226	0.012092
C	-0.673410	1.394983	-0.094376
C	2.506136	-1.527857	0.013797
H	-0.173690	-1.952608	0.104254
H	2.724623	1.188977	-0.146852
H	0.776081	2.332197	1.693737
H	0.896367	2.854375	-0.269961
H	-4.483587	-1.110160	0.024190
H	-1.475368	2.120704	-0.141297
H	3.481621	-1.072182	-0.164720
H	2.345659	-2.297389	-0.745622
H	2.541889	-2.026539	0.986600

**Vibrational frequencies**

-953.563	110.3443	130.9869
141.0807	206.4423	290.1281
339.5051	369.7694	417.5262
472.9983	516.2084	536.2535
557.0067	599.4887	670.8844
699.4633	703.2014	735.3059
853.6926	903.6072	920.9736
929.3979	1011.782	1026.357
1057.715	1073.544	1109.688
1174.137	1197.535	1276.513
1306.551	1340.742	1426.622
1450.943	1493.652	1505.301
1523.678	1634.298	1652.506
2245.909	3050.483	3117.773
3137.153	3191.33	3202.058
3205.782	3228.214	3484.993

**i95 - p2**

**Cartesian coordinates**

C	0.046051	-0.887911	-0.022735
C	1.373692	-0.495859	-0.051911
C	1.668134	0.882879	-0.032202
C	0.633860	1.827768	-0.085432
C	-0.991546	0.054665	-0.012959
C	-2.353221	-0.380346	0.020017
C	-3.496383	-0.748043	0.050689
C	-0.685592	1.420646	-0.055032
C	2.491704	-1.498974	-0.042370
H	-0.205488	-1.942790	-0.014391
H	2.692966	1.205614	-0.183481
H	2.154077	0.995183	1.813364
H	0.874422	2.883433	-0.127859
H	-4.508382	-1.073148	0.078653
H	-1.489241	2.146446	-0.073628
H	3.021934	-1.463629	0.915051
H	3.220344	-1.285816	-0.828960
H	2.119174	-2.514244	-0.187143

**Vibrational frequencies**

-820.997	125.9235	133.9904
140.5449	199.333	294.0968
331.5732	369.6567	410.1643
462.1031	477.134	533.2581
556.3067	604.0583	667.5063
701.5879	722.0205	730.8019
825.1793	908.1189	927.1103
971.3792	1007.335	1019.575
1026.417	1069.247	1115.935
1182.417	1197.895	1278.125
1307.061	1344.436	1415.109
1459.317	1490.357	1508.537
1521.666	1622.282	1662.876
2238.111	3046.209	3111.677
3143.281	3191.643	3198.764
3209.856	3228.536	3484.883

**i99 - i95**

**Cartesian coordinates**

C	-0.017883	-0.930845	0.026877
C	-1.399147	-0.553587	-0.053880
C	-1.760093	0.887160	0.239382
C	-0.634986	1.835968	-0.062246
C	0.979102	0.008105	-0.008396
C	2.348920	-0.372286	0.029515
C	3.513929	-0.673242	0.063576
C	0.633983	1.420274	-0.138642
C	-2.498103	-1.538064	-0.018876
H	0.238778	-1.984915	0.052238
H	-1.845684	-0.934548	-1.136451
H	-2.665551	1.169258	-0.308646
H	-2.028794	0.962702	1.306853
H	-0.871604	2.889932	-0.159438
H	4.541697	-0.942574	0.096064
H	1.439142	2.125592	-0.309085
H	-2.283186	-2.597901	-0.042083
H	-3.519125	-1.188449	0.036683

**Vibrational frequencies**

-1893.75	107.5109	134.3815
144.4578	281.2424	329.3739
410.6628	417.7258	446.7809
491.8269	513.2004	551.1604
596.8492	608.3638	618.5223
671.7198	710.4784	755.8707
856.0302	876.0107	942.9849
953.0531	981.3543	993.6757
1023.66	1152.792	1161.766

1207.806	1243.927	1277.391
1312.848	1370.559	1414.603
1435.839	1448.956	1480.365
1563.759	1703.25	2208.166
2241.867	2962.47	3060.586
3177.817	3190.485	3193.28
3216.26	3300.395	3486.74

**i92 - p62**

**Cartesian coordinates**

C	-0.026988	-0.938631	0.087552
C	-1.448931	-0.614013	-0.010338
C	-1.828365	0.825001	0.255939
C	-0.740231	1.805694	-0.076066
C	0.923423	0.026381	-0.031870
C	2.310283	-0.303742	-0.032852
C	3.485336	-0.555930	-0.033256
C	0.535381	1.431754	-0.187673
C	-2.351158	-1.552484	-0.307993
H	0.024262	-1.085862	2.327933
H	0.264861	-1.982776	0.100596
H	-2.752999	1.077832	-0.269589
H	-2.052487	0.929815	1.328694
H	-1.013294	2.850481	-0.178713
H	4.523524	-0.785674	-0.032416
H	1.317261	2.153703	-0.390442
H	-2.061753	-2.589622	-0.438159
H	-3.401866	-1.312079	-0.428566

**Vibrational frequencies**

-490.329	98.6023	119.9241
146.1305	186.2216	246.316
300.0253	377.9369	407.5484
427.5067	515.7125	554.3431
557.3049	609.2912	661.0581
683.7191	718.6564	721.8179
770.5335	868.3028	904.2931
926.8322	953.7999	969.4299
982.4674	1008.909	1033.198
1178.187	1209.114	1227.346
1307.738	1347.607	1368.77
1439.175	1450.469	1465.19
1582.999	1704.71	1728.058
2230.473	3002.958	3096.299
3160.099	3195.942	3201.282
3220.182	3249.051	3484.119

**i92 - p8**

**Cartesian coordinates**

C	-0.025503	-0.958092	0.362475
C	-1.450513	-0.621457	-0.008689
C	-1.801354	0.800400	0.012781
C	-0.842138	1.749232	-0.099909
C	0.969516	0.127882	0.014822
C	2.345125	-0.232671	-0.036421
C	3.497036	-0.576319	-0.068043
C	0.559324	1.398734	-0.170277
C	-2.347330	-1.556387	-0.328334
H	0.024837	-1.103049	1.451910
H	0.277403	-1.906347	-0.086727
H	-2.850114	1.069166	-0.052733
H	-2.107086	0.951825	2.184677
H	-1.118462	2.794956	-0.168587
H	4.519309	-0.867099	-0.100899
H	1.287439	2.174653	-0.374778
H	-2.076549	-2.604401	-0.396178
H	-3.381756	-1.297635	-0.527115

**Vibrational frequencies**

-547.531	88.2193	129.8122
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644.1613	675.2751	689.0683
708.8668	774.7234	833.4756
960.9241	967.2357	1039.845
1049.421	1063.184	1126.399
1180.596	1244.753	1315.788
1369.725	1401.113	1431.512
1479.199	1495.324	1505.582
1512.15	2176.574	2301.326
3055.823	3125.367	3128.294
3148.547	3160.574	3205.338
3217.694	3262.542	3487.227

**i16 – p24**

**Cartesian coordinates**

C	-2.929029	0.304304	-0.931581
C	-1.930893	-0.100447	-0.131256
C	-0.798329	-1.070674	-0.188747
C	-1.681838	-0.903909	1.071966
C	1.749250	-0.382909	-0.140454
C	3.073641	-0.027746	-0.117083
C	4.235040	0.285249	-0.095650
C	0.581443	-0.682605	-0.155395
C	-0.897213	1.943378	0.461055
H	-2.770476	0.434583	-1.996101
H	-3.877968	0.624492	-0.515005
H	-0.991078	-1.960042	-0.782303
H	-1.201883	-0.449823	1.929536
H	-2.368451	-1.712149	1.300601
H	5.261975	0.559652	-0.076809
H	-0.170891	1.635183	1.203288
H	-1.783025	2.458695	0.810801
H	-0.510635	2.221565	-0.511133

**Vibrational frequencies**

-480.666	62.5593	67.9827
107.5803	172.5291	190.6576
224.2591	250.0881	301.7623
344.0295	440.2564	485.0236
502.0729	531.3928	548.1846
564.4048	586.8566	673.3856
692.4625	700.5638	749.8015
853.0985	871.9041	893.1656
937.5578	1001.594	1051.299
1081.533	1104.674	1130.379
1222.987	1360.046	1415.165
1425.255	1450.273	1483.16
1699.133	2203.51	2398.063
3107.863	3146.569	3150.754
3157.355	3240.704	3245.842
3278.371	3281.778	3488.503

**i31 – p60**

**Cartesian coordinates**

C	2.661932	-1.270771	-0.817693
C	1.811018	-0.680284	0.016782
C	0.857114	0.457488	0.112281
C	1.620274	-0.090159	1.345599
C	-1.751636	0.035777	-0.001270
C	-3.105556	-0.171059	-0.065598
C	-4.293520	-0.351624	-0.122627
C	-0.558240	0.198138	0.058986
C	1.289658	1.791758	-0.473165
H	2.511618	-1.221353	-1.890440
H	3.477700	-1.879900	-0.444167
H	0.528262	-2.186645	0.226791
H	1.030388	-0.623485	2.080998
H	2.413305	0.534668	1.744957
H	-5.343042	-0.512922	-0.175182

H	0.784505	2.614464	0.038339
H	1.042028	1.841744	-1.535819
H	2.368976	1.917847	-0.365247

**Vibrational frequencies**

-820.056	74.6589	81.9389
178.5057	207.1743	225.9952
242.6337	289.3149	319.0042
368.6932	446.4323	478.4552
490.7766	508.4058	551.471
571.1339	589.0306	662.0513
678.7621	710.6752	765.1793
849.9684	910.6462	932.3162
970.2407	1013.718	1058.346
1080.962	1111.065	1132.567
1234.422	1328.177	1419.067
1440.351	1473.73	1492.109
1508.975	1774.547	2201.875
2395.652	3051.704	3131.697
3139.096	3142.145	3155.107
3238.502	3250.194	3485.36

**i31 – i34**

**Cartesian coordinates**

C	2.845907	-0.989108	-0.828085
C	1.704512	-1.026207	-0.022604
C	0.778710	0.479924	0.235004
C	1.549797	-0.281997	1.261732
C	-1.803073	0.068276	0.020266
C	-3.147609	-0.150292	-0.098748
C	-4.331982	-0.343382	-0.203929
C	-0.612070	0.266466	0.130874
C	1.342459	1.739435	-0.370344
H	2.891184	-1.564003	-1.743769
H	3.684418	-0.343940	-0.592818
H	0.965696	-1.794210	-0.217914
H	0.976777	-0.769172	2.043958
H	2.445596	0.212864	1.628305
H	-5.377092	-0.512755	-0.299485
H	1.039867	2.607889	0.223163
H	0.980815	1.880097	-1.390626
H	2.432828	1.704542	-0.395814

**Vibrational frequencies**

-584.34	73.0477	84.3017
125.5178	179.1415	221.128
238.0727	297.3019	344.2902
435.637	444.2038	485.348
503.5378	553.1018	589.2808
604.1542	668.7134	691.5744
711.0875	864.291	908.3294
916.8044	1006.657	1018.587
1055.618	1099.983	1160.623
1173.914	1258.593	1291.718
1371.88	1407.739	1417.136
1475.887	1488.219	1501.353
1504.103	2181.078	2317.664
3048.296	3122.071	3125.947
3150.819	3162.142	3196.606
3212.978	3264.597	3485.597

**i74 – p42**

**Cartesian coordinates**

C	-1.198797	-1.837713	0.083658
C	-1.686302	-0.599130	-0.009917
C	-0.780957	0.573523	-0.090578
C	-1.224081	1.842555	-0.184152
C	1.820468	0.148430	-0.028650
C	3.172318	-0.073118	0.000199
C	4.358729	-0.270490	0.025168
C	0.629557	0.342637	-0.055098
C	-3.166834	-0.334241	-0.032734
H	-1.863156	-2.692316	0.143369
H	-0.133077	-2.032719	0.103292
H	-2.279815	2.071497	-0.248344
H	-0.527353	2.667358	-0.259202
H	5.407514	-0.444307	0.048226
H	-3.465473	0.308161	0.801462
H	-3.722882	-1.269053	0.041186
H	-3.465299	0.167691	-0.958243
H	-1.495064	2.468969	2.080872

C	-1.198797	-1.837713	0.083658
C	-1.686302	-0.599130	-0.009917
C	-0.780957	0.573523	-0.090578
C	-1.224081	1.842555	-0.184152
C	1.820468	0.148430	-0.028650
C	3.172318	-0.073118	0.000199
C	4.358729	-0.270490	0.025168
C	0.629557	0.342637	-0.055098
C	-3.166834	-0.334241	-0.032734
H	-1.863156	-2.692316	0.143369
H	-0.133077	-2.032719	0.103292
H	-2.279815	2.071497	-0.248344
H	-0.527353	2.667358	-0.259202
H	5.407514	-0.444307	0.048226
H	-3.465473	0.308161	0.801462
H	-3.722882	-1.269053	0.041186
H	-3.465299	0.167691	-0.958243
H	-1.495064	2.468969	2.080872

**Vibrational frequencies**

-384.443	46.9094	71.4908
108.7231	140.6717	183.5262
223.6153	233.9912	290.1881
330.58	376.3497	404.1101
453.2549	517.4928	544.7932
594.7023	616.9999	671.9896
678.8121	712.8755	739.7803
795.9967	838.4254	944.6161
953.4977	975.3338	1030.62
1073.139	1080.988	1232.585
1387.536	1420.148	1437.475
1454.463	1489.215	1509.373
1638.772	1720.426	2198.758
2382.008	3047.504	3108.991
3149.271	3166.895	3184.324
3257.943	3280.217	3482.764

**i74 – p27**

**Cartesian coordinates**

C	2.402485	1.001667	-1.339089
C	1.629098	0.267645	-0.587396
C	0.724976	-0.659492	-0.247925
C	1.139598	-2.036608	0.212965
C	-1.821288	-0.043290	-0.084207
C	-3.152249	0.261323	0.002800
C	-4.323760	0.527793	0.081004
C	-0.642531	-0.305312	-0.167406
C	2.258695	1.056562	1.619009
H	3.049274	1.773486	-0.941001
H	2.403570	0.844885	-2.414607
H	0.948681	-2.157515	1.283950
H	2.201615	-2.198199	0.026707
H	0.564220	-2.800585	-0.315581
H	-5.358558	0.761403	0.151372
H	1.687594	0.416881	2.279296
H	1.890558	2.061523	1.456812
H	3.322912	0.876390	1.534525

**Vibrational frequencies**

-465.374	34.4127	70.0341
88.4158	102.6407	145.1266
178.3673	179.132	236.6551
259.2539	329.774	409.1004
460.5985	485.064	500.2599
524.4756	559.3174	577.4634
645.0624	672.141	690.8971
700.7048	779.5225	908.6649
914.4472	1004.823	1052.149
1065.646	1242.393	1327.004



3146.93	3167.131	3182.681	706.5646	713.6599	759.9499	H	-0.181026	-2.002474	-0.695103				
3187.382	3256.889	3483.934	837.1663	863.8148	937.9524	<b>Vibrational frequencies</b>							
<b>i33 – p12</b>							-1884.89	56.7974	63.2331				
<b>Cartesian coordinates</b>							111.2341	149.5403	168.0998				
C	0.783357	2.024239	-0.290585	1076.309	1159.489	1259.146	200.0614	237.9777	318.0896				
C	1.712353	1.220366	0.229850	1347.457	1416.818	1444.171	367.9601	425.6331	466.305				
C	1.794346	-0.233236	0.096333	1466.037	1502.671	1521.603	520.4439	524.1073	541.8583				
C	0.734294	-1.064267	-0.113352	1589.408	1676.945	2198.78	569.0163	635.8724	706.4326				
C	-1.818435	-0.459873	0.014231	2374.04	3062.786	3134.475	734.1208	785.5673	822.0274				
C	-3.152959	-0.162447	0.087244	3147.26	3154.774	3172.43	885.7295	981.1614	1001.847				
C	-4.325507	0.100568	0.151793	3189.812	3246.207	3485.572	1020.538	1043.213	1069.171				
C	-0.637257	-0.703673	-0.053363	<b>i18 – p10</b>									
C	3.178665	-0.811583	0.170791	<b>Cartesian coordinates</b>									
H	-0.041209	1.651301	-0.885337	C	-1.209413	-1.300669	0.746684	1331.951	1427.992	1449.334			
H	0.841278	3.096243	-0.141258	C	-1.963147	-0.415890	0.084371	1473.851	1483.845	1509.866			
H	2.539572	1.672488	0.773821	C	-3.268118	-0.807047	-0.562925	1627.074	1849.104	2092.35			
H	0.853907	-1.230559	-2.153192	C	-1.612456	0.997854	-0.027273	2205.348	3021.534	3087.427			
H	0.922974	-2.133672	-0.138250	C	-0.381293	1.573965	0.011629	3137.534	3159.364	3166.997			
H	-5.362211	0.329046	0.211115	C	1.940972	0.347557	-0.087049	3193.961	3252.449	3485.085			
H	3.651232	-0.547542	1.122541	C	3.155832	-0.280850	-0.150243	<b>i33 – i37</b>					
H	3.808053	-0.399673	-0.624939	C	4.222684	-0.834573	-0.205389	<b>Cartesian coordinates</b>					
H	3.173268	-1.898196	0.077841	C	0.861346	0.885013	-0.025875	C	-0.797392	2.059062	-0.020389		
<b>Vibrational frequencies</b>							-1.511167	-2.339833	0.820412	C	-1.844379	1.211164	0.018731
-697.434	62.8128	66.606	-773.672	36.5847	65.9171	-0.291289	-1.016419	1.244753	C	-1.858119	-0.225246	-0.040825	
105.727	144.5543	198.7876	124.3518	171.2017	196.3509	H	-3.245970	-0.605138	-1.638114	C	-0.730331	-1.052488	-0.062975
205.7484	255.0536	298.5482	210.3688	281.9972	300.3323	H	-4.098340	-0.231320	-0.140910	C	1.859883	-0.434543	-0.140886
305.266	353.5323	415.554	352.2657	383.9561	436.27	H	-3.479323	-1.867209	-0.417287	C	3.179138	-0.156818	-0.021886
442.6833	482.8611	551.1374	448.4308	533.185	547.6066	H	-2.449557	1.681017	-0.149647	C	4.360424	0.097533	0.054074
562.0669	576.0732	679.8838	601.1207	644.0396	686.3835	H	-0.315854	2.646304	-0.144834	C	0.654552	-0.692843	-0.001441
702.8744	717.1921	801.0146	701.7785	715.1539	747.3047	H	5.166141	-1.322305	-0.256139	C	-3.208247	-0.892888	0.014715
836.339	879.458	980.9969	822.4695	905.6561	959.0583	H	-0.253086	2.062748	1.978180	H	-0.967966	3.127135	0.046717
1014.502	1032.625	1054.833	985.758	1001.271	1038.174	H	0.226493	1.730155	-0.130542	H	0.226493	1.730155	-0.130542
1103.976	1192.063	1228.607	1073.893	1164.106	1260.702	H	-2.832994	1.657402	0.115663	H	-2.832994	1.657402	0.115663
1351.577	1374.984	1414.029	1276.552	1416.862	1447.845	H	-0.887583	-2.122949	-0.167794	H	-0.887583	-2.122949	-0.167794
1469.26	1482.003	1492.965	1454.495	1489.512	1505.515	H	5.397686	0.317846	0.128425	H	5.397686	0.317846	0.128425
1608.207	1705.757	2197.751	1593.022	1704.933	2198.539	H	-3.875887	-0.490864	-0.753429	H	-3.875887	-0.490864	-0.753429
2373.169	3044.5	3105.342	2375.195	3045.536	3107.688	H	-3.693463	-0.724151	0.983563	H	-3.693463	-0.724151	0.983563
3146.742	3152.659	3176.845	3145.564	3168.639	3170.446	H	-3.136387	-1.971602	-0.136862	H	-3.136387	-1.971602	-0.136862
3177.738	3270.385	3485.305	3189.037	3265.289	3485.251	H	0.076937	-1.000570	1.119550	<b>Vibrational frequencies</b>			
<b>i17 – p10</b>							-1847.03	63.8944	65.8913				
<b>Cartesian coordinates</b>							113.0169	149.5125	192.3551				
C	-3.389370	-0.699998	-0.134233	1073.893	1164.106	1260.702	207.6081	269.3543	336.8339				
C	-2.083380	-0.409865	-0.025862	1276.552	1416.862	1447.845	345.8605	418.1046	420.3243				
C	-1.688745	0.987825	-0.118572	1454.495	1489.512	1505.515	463.7616	536.4197	545.6339				
C	-0.452263	1.552753	-0.038905	1593.022	1704.933	2198.539	559.1574	665.8547	720.7577				
C	1.904810	0.390724	-0.040614	2375.195	3045.536	3107.688	723.6606	786.4488	834.9962				
C	3.138678	-0.202269	-0.053731	3145.564	3168.639	3170.446	919.0714	975.4777	1020.262				
C	4.221638	-0.726819	-0.065988	3189.037	3265.289	3485.251	1028.739	1056.233	1091.625				
C	0.803738	0.886416	-0.026186	<b>i33 – i80</b>									
C	-1.059798	-1.489619	0.198447	<b>Cartesian coordinates</b>									
H	-3.749146	-1.720776	-0.069928	C	-3.540618	1.004882	0.147946	1191.863	1249.309	1340.985			
H	-4.131838	0.075570	-0.289703	C	-2.901776	-0.164458	-0.046551	1362.793	1424.644	1453.764			
H	-2.511990	1.688231	-0.227353	C	-1.480477	-0.397082	-0.077840	1489.844	1492.729	1513.52			
H	-0.385331	2.625521	-0.194471	C	-0.579783	0.666441	-0.183376	1635.875	1849.065	2092.291			
H	-0.395927	2.083794	1.917723	C	2.061646	0.322489	-0.158696	2203.958	3028.341	3090.453			
H	5.179143	-1.189120	-0.076749	C	3.396917	0.164703	-0.001436	3132.747	3141.298	3167.82			
H	-0.487590	-1.302536	1.110669	C	4.592334	0.011228	0.111623	3181.163	3280.773	3481.824			
H	-0.342988	-1.533561	-0.624423	C	0.842309	0.534178	-0.073932	<b>i33 – i36</b>					
H	-1.546184	-2.462014	0.288101	C	-0.951066	-1.794776	0.053371	<b>Cartesian coordinates</b>					
<b>Vibrational frequencies</b>							-4.622021	1.055333	0.119946	C	-2.284315	1.736583	-0.256318
-765.794	55.2973	67.2139	3189.037	3265.289	3485.251	H	-3.015846	1.932108	0.352427	C	-2.500891	0.300198	-0.571349
128.7699	206.4582	221.3793	3145.564	3168.639	3170.446	H	-3.513885	-1.052074	-0.192704				
277.877	300.0527	315.3119	3189.037	3265.289	3485.251	H	-0.933780	1.668257	-0.404765				
374.0465	397.0581	442.36	3145.564	3168.639	3170.446	H	0.221198	0.916453	0.992398				
454.3396	532.8169	547.9078	3145.564	3168.639	3170.446	H	5.641517	-0.122767	0.217383				
598.2815	653.5184	676.5848	3189.037	3265.289	3485.251	H	-1.748951	-2.531827	-0.051099				
			3189.037	3265.289	3485.251	H	-0.484118	-1.948644	1.034865				

C	-1.631707	-0.532011	0.001928						
C	-0.657503	0.211079	0.888613	1466.545	1486.066	1509.996	406.5828	442.8593	448.9105
C	1.888714	0.137062	0.224483						
C	3.208918	0.108976	-0.133535	1638.246	2143.245	2171.198	513.0604	547.0733	551.6735
C	4.370818	0.083354	-0.448830						
C	0.721111	0.154390	0.546096	2280.128	3038.863	3108.927	655.3306	666.3067	690.4911
C	-1.553225	-2.015924	-0.145503						
H	-3.049270	2.258339	0.318470	3143.01	3161.295	3171.389	733.0134	735.9105	790.2311
H	-1.824112	2.356188	-1.026157						
H	-3.306060	-0.036758	-1.218880	3208.12	3256.347	3486.891	891.0695	897.2325	979.7172
H	-1.181662	1.375364	0.595845						
H	-0.836084	0.091525	1.960908				997.6162	1037.119	1072.219
H	5.397061	0.060570	-0.725505						
H	-2.328340	-2.387969	-0.818397						
H	-1.666107	-2.510836	0.824559						
H	-0.576945	-2.308662	-0.544353						
<b>Vibrational frequencies</b>									
	-1845.26	55.3446	70.1361						
	160.8238	185.1157	191.0727						
	234.3106	328.7434	342.305						
	386.1716	434.6659	509.478						
	536.6317	575.671	600.1859						
	632.2942	668.2097	687.167						
	760.9032	826.6062	891.3275						
	919.3062	939.7849	1037.433						
	1053.182	1076.411	1106.866						
	1207.745	1212.218	1291.335						
	1339.484	1388.688	1423.176						
	1451.617	1483.673	1494.69						
	1654.52	1756.016	2183.827						
	2327.812	3041.218	3092.028						
	3097.88	3104.377	3136.045						
	3177.194	3179.461	3487.577						
<b>i33 – i76</b>									
<b>Cartesian coordinates</b>									
C	-1.698667	2.054248	-0.017544				1152.952	1270.404	1288.06
C	-2.126791	0.868048	-0.470230						
C	-1.712637	-0.436051	0.011203				1415.03	1432.082	1441.573
C	-0.715713	-0.549558	1.145436						
C	1.778712	-0.162718	0.289210				1487.741	1504.792	1507.616
C	3.057008	0.042574	-0.165830						
C	4.177812	0.222514	-0.563141				1635.685	1854.771	2092.623
C	0.657223	-0.342286	0.690153						
C	-1.919169	-1.645103	-0.832074				2201.003	3045.58	3108.736
H	-2.084609	2.975647	-0.435359						
H	-0.942057	2.144721	0.754107				3140.795	3169.057	3174.813
H	-2.857537	0.853335	-1.276838						
H	-0.950333	0.178538	1.928216				3194.112	3278.152	3482.743
H	-0.790509	-1.540570	1.606140						
H	5.167544	0.382254	-0.916991						
H	-2.377730	-1.547888	-1.806195						
H	-2.711543	-1.185157	0.171620						
H	-1.439897	-2.570886	-0.547802						
<b>Vibrational frequencies</b>									
	-1906.56	43.3365	67.6483						
	147.2432	167.7906	182.2453						
	277.5961	335.6338	358.3721						
	384.7065	401.9852	471.8126						
	543.7728	550.3315	573.8001						
	645.0127	676.3837	689.6775						
	706.7741	779.5712	789.7479						
	904.3886	928.7846	957.7609						
	1022.941	1061.714	1162.944				-1830.74	42.2139	66.5805
	1182.439	1209.989	1296.476				121.9604	126.5917	203.007
	1328.175	1346.232	1365.228				249.9543	271.7918	363.6299
	1433.465	1467.675	1487.674				376.2883	446.172	488.3108
	1668.835	2202.726	2221.343				516.7338	547.2715	620.7105
	2403.715	3050.101	3093.079				625.2575	647.2538	704.4158
	3155.57	3165.233	3176.343				717.8197	723.249	874.2828
	3250.873	3300.229	3486.064				899.2982	908.9028	961.5263
							1032.64	1065.462	1120.98
							1207.765	1249.323	1283.402
							1412.924	1429.672	1445.748
							1470.077	1485.094	1503.997
							1639.57	2162.626	2168.04
							2272.879	3040.886	3101.698
							3142.293	3175.441	3181.715
							3196.329	3279.274	3484.788
<b>i33 – i81</b>									
<b>Cartesian coordinates</b>									
C	-3.462881	1.056769	-0.299805						
C	-2.897870	-0.136367	-0.043766						
C	-1.494660	-0.414468	0.157762						
C	-0.510233	0.692479	0.284329						
C	2.069471	0.355374	0.047536						
C	3.416610	0.176996	-0.074067						
C	4.606913	0.016319	-0.181083						
C	0.867892	0.515780	0.144024						
C	-0.970216	-1.804904	-0.061777						
H	-4.537087	1.148225	-0.401267						
H	-2.883786	1.963803	-0.432663						
H	-3.545322	-1.006891	0.033239						
H	-0.897836	1.702836	0.337782						
H	-1.045511	0.059375	1.296208						
H	5.656023	-0.124335	-0.278974						
H	-1.716624	-2.550596	0.218973						
H	-0.056974	-1.991137	0.507742						
H	-0.723049	-1.949153	-1.119953						
<b>Vibrational frequencies</b>									
	-1848.51	60.6906	68.4227						
	145.551	168.1621	193.5467						
	210.8116	254.0692	355.9805						
	372.2651	413.9386	488.8383						
	515.5185	527.2377	564.2172						
	648.2953	654.3556	719.3587						
	764.2031	788.993	810.5391						
	888.3447	998.4324	1004.374						
	1049.512	1069.841	1180.508						
	1231.654	1271.428	1302.373						
	1335.366	1430.262	1437.27						
<b>i33 – i81</b>									
<b>Cartesian coordinates</b>									
C	-1.197072	-1.450297	0.036155				1207.765	1249.323	1283.402
C	-2.039933	-0.394712	0.020940						
C	-1.634146	0.984717	0.057923				1412.924	1429.672	1445.748
C	-0.352734	1.535162	0.046199						
C	2.026258	0.338655	0.115332				1470.077	1485.094	1503.997
C	3.241331	-0.247910	0.017823						
C	4.327706	-0.778996	-0.041657				1639.57	2162.626	2168.04
C	0.912894	0.869737	-0.011959						
C	-3.534347	-0.616430	-0.047810				2272.879	3040.886	3101.698
H	-1.589483	-2.460262	-0.004804						
H	-0.123966	-1.342357	0.104074				3142.293	3175.441	3181.715
H	-2.431978	1.720420	0.043641						
H	-0.266145	2.615057	0.128953				3196.329	3279.274	3484.788
H	5.281190	-1.245417	-0.099735						
H	0.397753	1.273062	-1.137029						
H	-3.955721	-0.165354	-0.951376						
H	-4.032866	-0.155136	0.810238						
H	-3.778538	-1.679567	-0.051640						
<b>Vibrational frequencies</b>									
	-1843.54	40.915	64.6459						
	100.4231	146.0538	199.6493						
	234.5299	269.3216	364.3803						
<b>i33 – i81</b>									
<b>Cartesian coordinates</b>									
C	-2.026089	1.016196	0.964541						
C	-2.251224	-0.163477	0.077414						
C	-1.301365	-0.306070	-0.847231						
C	-0.261421	0.778020	-0.800968						
C	2.204064	0.110124	-0.158827						
C	3.481084	-0.230824	0.195166						
C	4.605179	-0.529485	0.507089						
C	1.075510	0.411255	-0.478183						
C	-3.443010	-1.050110	0.263267						
H	-1.640711	0.818155	1.964938						
H	-2.763638	1.818406	0.935140						





**Vibrational frequencies**

-1892.15	42.483	65.4693
131.277	149.5104	198.4216
293.0014	337.5714	359.8567
385.3841	423.414	466.8439
537.2632	554.3459	580.0048
649.997	683.8569	688.8758
703.735	783.7294	788.7991
891.5825	925.0674	961.0506
1005.991	1067.543	1152.168
1185.313	1222.873	1260.093
1336.396	1350.404	1387.076
1454.223	1462.356	1476.363
1652.258	2204.012	2232.664
2404.907	3042.439	3090.704
3159.354	3170.06	3184.691
3256.495	3303.101	3487.797

**i25 – i22****Cartesian coordinates**

C	0.418454	-1.024731	-0.882702
C	1.500239	-0.554381	-0.210713
C	1.755975	0.869161	-0.187643
C	0.775902	1.794005	-0.047948
C	-1.255516	0.359771	0.020728
C	-2.471256	-0.238602	0.136507
C	-3.511238	-0.867076	0.175453
C	-0.624310	1.515066	0.216731
C	2.378731	-1.434648	0.635264
H	0.130145	-2.069182	-0.820713
H	-0.018192	-0.453504	-1.691696
H	2.789616	1.206024	-0.146650
H	1.067722	2.836526	0.030970
H	-4.435382	-1.389958	0.227561
H	-1.180646	2.323180	0.693916
H	2.247197	-1.212104	1.699276
H	3.433701	-1.260166	0.399383
H	2.163954	-2.492197	0.473895

**Vibrational frequencies**

-400.118	84.3783	111.4333
142.3776	193.6113	232.7751
309.3213	363.9215	407.2152
457.1501	487.27	507.7664
554.4027	559.6334	666.9891
723.9112	735.1651	769.122
855.7425	881.44	912.5997
952.9715	996.1938	998.9333
1034.625	1069.24	1083.428
1231.277	1283.148	1317.68
1411.077	1428.655	1465.148
1494.566	1503.197	1554.73
1638.666	1716.723	2076.097
3040.257	3100.551	3113.367
3140.173	3156.387	3159.97
3194.954	3250.958	3476.472

**i16 – i109****Cartesian coordinates**

C	-3.010787	-0.129100	-0.738512
C	-1.710172	0.098217	-0.059780
C	-0.602581	-0.860840	-0.372057
C	-1.996037	-0.463513	1.285640

C	1.922525	-0.303398	-0.132385
C	3.245120	-0.009622	-0.016119
C	4.419150	0.252308	0.088541
C	0.732635	-0.567941	-0.235278
C	-1.288076	1.561295	-0.031289
H	-3.789503	0.616512	-0.633873
H	-3.277683	-1.112518	-1.109151
H	-0.881983	-1.870855	-0.657353
H	-1.865017	0.121631	2.191430
H	-2.353253	-1.481289	1.369480
H	5.453426	0.479512	0.182498
H	-0.416502	1.704257	0.611428
H	-2.105766	2.178104	0.350495
H	-1.034395	1.900227	-1.037522

**Vibrational frequencies**

-589.744	58.376	71.3639
153.1319	200.9756	242.3129
255.6531	315.9055	349.9578
373.1262	388.7988	412.6101
467.8156	514.8791	524.3297
540.985	567.4582	637.8205
646.7441	679.9645	696.6642
772.6657	810.1361	928.4125
944.7945	1002.399	1015.968
1192.947	1220.883	1248.628
1321.704	1407.487	1428.656
1452.025	1468.076	1497.431
1501.369	2116.455	2202.06
3059.356	3138.312	3148.043
3149.423	3157.893	3179.613
3272.323	3276.622	3482.301

**i34 – p53****Cartesian coordinates**

C	2.949654	-1.666779	-0.449636
C	1.800316	-1.230978	0.045719
C	0.660776	0.996927	0.205913
C	1.644651	0.035952	0.842751
C	-1.816247	0.122523	0.038934
C	-3.097238	-0.354741	-0.045213
C	-4.220960	-0.777989	-0.120131
C	-0.688055	0.549894	0.104644
C	1.024866	2.196328	-0.276054
H	3.006501	-2.589875	-1.015186
H	3.876640	-1.119183	-0.305369
H	0.888662	-1.800486	-0.121347
H	1.280923	-0.212858	1.847135
H	2.611269	0.533010	0.954958
H	-5.213170	-1.154247	-0.188744
H	0.299502	2.873954	-0.708827
H	1.659176	1.693841	-2.378078
H	2.043909	2.549022	-0.166107

**Vibrational frequencies**

-459.282	40.1195	75.014
81.8184	107.539	161.0976
193.9174	216.193	270.7945
326.8762	365.4825	417.672
506.0493	532.7751	592.4997
597.0191	623.3864	686.6232
697.4457	708.2858	779.5879
919.1501	945.3002	958.3865
969.0318	976.9374	1046.519
1076.336	1135.951	1245.515
1315.571	1335.128	1339.285
1439.289	1461.882	1478.196

1658.217	1739.404	2195.773
2369.779	3045.602	3110.735
3150.434	3166.993	3171.953
3241.705	3264.883	3483.118

**i34 – p13****Cartesian coordinates**

C	2.856188	-2.001906	-0.114414
C	1.762052	-1.252125	0.009948
C	0.694756	1.009450	-0.045995
C	1.791724	0.205237	0.020056
C	-1.746494	0.039898	-0.007866
C	-3.021939	-0.455796	0.005831
C	-4.142750	-0.894306	0.017390
C	-0.614512	0.467056	-0.020511
C	0.803547	2.509371	-0.099435
H	2.799340	-3.083633	-0.131868
H	3.842424	-1.555902	-0.201471
H	0.787651	-1.723690	0.100041
H	2.167927	0.528858	2.032608
H	2.766188	0.674563	-0.086475
H	-5.132273	-1.283501	0.027996
H	0.345699	2.956359	0.787883
H	0.279349	2.904842	-0.973411
H	1.848259	2.820818	-0.145328

**Vibrational frequencies**

-668.287	58.4782	94.509
124.022	148.2808	172.3508
192.0524	241.6721	262.379
311.2733	361.4683	381.0851
432.8839	522.7	534.5905
604.964	622.7644	656.5444
674.7771	692.3889	706.6314
938.9811	949.0036	963.838
1038.827	1043.403	1057.26
1070.462	1185.795	1258.991
1332.995	1385.635	1419.439
1453.444	1478.684	1499.387
1605.671	1718.477	2189.729
2347.986	3051.533	3119.805
3145.832	3153.064	3169.743
3182.975	3249.933	3482.544

**i34 – p51****Cartesian coordinates**

C	1.693037	-2.102926	-0.596974
C	2.588788	-1.493044	0.132272
C	0.782713	1.058306	0.207218
C	1.622695	0.637067	1.173705
C	-1.704716	0.205163	0.111242
C	-2.997055	-0.241828	0.046741
C	-4.132331	-0.637332	-0.012255
C	-0.560328	0.592583	0.175961
C	1.215468	1.956216	-0.921853
H	1.898743	-3.059610	-1.080184
H	0.699745	-1.683672	-0.748425
H	3.610534	-1.696830	0.425423
H	1.276501	0.012060	1.986670
H	2.633707	1.022895	1.228669
H	-5.134914	-0.987395	-0.065004
H	2.252001	2.269183	-0.787792
H	0.582424	2.845777	-0.977251
H	1.131635	1.432356	-1.878438

**Vibrational frequencies**

-175.149	34.5784	51.07
81.3721	97.5592	115.7334
136.8228	174.1994	234.5066
274.7118	313.546	367.8684

502.7337	510.4316	579.7824
602.6983	633.8541	668.6514
690.3536	752.5632	776.1321
867.6618	902.3371	935.1718
961.8857	1027.475	1069.63
1071.905	1096.764	1340.754
1389.779	1413.929	1432.491
1477.143	1497.428	1628.609
1668.575	2189.884	2350.274
3050.437	3086.695	3116.543
3149.084	3169.888	3172.23
3236.715	3271.47	3483.991

**i17 - i19**

**Cartesian coordinates**

C	3.382475	1.318034	-0.097360
C	2.550635	0.257005	-0.025762
C	1.137094	0.452660	0.171789
C	0.123839	-0.638546	0.158654
C	-2.437822	-0.150351	0.010481
C	-3.776287	0.106465	-0.064643
C	-4.958379	0.334117	-0.130793
C	-1.246296	-0.383461	0.061625
C	3.068648	-1.151762	-0.155383
H	4.446285	1.186958	-0.254469
H	3.011807	2.333411	-0.009868
H	0.738001	1.460441	0.187737
H	0.475659	-1.655056	0.028346
H	0.662798	-0.161532	1.237819
H	-6.000820	0.532982	-0.192691
H	2.627669	-1.652617	-1.023338
H	2.822762	-1.751721	0.727802
H	4.152390	-1.157829	-0.272983

**Vibrational frequencies**

-1858.85	61.1016	64.769
160.2214	167.7571	197.3762
236.5028	252.6117	376.5579
384.8562	478.8748	490.0709
497.7693	521.4855	573.572
634.656	666.0525	714.3557
764.7873	796.4727	812.7466
866.5008	874.7824	984.0101
1034.656	1067.162	1139.603
1197.32	1249.968	1296.74
1352.597	1409.775	1438.195
1482.292	1497.304	1504.244
1627.923	2155.755	2174.088
2290.253	3037.262	3097.075
3148.36	3160.233	3205.514
3213.959	3253.313	3483.968

**i80 - i83**

**Cartesian coordinates**

C	3.649802	-0.341761	0.099291
C	2.658271	0.471974	-0.257181
C	1.228256	0.255513	0.013043
C	0.664019	-0.983551	0.019041
C	-1.613570	-0.124542	-0.050438
C	-2.990086	0.011139	-0.044903
C	-4.180244	0.228199	-0.027514
C	-0.765408	-1.166705	0.011230
C	0.369540	1.429569	0.190362
H	4.680421	-0.104873	-0.136492
H	3.468040	-1.258917	0.650214
H	2.899061	1.407276	-0.759093
H	1.286357	-1.860475	-0.118525

H	-5.229833	0.396971	-0.013562
H	-1.152513	-2.182190	-0.041322
H	0.688279	2.342243	-0.313531
H	0.055945	1.617380	1.218795
H	-0.819231	0.963574	-0.204065

**Vibrational frequencies**

-1612.87	60.0489	111.1126
126.0137	187.9645	234.8331
311.5042	341.3186	415.7635
445.4812	503.3082	528.627
549.2664	580.6384	630.8306
661.6214	694.6351	703.2214
851.972	859.748	936.1044
957.6856	1000.212	1013.655
1038.296	1048.68	1068.382
1154.723	1241.404	1302.016
1324.761	1332.424	1382.623
1456.745	1472.213	1528.823
1577.253	1688.584	1711.544
2142.513	3090.594	3153.42
3157.678	3164.731	3168.109
3212.139	3247.329	3477.821

**i80 - p55**

**Cartesian coordinates**

C	-3.497668	-0.891553	-0.219399
C	-2.662792	0.097340	-0.533676
C	-1.322714	0.301657	0.054900
C	-0.598774	1.328783	-0.355720
C	-0.840606	-0.675714	1.095826
H	-4.465364	-0.976785	-0.699798
H	-3.248959	-1.646734	0.518086
H	-2.964601	0.825604	-1.282106
H	-0.779058	2.090842	-1.104289
H	-0.757762	-1.678427	0.665769
H	-1.550369	-0.729273	1.926740
H	0.132714	-0.384405	1.485536
C	2.319298	0.668174	0.095653
C	2.901229	-0.525608	-0.225040
C	3.414820	-1.579888	-0.499651
C	1.681426	1.670683	0.347708
H	3.870345	-2.509623	-0.742497
H	1.397737	2.645563	0.668952

**Vibrational frequencies**

-321.182	23.1253	41.1284
82.1296	117.2782	167.3216
208.4541	234.7511	260.0069
309.725	419.1749	432.107
504.0435	525.4432	533.648
652.9911	672.9182	678.6251
684.4609	699.6472	767.0813
800.5302	909.5025	925.639
960.6921	1006.263	1044.812
1066.177	1084.177	1267.125
1338.218	1410.173	1448.58
1487.951	1500.629	1666.15
1713.653	2076.533	2256.393
3051.293	3112.238	3160.943
3174.583	3177.29	3216.061
3251.358	3451.947	3483.236

**i80 - p11**

**Cartesian coordinates**

C	-3.827860	-0.371616	0.000277
C	-2.791278	0.465935	0.000506
C	-1.380121	0.069159	-0.000052
C	-0.448668	1.046385	0.000098
C	2.068327	0.309942	0.000061
C	3.351287	-0.150299	0.000258
C	4.483344	-0.563762	0.000452
C	0.955983	0.812629	-0.000254
C	-1.042713	-1.391095	-0.000691
H	-4.844657	0.002679	0.000771
H	-3.702594	-1.448846	-0.000438
H	-2.979562	1.536869	0.001217
H	-0.770203	2.081867	0.000541
H	5.482003	-0.929180	0.000646
H	-1.469671	-1.878436	-0.882276
H	-1.469050	-1.879021	0.880871
H	0.033208	-1.557108	-0.001129
H	1.510720	2.707503	-0.004134

**Vibrational frequencies**

-811.331	17.6809	70.5524
76.1346	124.9925	167.8868
208.4906	227.3583	293.1242
378.2977	395.5478	443.571
474.5758	478.8841	561.74
577.4634	626.2041	669.4346
674.7761	684.3696	780.2861
838.0755	887.0905	949.3043
997.5771	1022.34	1065.253
1096.16	1223.5	1247.077
1345.009	1388.293	1438.592
1454.489	1487.915	1501.044
1669.21	1720.84	2160.135
2282.602	3056.614	3116.603
3164.286	3171.42	3176.091
3193.85	3257.119	3480.995

**i14 - i73**

**Cartesian coordinates**

C	-3.153444	-0.287238	0.001750
C	-1.788683	-0.463433	0.054018
C	-0.831121	0.703443	0.053666
C	-1.219037	2.030385	-0.124705
C	1.758424	0.186982	0.028872
C	3.105079	-0.064844	0.001010
C	4.287355	-0.286594	-0.022897
C	0.571851	0.404865	0.051228
C	-1.189473	-1.842166	-0.099341
H	-3.802803	-1.151579	-0.036027
H	-3.620394	0.686651	0.058200
H	-1.314638	0.121820	1.175132
H	-2.251981	2.301207	-0.291933
H	-0.477617	2.814756	-0.077408
H	5.332619	-0.480018	-0.046297
H	-0.852685	-1.987216	-1.129419
H	-1.933187	-2.603716	0.136691
H	-0.325018	-1.990301	0.549441

**Vibrational frequencies**

-1851.7	56.1713	71.5715
114.8715	128.8505	220.4117
272.6204	308.0317	390.4486
400.4671	413.9719	496.6837
509.1355	540.7163	555.7815
590.2738	634.2215	661.5292
666.8396	706.4653	716.4058
746.431	825.1214	956.1697
1023.952	1041.402	1066.245



2372.222	3046.997	3107.277	1441.906	1503.631	1511.787	1494.89	2199.292	2228.682
			1944.063	2189.682	2344.851	2394.065	2997.59	3062.906
3157.825	3160.81	3169.639	3053.532	3106.285	3114.607	3066.921	3083.607	3118.304
			3127.278	3157.803	3175.493	3122.703	3213.041	3484.347
3185.966	3256.782	3488.829	3277.67	3284.353	3486.11			

**i36 – i38**

**Cartesian coordinates**

C	-3.653847	-0.404523	-0.726532
C	-2.770951	-0.238506	0.463117
C	-1.353874	0.140412	0.298391
C	-0.388997	-0.794013	0.337002
C	2.178611	-0.320934	0.034649
C	3.517788	-0.082123	-0.126573
C	4.693826	0.129682	-0.269392
C	0.995610	-0.525133	0.173932
C	-1.074492	1.602248	0.073339
H	-4.609276	-0.859062	-0.457735
H	-3.173156	-1.026904	-1.489068
H	-3.875480	0.561415	-1.206893
H	-3.215323	-0.143567	1.449989
H	-0.660396	-1.832355	0.503466
H	5.732927	0.314384	-0.397276
H	-1.608537	1.955038	-0.814787
H	-0.009882	1.800180	-0.056702
H	-1.442923	2.188211	0.921404

**Vibrational frequencies**

-175.469	61.3569	71.6754
97.177	158.0712	173.6561
200.9579	230.8213	271.3662
374.4453	425.9549	466.5731
494.508	547.7944	566.1216
576.0611	694.1293	711.1923
793.6041	823.3514	891.8261
978.0168	987.8709	1033.958
1076.786	1114.941	1201.164
1234.391	1335.589	1377.269
1407.549	1412.031	1476.03
1484.888	1487.875	1490.549
1700.574	2196.558	2377.593
2986.657	3044.469	3067.522
3105.605	3132.291	3150.926
3169.703	3180.957	3484.947

**i38 – p20**

**Cartesian coordinates**

C	-3.679688	0.235549	0.572943
C	-2.511703	-0.701494	0.508313
C	-1.390124	-0.584400	-0.157682
C	-0.276957	-1.026714	-0.756710
C	2.153579	-0.311929	-0.086882
C	3.425881	0.059609	0.253227
C	4.545220	0.388488	0.550431
C	1.027449	-0.641977	-0.382880
C	-1.160150	1.799408	-0.556281
H	-3.715822	0.738701	1.544729
H	-4.612220	-0.324564	0.465710
H	-3.640589	0.992951	-0.207787
H	-2.589422	-1.606050	1.112630
H	-0.375430	-1.661775	-1.634172
H	5.534961	0.676277	0.811086
H	-1.608203	2.204937	0.342329
H	-1.714454	1.884794	-1.483100
H	-0.079862	1.795491	-0.618295

**Vibrational frequencies**

-455.507	33.774	55.6708
122.071	143.923	159.043
173.372	228.7122	271.1933
286.5026	336.9626	407.8834
421.6106	437.0953	493.0006
535.757	538.9307	589.895
676.4761	684.9734	705.2778
774.4474	814.6342	849.6451
901.2777	1064.332	1079.495
1146.227	1216.925	1306.477
1417.147	1421.777	1428.596

**i38 – p11**

**Cartesian coordinates**

C	-3.817264	0.121084	-0.115688
C	-2.696351	-0.612154	-0.063751
C	-1.339274	-0.076319	-0.055739
C	-0.306624	-0.946635	-0.010264
C	2.233751	-0.293098	0.014634
C	3.562333	0.036711	0.028459
C	4.729922	0.328119	0.040957
C	1.058947	-0.579305	0.002415
C	-1.143590	1.409684	-0.090709
H	-4.790543	-0.353337	-0.143690
H	-3.797034	1.201108	-0.207787
H	-4.260396	0.564193	2.083409
H	-2.781773	-1.694518	-0.007876
H	-0.512225	-2.013318	0.019020
H	5.762196	0.582686	0.052517
H	-1.634850	1.877196	0.768123
H	-1.589935	1.834844	-0.994586
H	-0.086539	1.672619	-0.071012

**Vibrational frequencies**

-424.875	56.6399	64.7463
114.235	153.7136	177.5306
203.6206	215.1626	267.9262
291.4793	376.5355	413.4933
422.0304	478.1054	541.6243
575.9384	597.9118	676.4726
698.2499	709.1641	798.4265
832.6985	878.1753	955.9701
995.2136	1020.354	1066.039
1092.156	1224.717	1247.071
1333.844	1387.245	1437.197
1455.947	1489.793	1496.741
1658.913	1674.807	2196.43
2367.719	3050.513	3112.635
3157.095	3165.072	3174.144
3175.45	3261.853	3486.609

**i116 – i114**

**Cartesian coordinates**

C	1.420356	0.549712	-1.048552
C	2.288433	-0.106075	0.013614
C	1.374938	0.385637	1.102710
C	0.485656	1.109136	0.086166
C	-2.004876	0.185988	0.015219
C	-3.285236	-0.305668	-0.014714
C	-4.407934	-0.737048	-0.040339
C	-0.878183	0.615375	0.039475
C	3.097953	-1.352842	-0.058310
H	0.894686	-0.188076	-1.661894
H	1.881700	1.291087	-1.704656
H	2.556752	0.858942	0.842001
H	1.129157	-0.044236	2.066079
H	0.471482	2.199983	0.169781
H	-5.399308	-1.120319	-0.063574
H	3.607124	-1.542617	0.890543
H	3.855673	-1.298528	-0.844423
H	2.456078	-2.221531	-0.265468

**Vibrational frequencies**

-1934.15	41.5377	87.062
131.2845	211.8684	230.8909
248.9485	300.9266	325.5911
415.0424	480.3191	531.8651
582.2577	623.2129	642.038
678.3004	681.2717	726.1883
867.872	918.9887	943.5979
964.225	988.5334	1054.409
1125.649	1128.963	1186.786
1208.559	1222.971	1247.905
1261.169	1346.146	1380.113
1427.326	1485.813	1489.933

**i32 – i82**

**Cartesian coordinates**

C	-3.354985	-0.821193	-0.583880
C	-2.431827	0.344157	-0.699813
C	-1.426857	0.305278	0.174707
C	-0.342872	1.345006	0.311419
C	2.084679	0.294139	-0.012169
C	3.328133	-0.261866	-0.181813
C	4.416869	-0.750259	-0.331245
C	0.992812	0.780335	0.135597
C	-1.470094	-0.905603	1.051479
H	-3.354635	-1.534087	-1.409369
H	-4.358630	-0.621709	-0.206003
H	-2.567986	1.137100	-1.430046
H	-0.497044	2.143855	-0.421016
H	-0.397214	1.806413	1.305346
H	5.378416	-1.183834	-0.464018
H	-1.680382	-0.735660	2.108707
H	-0.683710	-1.644839	0.895581
H	-2.613967	-1.347196	0.435129

**Vibrational frequencies**

-1876.94	46.0116	65.2212
149.7518	177.266	241.713
306.4395	324.0528	351.5415
386.7741	451.0562	557.5192
559.6374	587.4197	604.5448
690.8313	710.1137	715.6657
734.9525	844.8965	878.2602
927.8085	962.4154	1027.119
1055.616	1073.359	1114.293
1169.067	1209.644	1217.614
1334.911	1348.525	1369.262
1452.294	1454.178	1468.1
1664.559	1753.771	2203.481
2406.068	3037.072	3087.058
3087.993	3091.814	3166.194
3168.212	3175.455	3487.114

**i32 – i78**

**Cartesian coordinates**

C	3.812145	-0.004408	-0.636110
C	2.660422	0.618525	-0.300314
C	1.532375	0.004107	0.315854
C	0.334415	0.817466	0.726302
C	-2.105550	0.146883	0.034930
C	-3.423846	0.019227	-0.233174
C	-4.610528	-0.070096	-0.462364
C	-0.867834	0.042646	0.203096
C	1.233819	-1.374206	0.309136
H	3.979085	-1.053201	-0.416407
H	4.612094	0.530687	-1.132987
H	2.577980	1.686038	-0.496174
H	0.234086	0.885818	1.816431
H	0.361416	1.839719	0.338682
H	-5.650896	-0.155457	-0.664016
H	1.852424	-2.052348	-0.273727
H	-0.159909	-1.054147	-0.116440
H	0.801209	-1.827965	1.200498

**Vibrational frequencies**

-2304.53	37.6947	77.4712
138.4023	187.2794	246.2531
304.9645	340.3951	350.5701
406.9894	458.4213	510.6367
541.1932	599.0987	600.1184
654.6872	685.1156	694.7246
812.5882	883.5928	904.8732
912.5406	977.5126	996.8768
1015.527	1084.777	1089.633
1135.563	1214.975	1226.219
1301.994	1315.214	1410.378
1460.968	1462.212	1523.166
1572.451	1601.289	1997.662
2156.124	3042.519	3100.671
3109.089	3153.715	3163.515
3194.735	3253.284	3478.996

**i22 – p10**

**Cartesian coordinates**

C	3.424252	-0.625613	-0.168583
C	2.117292	-0.370343	-0.039015
C	1.680590	1.026568	-0.114325
C	0.449144	1.552081	-0.018130
C	-1.902335	0.392241	-0.023036
C	-3.131297	-0.191589	-0.099087
C	-4.216628	-0.710347	-0.175015
C	-0.792459	0.866719	0.158155
C	1.119852	-1.473908	0.184307
H	3.811138	-1.637318	-0.117913

H	4.145454	0.169467	-0.326489	913.6217	971.0725	986.8006	C	-3.171861	-0.075976	0.029036
H	2.484089	1.741817	-0.268317	1017.03	1050.814	1094.823	C	-4.354000	-0.297489	0.047996
H	0.349192	2.631814	-0.083577	1144.075	1221.379	1255.234	C	-0.638859	0.396182	-0.012794
H	-5.173983	-1.168123	-0.243597	1299.887	1353.351	1382.214	C	3.170305	-0.246906	0.098481
H	0.379646	-1.505685	-0.618609	1463.519	1465.298	1529.952	H	1.910574	-2.606488	-0.295005
H	0.572580	-1.324111	1.118563	1569.302	1592.059	2001.376	H	0.175780	-1.959256	-0.409987
H	1.624606	-2.440067	0.230370	2157.857	3050.323	3100.54	H	1.487300	-0.654657	1.930833
H	-0.683180	0.737353	2.077930	3114.036	3161.368	3170.482	H	2.257697	2.154946	-0.149520
				3189.57	3259.959	3479.818	H	0.499961	2.735434	-0.200480
							H	-5.399195	-0.492201	0.066518
							H	3.505661	0.191817	-0.846862
							H	3.721869	-1.173420	0.259024
							H	3.424730	0.446145	0.902417
<b>Vibrational frequencies</b>										
	-879.939	40.1317	56.9335							
	114.3343	127.6555	204.2001							
	274.985	277.8596	294.4015							
	393.9808	409.3121	429.6946							
	450.2076	537.8368	542.2026							
	593.7624	663.7043	673.089							
	714.9244	716.2553	757.1559							
	801.6537	860.226	943.3192							
	993.6415	1008.197	1056.84							
	1078.044	1163.598	1267.639							
	1352.417	1415.612	1442.322							
	1466.825	1492.028	1510.727							
	1678.349	1721.242	2155.169							
	2271.293	3060.874	3131.18							
	3147.676	3156.2	3166.118							
	3185.832	3245.49	3483.717							
<b>i19 - p9</b>										
<b>Cartesian coordinates</b>										
C	-3.011009	1.250219	-0.189032							
C	-2.529614	0.008549	-0.102445							
C	-1.079926	-0.263946	-0.112962							
C	-0.124848	0.594734	0.316859							
C	2.442315	0.135239	0.065244							
C	3.783024	-0.102679	-0.069694							
C	4.961847	-0.313697	-0.190073							
C	1.255808	0.343012	0.175939							
C	-3.429825	-1.196616	-0.046489							
H	-4.079304	1.436124	-0.187570							
H	-2.360776	2.112270	-0.286155							
H	-0.761626	-1.175366	-0.613115							
H	-1.039620	-1.569447	1.572633							
H	-0.407750	1.512401	0.824868							
H	6.003299	-0.498641	-0.298430							
H	-3.305650	-1.726289	0.903094							
H	-3.176883	-1.903255	-0.843343							
H	-4.478317	-0.916694	-0.156069							
<b>Vibrational frequencies</b>										
	-627.622	56.1583	65.9894							
	98.8618	173.7025	180.3093							
	202.8357	264.7487	293.2789							
	362.5184	399.1923	400.078							
	491.2351	499.1492	531.3743							
	563.9465	574.1058	695.9511							
	705.8498	712.2801	778.532							
	876.9126	909.0287	939.6733							
	990.9607	1009.503	1030.177							
	1078.259	1214.6	1246.747							
	1307.641	1348.678	1418.144							
	1450.171	1483.367	1500.048							
	1624.579	1719.689	2192.715							
	2352.675	3045.959	3107.289							
	3148.774	3163.501	3174.012							
	3182.314	3251.651	3484.006							
<b>i73 - p6</b>										
<b>Cartesian coordinates</b>										
C	-1.449467	-1.406742	-1.238999							
C	-1.838666	-0.298121	-0.551209							
C	-0.906661	0.812904	-0.232221							
C	-1.331984	2.068966	-0.047792							
C	1.651759	0.209011	-0.027685							
C	2.979101	-0.112189	0.086601							
C	4.143795	-0.395262	0.188505							
C	0.484500	0.500147	-0.124334							
C	-2.112510	-0.984770	1.590270							
H	-0.400805	-1.642626	-1.379971							
H	-2.181469	-2.119445	-1.597631							
H	-2.886914	-0.015618	-0.562660							
H	-2.386875	2.309235	-0.121402							
H	-0.641231	2.871937	0.174863							
H	5.173790	-0.642906	0.280520							
H	-1.081053	-1.191502	1.850471							
H	-2.764617	-1.843160	1.478894							
H	-2.550036	-0.089577	2.018098							
<b>Vibrational frequencies</b>										
	-529.588	46.7891	71.7765							
	116.939	134.1659	157.3206							
	211.7147	248.8056	297.7353							
	317.932	437.9405	497.5659							
	525.6165	544.8659	556.1276							
	565.758	615.9609	652.4164							
	685.885	694.1524	701.1782							
	736.8657	851.1742	881.7316							
	905.622	941.3221	987.066							
	1053.236	1101.201	1283.706							
	1343.137	1408.34	1416.745							
	1431.191	1455.741	1563.051							
	1690.971	2200.919	2387.783							
	3096.148	3161.976	3168.619							
	3175.977	3261.388	3262.272							
	3266.115	3268.798	3484.83							
<b>i72 - p41</b>										
<b>Cartesian coordinates</b>										
C	0.970592	-1.911151	0.221100							
C	1.855972	-0.969951	0.000786							
C	0.772708	0.887409	-0.464979							
C	1.364881	1.914086	0.467468							
C	-1.747154	0.267466	-0.169845							
C	-3.059137	-0.067242	-0.003181							
C	-4.217731	-0.365363	0.146640							
C	-0.582036	0.584096	-0.329192							
C	3.148481	-0.585434	-0.082536							
H	1.315897	-2.928480	0.377765							
H	-0.096389	-1.727594	0.247156							
H	1.131386	0.907809	-1.490563							
H	0.933471	2.901445	0.272368							
H	2.445415	1.978887	0.329014							
H	1.161175	1.658137	1.509547							
H	-5.240459	-0.623669	0.279537							
H	3.690233	-0.271331	0.803416							
H	3.619822	-0.418707	-1.045807							
<b>Vibrational frequencies</b>										
	-695.541	17.1153	67.5074							
	101.1302	166.5743	192.6951							
<b>i73 - p42</b>										
<b>Cartesian coordinates</b>										
C	1.229971	-1.764257	-0.256364							
C	1.687055	-0.525614	0.042861							
C	0.768816	0.651385	-0.032970							
C	1.202443	1.914791	-0.132534							
C	-1.824600	0.174164	0.006797							
<b>i33 - i78</b>										
<b>Cartesian coordinates</b>										
C	3.267386	-1.302303	-0.288410							
C	2.790185	-0.042724	-0.405649							
C	1.594279	0.461629	0.175317							
C	0.522066	-0.414016	0.766756							
C	-1.997091	-0.159104	0.080198							
C	-3.326035	-0.234644	-0.153895							
C	-4.518531	-0.326589	-0.348864							
C	-0.778578	0.114732	0.178978							
C	1.118786	1.772240	-0.032262							
H	4.197963	-1.588948	-0.762268							
H	2.757468	-2.063974	0.290782							
H	3.379705	0.678000	-0.968559							
H	0.653598	-1.474204	0.539555							
H	0.461206	-0.313926	1.856736							
H	-5.564429	-0.407458	-0.521612							
H	0.642708	2.298056	0.795535							
H	-0.221987	1.227856	-0.352618							
H	1.658973	2.429279	-0.710558							
<b>Vibrational frequencies</b>										
	-2304.34	39.601	81.1781							
	146.9251	192.1886	225.995							
	299.7287	332.6562	379.1508							
	436.0998	466.4725	505.6917							
	532.6808	578.2764	598.4076							
	663.5261	688.3757	691.3615							
	808.1972	885.9819	892.255							
<b>i73 - p42</b>										
<b>Cartesian coordinates</b>										
C	1.229971	-1.764257	-0.256364							
C	1.687055	-0.525614	0.042861							
C	0.768816	0.651385	-0.032970							
C	1.202443	1.914791	-0.132534							

207.5412	245.5369	255.402
262.9811	368.4324	398.6297
459.9712	487.7065	527.0387
563.7387	664.6014	685.0136
692.1044	759.8811	775.788
827.5274	927.2381	963.432
1016.905	1034.028	1043.154
1076.63	1111.22	1228.886
1383.742	1413.349	1439.815
1481.067	1492.999	1499.123
1868.645	2153.276	2252.96
3042.985	3113.317	3139.641
3141.977	3155.088	3167.299
3230.221	3247.843	3483.324

**i75 - i87**

**Cartesian coordinates**

C	0.032999	-1.131131	0.693666
C	1.333109	-0.804193	0.179884
C	1.860660	0.550211	0.568224
C	1.135985	1.676397	-0.242309
C	-1.150436	0.522955	-0.100029
C	-2.454111	0.052726	-0.112655
C	-3.567883	-0.401490	-0.100112
C	-0.297556	1.409097	-0.292886
C	1.981109	-1.582783	-0.714803
H	-0.470644	-2.016374	0.318886
H	-0.220346	-0.836503	1.705964
H	1.685565	0.730599	1.632553
H	2.934313	0.628690	0.384186
H	1.347477	2.648969	0.210304
H	1.531291	1.702881	-1.263090
H	-4.558867	-0.786567	-0.098030
H	2.942917	-1.292918	-1.123766
H	1.565036	-2.529506	-1.040886

**Vibrational frequencies**

-689.964	75.596	128.2958
148.1971	189.9931	323.4004
342.5288	418.4678	423.0021
462.145	523.3619	536.4044
649.5178	659.9153	663.0994
687.8182	691.8012	719.3485
804.2074	872.6052	899.4566
908.667	942.9894	982.2696
1022.781	1055.802	1151.646
1186.802	1215.493	1304.381
1325.169	1375.795	1430.67
1474.678	1488.137	1512.798
1606.219	2011.784	2253.202
3061.865	3070.773	3104.468
3128.765	3148.294	3156.868
3246.166	3249.003	3483.358

**i75 - p44**

**Cartesian coordinates**

C	1.570377	-1.009845	-1.303039
C	2.168687	-0.833245	-0.122839
C	1.464983	1.233005	0.567982
C	0.350169	1.718139	-0.312354
C	-1.904075	0.333645	-0.004706
C	-3.063854	-0.383116	0.154434
C	-4.079786	-1.011912	0.292139
C	-0.888294	0.964891	-0.149160
C	2.946330	-1.159728	0.880370
H	2.077941	-0.739396	-2.223383
H	0.522126	-1.283106	-1.359916
H	1.207603	0.950968	1.582615
H	2.425999	1.718399	0.433527
H	0.141274	2.778363	-0.108127
H	0.657570	1.667084	-1.363489
H	-4.979663	-1.564680	0.414833
H	3.169088	-0.488608	1.700396
H	3.390841	-2.150033	0.906576

**Vibrational frequencies**

-566.645	28.5968	47.1749
101.8377	137.0213	156.9332
196.0134	220.6379	272.2317
335.1211	343.0944	375.8595
473.4899	530.8972	548.0837
572.6427	684.0725	686.7239
696.7914	768.0624	792.8388
804.4571	904.4901	904.7496
991.8312	1021.989	1025.882
1065.176	1115.17	1175.762
1233.789	1358.993	1430.433
1454.577	1465.265	1479.816
1921.568	2203.452	2406.619
3009.909	3060.596	3140.545
3146.039	3154.386	3236.866
3241.837	3248.943	3485.001

**i82 - p48**

**Cartesian coordinates**

C	-3.644900	0.515472	-0.387288
C	-2.768249	-0.293942	0.516224
C	-1.550936	-0.749644	0.154509
C	-0.408137	1.139173	0.057455
C	2.103983	0.454814	0.009806
C	3.413275	0.076268	-0.013962
C	4.570700	-0.262724	-0.034830
C	0.941242	0.822864	0.030655
C	-0.734256	-1.716979	-0.181719
H	-3.520307	1.590315	-0.197429
H	-4.699033	0.283171	-0.215013
H	-3.413328	0.330021	-1.437876
H	-3.035983	-0.347802	1.569372
H	-0.868260	1.459003	-0.871743
H	-0.790718	1.610847	0.955531
H	5.591831	-0.557911	-0.053089
H	-1.130516	-2.716036	-0.335154
H	0.329974	-1.563415	-0.319698

**Vibrational frequencies**

-679.255	27.9751	60.3336
93.8803	149.9129	176.793
186.9337	207.1013	267.328
341.1739	348.0121	434.895
505.6365	514.4329	533.0372
608.5972	645.8711	646.1733
674.4851	724.3055	795.9536
831.2941	898.8577	939.2811
1025.156	1038.423	1073.87
1101.182	1143.72	1261.569
1360.191	1416.497	1460.273
1466.137	1494.573	1504.435
1887.927	2143.909	2235.32
3017.751	3093.345	3135.741
3145.168	3148.561	3157.995
3234.98	3236.453	3486.121

**i82 - p49**

**Cartesian coordinates**

C	-3.805590	0.180644	-0.407443
C	-2.755110	-0.444389	0.136879
C	-1.364576	0.036198	0.093027
C	-0.330191	-1.076701	0.040651
C	2.209676	-0.292577	-0.012320
C	3.523264	0.104753	-0.040796
C	4.674093	0.452386	-0.065913
C	1.058229	-0.644098	0.012792
C	-1.048403	1.329733	0.119130
H	-4.801647	-0.240302	-0.340195
H	-3.683079	1.074272	-1.009882
H	-4.417489	1.604842	1.182586
H	-2.919943	-1.388841	0.653003
H	-0.477397	-1.732956	0.907761
H	-0.524196	-1.699884	-0.840774
H	5.692082	0.758522	-0.088714
H	-1.818803	2.086882	0.208574
H	-0.017877	1.661768	0.071600

**Vibrational frequencies**

-473.922	36.1719	63.4557
92.8036	145.6238	166.9919
211.5069	250.6863	289.4628
329.9565	361.628	400.3252
442.1295	542.6326	550.3987
588.2741	674.0532	685.84
689.1781	755.0876	785.739
858.6005	939.5894	960.4708
963.2781	967.9927	1030.527
1100.85	1177.621	1212.193
1245.064	1333.8	1368.948
1439.776	1458.471	1467.04
1673.129	1725.354	2206.249
2409.572	3036.213	3068.308
3151.106	3164.33	3167.049
3256.166	3257.936	3487.312

**i109 - p23**

**Cartesian coordinates**

C	1.903467	-0.832845	1.118101
C	1.529346	-0.316970	-0.203342
C	0.500048	-0.271302	-1.073213
C	2.898019	-0.827443	-0.053745
C	-1.994960	-0.113569	-0.287996
C	-3.297313	-0.029870	0.122341
C	-4.443233	0.045322	0.484628
C	-0.841360	-0.190046	-0.648789
C	1.863843	2.075452	0.186750
H	2.089840	-0.139115	1.928927
H	1.467749	-1.779415	1.420753
H	0.695537	-0.211434	-2.139879
H	3.722132	-0.126226	0.003661
H	3.136639	-1.772703	-0.530305
H	-5.455221	0.112738	0.803383
H	2.025743	2.409712	-0.829626
H	2.721227	2.032340	0.848098

H	0.889211	2.241723	0.626579
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**Vibrational frequencies**

-430.658	51.377	63.0883
102.2601	139.7929	177.339
196.5975	222.5858	294.81
336.8506	423.1601	444.4721
453.4283	480.5691	546.2907
551.9447	671.1706	676.5881
735.2515	771.1576	777.0394
788.7518	799.7113	930.5119
1013.461	1051.128	1060.472
1081.079	1090.578	1168.217
1222.842	1361.306	1409.136
1425.82	1454.492	1478.146
1708.394	2186.744	2335.865
3104.375	3141.624	3144.524
3177.47	3225.098	3235.55
3274.484	3286.184	3485.483

**i21 - p45**

**Cartesian coordinates**

C	3.122474	-1.300849	0.323424
C	2.407370	-0.003299	0.061642
C	1.153719	0.012830	-0.342515
C	0.055995	0.058458	-1.067971
C	-2.423062	0.014215	-0.199696
C	-3.722470	-0.009883	0.232270
C	-4.864711	-0.031599	0.610558
C	-1.271856	0.033357	-0.562171
C	3.123304	1.267581	0.430724
H	3.316027	-1.412046	1.396013
H	4.090815	-1.304378	-0.186565
H	2.541684	-2.159108	-0.013529
H	0.327144	-0.190726	1.493800
H	0.161152	0.119646	-2.149734
H	-5.873338	-0.051523	0.946233
H	3.324107	1.286324	1.507529
H	2.540824	2.151414	0.171635
H	4.088625	1.315525	-0.082968

**Vibrational frequencies**

-703.409	39.5468	63.5107
66.5374	149.0612	165.2979
169.8742	209.1934	246.438
281.3273	325.9993	416.1918
438.2856	474.431	519.0481
548.5183	565.906	591.2546
677.1865	681.0574	772.5339
798.2745	833.4148	970.9108
987.7208	1023.69	1096.856
1196.415	1234.077	1252.224
1402.297	1416.063	1446.152
1475.851	1485.448	1495.043
1518.375	2007.452	2201.261
2386.329	3039.413	3042.313
3103.321	3105.704	3144.707
3150.666	3154.716	3485.529

**i78 - i101**

**Cartesian coordinates**

C	-0.035035	1.480772	0.776294
C	1.035483	1.313455	-0.044115
C	1.787251	0.073408	-0.093348
C	1.147129	-1.110030	0.595113
C	-1.200157	-0.378186	0.062811
C	-2.513942	-0.166246	-0.255997
C	-3.660467	0.134528	-0.511561
C	-0.295404	-1.329620	0.161416
C	2.921584	-0.047493	-0.799809
H	-0.658700	2.363757	0.696842
H	-0.154570	0.905577	1.686632
H	1.250139	2.059739	-0.803118
H	1.728128	-2.011739	0.396467
H	1.167163	-0.962680	1.683340
H	-4.672191	0.366245	-0.741227
H	-0.578410	-2.355728	-0.073112
H	3.353012	0.	





C	0.582636	-0.504088	0.688259	534.4399	593.9815	594.1112
C	-1.445960	-1.387899	-1.241675	682.6209	699.6837	705.7617
H	-1.827872	3.182476	-0.145160	731.5039	859.9675	871.5336
H	-0.580478	1.949198	0.442869	927.0192	946.5461	967.4052
H	-3.395630	1.179408	-0.689941	990.0815	1052.547	1066.613
H	-2.783055	-1.213752	0.376311	1192.399	1203.275	1221.236
H	-1.109211	-0.103875	1.843209	1234.335	1253.195	1269.103
H	-0.695277	-1.801740	1.696296	1377.371	1441.924	1458.812
H	5.037900	0.679846	-0.796131	1480.314	1734.768	2202.236
H	-2.213029	-1.653803	-1.958773	2399.674	3075.499	3078.848
H	-0.422593	-1.329985	-1.595638	3097.519	3138.174	3140.052
				3158.628	3249.737	3485.235

C	-1.389566	0.057336	0.109877			
C	-0.356467	0.946655	0.002692			
C	2.179961	0.301707	-0.030540			
C	3.507162	-0.027803	-0.051339			
C	4.674985	-0.319595	-0.069718			
C	1.003752	0.589380	-0.012452			
C	-1.161140	-1.428156	0.063640			
H	-4.819072	0.289928	-0.346157			
H	-3.801578	-1.251108	-0.301202			
H	-2.861864	1.654772	0.031029			
H	-1.450262	0.154038	2.114502			
H	-0.577971	2.008714	-0.053419			
H	5.707152	-0.574480	-0.086031			
H	-1.828219	-1.952868	0.749469			
H	-0.131095	-1.674952	0.319064			
H	-1.361125	-1.796043	-0.948265			

**Vibrational frequencies**

-425.499	46.4503	52.3757
79.8048	138.9609	185.4675
204.1531	210.4521	282.7495
348.9048	352.9079	391.0323
524.1157	542.7839	554.3999
577.7414	678.6862	689.5627
749.5186	816.1953	877.3895
900.6722	915.0683	943.5788
954.8528	989.8723	1074.842
1106.994	1178.192	1243.473
1295.341	1367.263	1406.683
1437.13	1473.571	1600.232
1666.544	2203.265	2405.807
3045.539	3091.187	3094.364
3163.387	3178.768	3184.137
3229.086	3261	3484.993

**i81 - p4**

**Cartesian coordinates**

C	3.712144	-0.540995	0.740305
C	2.730622	-0.582919	-0.158627
C	1.336598	-0.258745	0.137084
C	0.318372	-0.625704	-0.703258
C	-2.207868	-0.281698	-0.120610
C	-3.527817	-0.091100	0.179122
C	-4.690345	0.080002	0.443728
C	-1.036833	-0.449865	-0.386975
C	1.447905	2.081261	-0.213937
H	4.730096	-0.805789	0.481136
H	3.524734	-0.242263	1.767362
H	2.947410	-0.886993	-1.180432
H	1.095022	0.002376	1.162553
H	0.551089	-1.019091	-1.689258
H	-5.717219	0.231368	0.673775
H	2.162445	2.322258	0.563513
H	0.405791	2.321400	-0.043184
H	1.803966	2.095318	-1.236461

**Vibrational frequencies**

-821.937	61.1575	65.5074
134.1068	195.7677	205.1255
222.0319	288.4737	338.0694
383.8087	400.5308	421.5451
434.4579	484.2157	542.5773
572.4429	597.9395	674.9821
692.9673	697.4988	797.5107
823.7066	857.9237	962.0697
992.2735	1029.008	1050.462
1088.574	1228.606	1240.493
1339.944	1380.628	1426.086
1459.139	1485.56	1495.792
1586.407	1715.2	2188.541
2336.601	3055.01	3128.246
3160.451	3161.101	3173.625
3178.215	3252.9	3485.976

**i76 - p49**

**Cartesian coordinates**

C	-1.468236	2.043616	0.101191
C	-2.045396	0.967873	-0.424914
C	-1.740837	-0.433613	-0.074826
C	-0.726362	-0.704543	1.030464
C	1.778305	-0.244073	0.248394
C	3.068416	-0.007116	-0.154995
C	4.199687	0.200219	-0.506342
C	0.645318	-0.449926	0.600798
C	-2.112453	-1.435389	-0.906435
H	-1.741971	3.037347	-0.232405
H	-0.697891	1.980654	0.862012
H	-2.799664	1.092380	-1.197610
H	-3.211207	-0.575999	1.127939
H	-0.950571	-0.088065	1.906142
H	-0.814188	-1.746271	1.349753
H	5.200024	0.383139	-0.816693
H	-2.757049	-1.243514	-1.756608
H	-1.818132	-2.461961	-0.722548

**Vibrational frequencies**

-427.904	52.5092	67.9328
106.8688	126.6659	142.4609
195.8067	209.6894	253.7041
305.3843	410.4248	427.0494
467.3817	499.8088	514.7671
550.4806	574.2285	667.9501
686.3206	703.7274	768.5111
790.2184	840.4519	939.1701
954.0404	965.5805	1032.306
1189.294	1225.083	1279.951
1286.247	1339.351	1414.34
1423.337	1450.654	1557.058
1714.911	2180.763	2314.808
3103.659	3153.25	3166.193
3173.545	3186.278	3248.095
3277.27	3279.323	3483.916

**i19 - i14**

**Cartesian coordinates**

C	1.460459	1.247237	-0.049351
C	2.296364	0.169503	-0.372947
C	1.336250	-0.990803	-0.416371
C	0.404793	-0.365268	0.632841
C	-2.161425	-0.116957	0.191054
C	-3.493504	0.050234	-0.061148
C	-4.668037	0.200557	-0.286072
C	-0.983114	-0.288910	0.433862
C	3.735628	0.037181	-0.022237
H	0.601371	1.478399	-0.673851
H	1.844909	2.110881	0.496211
H	1.769528	-1.953302	-0.126735
H	0.822679	-1.123966	-1.373988
H	0.737494	-0.477616	1.660549
H	-5.704365	0.333951	-0.481358
H	4.294732	-0.435855	-0.837271
H	3.878542	-0.599290	0.863206
H	4.190625	1.010162	0.175445

**Vibrational frequencies**

-973.211	45.2773	66.0853
95.3388	131.4757	186.1143
220.9974	340.6148	363.4321
435.305	471.4581	504.8491
537.1345	573.2841	668.4713
704.4108	713.437	795.1917
827.7416	850.4061	921.4928
973.5974	981.1273	995.6962
1019.379	1050.604	1150.173
1225.787	1238.873	1310.394
1364.617	1394.748	1426.076
1470.573	1482.935	1492.827
1549.064	2168.24	2288.225
2999.78	3050.148	3064.822
3095.378	3100.409	3124.959
3177.573	3179.912	3484.023

**i114 - p86**

**Cartesian coordinates**

C	-1.341583	-1.091986	0.014654
C	-2.336782	0.000002	-0.307139
C	-1.341581	1.091985	0.014659
C	-0.454425	-0.000003	0.697405
C	2.143068	-0.000002	0.155585
C	3.484142	0.000000	-0.134584
C	4.659945	0.000003	-0.387562
C	0.964898	-0.000003	0.411050
C	-3.640533	0.000003	-0.574546
H	-0.861373	-1.500627	-0.878532
H	-1.682903	-1.912087	0.648345
H	-1.682899	1.912084	0.648354
H	-0.861369	1.500630	-0.878524
H	-0.615190	-0.000006	1.779733
H	5.699752	0.000005	-0.609476
H	-4.179025	0.927306	-0.736114
H	-4.460856	-0.000004	1.426996
H	-4.179027	-0.927297	-0.736120

**i81 - p52**

**Cartesian coordinates**

C	-1.033629	2.336508	-0.251654
C	-2.018854	1.620272	0.219327
C	-1.611039	-0.807048	0.384730
C	-0.640690	-0.965443	-0.547837
C	1.889338	-0.429518	-0.121068
C	3.210433	-0.149724	0.097255
C	4.373079	0.097807	0.289327
C	0.718880	-0.678334	-0.309417
C	-3.023001	-1.263486	0.173261
H	-1.089604	3.424965	-0.301867
H	-0.114453	1.876234	-0.609067
H	-2.998242	1.846122	0.622677
H	-1.315136	-0.556494	1.398805
H	-0.904283	-1.289862	-1.551363
H	5.400264	0.312878	0.459104
H	-3.741530	-0.586761	0.639096
H	-3.164278	-2.249704	0.628788
H	-3.259844	-1.343589	-0.889725

**Vibrational frequencies**

-278.584	31.1293	53.6567
83.6714	129.7035	148.0195
198.2048	219.1823	230.3702
240.5783	290.6666	375.7556
429.9831	472.8377	551.6773
559.572	689.5774	710.1578
771.6765	783.3766	790.8397
865.5445	940.0828	947.9159
959.8846	1045.801	1083.392
1131.191	1221.058	1300.6
1321.19	1395.257	1425.008
1484.531	1496.175	1619.232
1672.762	2185.968	2334.246
3042.567	3091.64	3111.682
3142.596	3169.788	3179.847
3189.834	3229.429	3484.532

**i116 - p21**

**Cartesian coordinates**

C	-1.713758	-0.593683	-1.040687
C	-2.424051	0.062306	0.134130
C	-1.668671	-0.585029	1.060787
C	-0.755530	-1.233850	0.032194
C	1.760424	-0.371499	0.006283
C	3.052520	0.090105	0.000983
C	4.184656	0.496589	-0.002600
C	0.623294	-0.772910	0.010977
C	-1.596863	2.195956	-0.021132
H	-1.228612	0.066687	-1.760152
H	-2.306802	-1.341634	-1.572200
H	-3.405213	0.514883	0.197719
H	-1.658930	-0.620922	2.142191
H	-0.775768	-2.328883	0.031278
H	5.184805	0.857171	-0.005430
H	-1.933488	2.632753	0.911392
H	-2.110100	2.510505	-0.923487
H	-0.538020	1.981530	-0.106931

**Vibrational frequencies**

-469.293	42.5878	66.9908
112.115	182.8834	208.2726
216.8705	255.804	352.4864
398.156	446.4482	484.8421

**Vibrational frequencies**

-495.025	49.223	80.0228
122.6873	140.9951	180.7028
230.2999	238.2336	343.2744
441.4503	478.0209	501.7073
536.2006	549.4728	588.6208
642.0641	675.445	679.433
780.2601	816.931	866.532
907.8489	920.0917	943.4131
998.9016	1015.732	1095.532
1118.025	1164.439	1198.949
1234.383	1303.006	1330.068
1420.572	1426.303	1481.404
1513.906	2199.481	2395.762
3065.031	3083.999	3095.272
3144.372	3210.416	3238.303
3260.345	3267.999	3484.14

***i115 - p84*****Cartesian coordinates**

C	3.469685	-0.674901	-0.423915
C	1.106571	-0.809871	-0.318312
C	0.344664	0.266059	-0.184226
C	3.881082	-0.241191	0.781361
C	-2.269502	-0.052776	0.008230
C	-3.625439	-0.219712	0.110332
C	-4.816315	-0.366387	0.200823
C	-1.072662	0.087029	-0.079244
C	0.853640	1.686832	-0.135924
H	3.461939	-1.732285	-0.662315
H	3.360668	0.005915	-1.260880
H	0.833683	-1.857185	-0.341769
H	4.078649	-0.932091	1.593069
H	3.984787	0.816226	0.998852
H	-5.868165	-0.497243	0.283397
H	0.395020	2.279414	-0.931708
H	1.936134	1.715834	-0.250607
H	0.586942	2.150914	0.817209

**Vibrational frequencies**

-280.284	30.1313	58.9617
73.2419	113.6474	146.3743
158.44	214.2213	236.3043
305.343	326.3872	373.2792
496.2056	502.4806	564.7598
590.2565	648.1198	689.8586
711.9988	752.2427	833.8646
876.6144	914.1731	936.2147
1022.287	1035.859	1060.56
1065.772	1238.582	1285.347
1334.007	1406.019	1468.417
1485.197	1487.799	1614.976
1663.469	2196.665	2375.275
3060.582	3126.166	3152.603
3165.023	3170.774	3228.792
3235.945	3260.594	3488.069

***i115 - p14*****Cartesian coordinates**

C	2.829899	-0.249108	0.026746
C	1.381316	-0.431207	-0.016591
C	0.450925	0.541021	0.020783
C	3.680907	-1.297946	0.112538
C	-2.106126	-0.088514	0.002366
C	-3.439905	-0.400278	-0.005045
C	-4.611809	-0.673081	-0.011017
C	-0.927311	0.176476	0.007609
C	0.728485	2.021813	0.064725
H	3.051199	0.280293	-1.813166
H	3.217599	0.745594	0.220023
H	1.036620	-1.459809	-0.073694
H	3.325560	-2.318721	0.018369
H	4.746418	-1.148562	0.233668
H	-5.647733	-0.912501	-0.016842
H	0.220990	2.518229	-0.766348
H	1.791937	2.245940	-0.005003
H	0.339125	2.454473	0.990308

**Vibrational frequencies**

-869.47	63.1492	79.5102
87.5732	99.8244	190.071
195.0101	258.5337	330.5596
369.917	397.0926	421.6836
451.0679	510.977	513.1863
592.9507	607.8829	658.2603
676.826	701.3315	733.952
908.6944	914.7973	936.2201
1005.351	1046.502	1066.126
1072.71	1188.923	1274.614
1302.892	1367.436	1429.323
1451.632	1482.081	1499.013
1603.19	1702.876	2197.101
2374.623	3056.94	3118.816
3161.371	3166.502	3182.605
3195.319	3261.313	3485.942

***i92 - i87*****Cartesian coordinates**

C	0.026077	-0.657451	1.005639
C	1.224288	-0.780793	0.089734
C	1.945682	0.520241	-0.156373
C	1.001145	1.711263	-0.183775
C	-0.909139	0.337496	0.330636
C	-2.190362	-0.064717	-0.084967
C	-3.277223	-0.450959	-0.441202
C	-0.376145	1.585778	0.057634
C	1.580014	-1.922253	-0.489915
H	-0.461953	-1.620176	1.156992
H	0.338284	-0.276819	1.986186
H	2.640938	0.710359	0.674045
H	2.554280	0.475365	-1.062897
H	1.451993	2.702019	-0.168340
H	0.104608	1.931020	-1.122038
H	-4.238492	-0.775667	-0.758261
H	2.415519	-1.971405	-1.180877
H	1.048795	-2.846331	-0.289293

**Vibrational frequencies**

-1567.29	75.1446	113.1169
162.2398	236.6846	370.5932
382.326	408.9075	479.062
521.9545	556.6361	569.5796
593.7099	664.1467	693.3726
714.6731	729.9273	815.4257
868.2204	905.4975	940.816
950.308	976.426	1005.259
1140.384	1165.679	1199.73
1212.799	1276.711	1297.367
1304.887	1317.062	1391.189
1446.595	1461.957	1475.253
1488.662	1745.874	2162.036
2175.543	3022.217	3038.072
3101.469	3136.331	3152.847
3155.173	3240.075	3481.4

***i101 - p64*****Cartesian coordinates**

C	-0.325769	1.202170	0.108080
C	1.022522	1.246463	0.025193
C	1.825497	0.035627	-0.047355
C	1.118720	-1.263335	0.278975
C	-1.045322	-0.081099	0.012303
C	-2.467493	-0.047531	-0.136274
C	-3.660637	0.013921	-0.257887
C	-0.363667	-1.234859	0.054770
C	3.125546	0.079787	-0.362706
H	-0.909969	2.113259	0.066388
H	-0.594245	1.467644	2.197708
H	1.531937	2.203133	-0.021264
H	1.574038	-2.094342	-0.266013
H	1.281931	-1.480524	1.346272
H	-4.717205	0.061396	-0.366813
H	-0.890004	-2.179762	-0.016756
H	3.628064	1.025478	-0.533908
H	3.719073	-0.823150	-0.456211

**Vibrational frequencies**

-593.038	61.6595	144.6672
165.1875	203.5443	281.6895
312.1779	379.5402	398.9622
410.1915	498.1183	532.5056
604.6974	642.2067	683.8759
706.3256	710.8882	719.3153
783.2907	829.6076	842.4515
920.2397	959.6515	964.5729
986.2959	1001.882	1063.482
1182.947	1194.473	1235.773
1311.05	1350.549	1364.311
1428.743	1456.241	1472.948
1595.863	1685.218	1716.624
2244.471	2998.378	3093.273
3156.746	3195.801	3210.201
3219.267	3246.73	3485.883

***i111 - p77*****Cartesian coordinates**

C	3.037880	-0.623217	0.138801
C	1.630914	-0.276831	-0.084838
C	0.697489	0.678509	0.007609
C	1.939026	-1.696461	0.073559
C	-1.856909	0.052346	0.006545
C	-3.190095	-0.260337	0.010598
C	-4.362124	-0.533281	0.013968
C	-0.678501	0.320712	0.003036
C	1.041424	2.143315	0.058096
H	3.733417	-0.574489	-0.691550
H	3.468012	-0.391268	1.108125
H	1.717586	-0.124924	-2.200099
H	1.921647	-2.335309	-0.802368
H	1.635544	-2.178855	0.997059

H	-5.398007	-0.772813	0.016426
H	0.593533	2.612565	0.938122
H	0.650677	2.657928	-0.824340
H	2.122972	2.278639	0.094375

**Vibrational frequencies**

-577.943	64.3237	85.8941
137.6265	162.6692	181.0704
224.7447	241.6836	275.1332
359.9863	387.6711	426.921
473.1528	523.4183	550.6325
601.3404	633.2499	674.8761
698.1439	760.9978	796.6158
885.0341	968.5232	1030.996
1049.119	1061.484	1075.397
1089.787	1096.12	1168.28
1190.455	1320.424	1419.716
1450.757	1473.625	1480.16
1499.624	1794.152	2195.126
2366.406	3053.761	3121.256
3135.409	3137.161	3153.724
3217.056	3227.538	3486.042

***i111 - p81*****Cartesian coordinates**

C	2.855765	-0.723839	-0.670306
C	1.472632	-0.713272	-0.066554
C	0.606921	0.501944	-0.137435
C	2.701403	-0.716271	0.818002
C	-1.981142	0.025575	-0.034911
C	-3.325403	-0.232345	0.016749
C	-4.506155	-0.458824	0.062318
C	-0.797996	0.263585	-0.081098
C	1.065617	1.762471	-0.220351
H	3.178141	-1.639112	-1.151042
H	3.193962	0.183408	-1.157081
H	0.923815	-1.645252	-0.119018
H	2.923711	-1.622145	1.368253
H	2.913126	0.206011	1.346670
H	-5.549870	-0.657593	0.104343
H	1.357317	2.345139	2.055355
H	0.383772	2.600840	-0.271554
H	2.126179	1.974569	-0.294415

**Vibrational frequencies**

-348.59	18.6805	71.638
105.2033	155.4314	178.783
218.1483	261.9135	300.3827
346.296	374.4538	497.1345
542.3237	590.5118	659.0984
682.3206	682.8545	707.9425
760.913	798.6258	837.2891
844.9309	927.0348	936.2958
961.4663	1059.758	1076.895
1083.453	1125.473	1132.79
1209.147	1230.353	1292.511
1437.691	1439.446	1478.561
1526.158	1659.935	2197.801
2376.048	3146.489	3154.949
3173.577	3198.117	3233.867
3248.726	3270.58	3483.934

***i111 - i115*****Cartesian coordinates**

C	2.915339	-0.446202	-0.530869
C	1.427881	-0.559313	-0.499442
C	0.561777	0.454295	-0.154292
C	2.906691	-1.014790	0.838035
C	-2.013289	-0.014513	-0.029836
C	-3.357857	-0.250138	0.032412
C	-4.543501	-0.458092	0.087526
C	-0.817639	0.187791	-0.084573
C	1.037670	1.848763	0.176944
H	3.387982	-1.073884	-1.284463
H	3.288088	0.574743	-0.594419
H	1.010027	-1.525901	-0.755777
H	2.950803	-2.084842	0.993660
H	2.804204	-0.366232	1.696977
H	-5.589452	-0.641198	0.135981
H	0.195		

1479.996	1497.619	1502.613	H	3.939642	-0.615511	0.714552	883.1431	905.2209	939.6606	
1518.863	2171.614	2295.172	H	3.200207	-0.454060	-1.398182	969.9907	1006.064	1043.651	
3035.632	3096.579	3099.541	H	0.951424	-0.525843	1.730323	1119.554	1165.808	1181.691	
3152.088	3164.465	3176.455	H	1.992050	-2.353774	0.466949	1201.257	1223.152	1262.436	
3206.053	3290.893	3487.023	H	0.893100	-2.059573	-0.908759	1281.251	1346.547	1372.454	
			H	-5.370971	0.322496	-0.492538	1425.434	1476.864	1492.318	
			H	0.785095	2.416354	-0.262377	1495.135	2199.194	2232.881	
			H	2.509895	2.382649	-0.691650	2393.594	3011.8	3065.24	
			H	2.002245	2.326752	1.009059	3069.375	3090.491	3119.033	
							3127.644	3203.993	3484.984	
<b>i21 - p10</b>			<b>Vibrational frequencies</b>				<b>i110 - p74</b>			
<b>Cartesian coordinates</b>						<b>Cartesian coordinates</b>				
C	-1.026425	-1.447025	-549.38	64.1209	79.4972	C	2.309352	-0.459340	-0.785445	
C	-2.034101	-0.332708	143.7646	174.3002	180.6218	C	1.740028	0.489839	-0.009552	
C	-1.611789	1.064787	236.6336	266.6778	305.1257	C	0.819484	-0.519726	0.694670	
C	-0.374120	1.592208	338.3259	402.0295	465.2782	C	1.558101	-1.609610	-0.164700	
C	1.967885	0.409589	525.137	544.221	597.2401	C	-1.764105	-0.167740	-0.189681	
C	3.197069	-0.192454	660.4617	705.4883	711.2405	C	-3.095237	0.031635	-0.076026	
C	4.276678	-0.724323	716.9455	885.4412	918.1466	C	-4.262200	0.208671	-0.307422	
C	0.868533	0.911943	923.0647	973.3516	986.7781	C	-0.594546	-0.343820	0.424080	
C	-3.353592	-0.589033	1022.641	1051.451	1115.531	C	1.652907	1.976539	-0.044385	
H	-0.336077	-1.368832	1168.078	1203.221	1218.948	H	3.067123	-0.416719	-1.558305	
H	-1.527180	-2.414972	1237.88	1296.923	1349.794	H	3.144324	0.431140	1.353344	
H	-0.421116	-1.414126	1411.759	1478.574	1479.868	H	0.986684	-0.614284	1.770733	
H	-2.428025	1.782067	1484.903	1682.713	2200.463	H	2.155006	-2.309173	0.427499	
H	-0.290712	2.674993	2397.216	3041.85	3060.332	H	0.901687	-2.169769	-0.834255	
H	5.231047	-1.193126	3084.713	3105.638	3138.82	H	-5.294040	0.365843	-0.509714	
H	-3.730023	-1.603017	3142.042	3223.668	3484.473	H	0.721395	2.270351	-0.539109	
H	-4.086455	0.210109				H	2.491560	2.403576	-0.597212	
H	-3.872282	-0.831009				H	1.643553	2.400339	0.961618	
<b>Vibrational frequencies</b>			<b>i108 - p73</b>			<b>Vibrational frequencies</b>				
	-342.537	37.2022	<b>Cartesian coordinates</b>				-751.227	66.4089	82.3764	
	126.4664	147.7892	C	2.773650	-0.551258	-0.156081	152.9006	182.7418	190.4944	
	198.6571	234.8698	C	1.716278	0.517743	-0.026261	256.4566	308.2577	391.4762	
	290.9106	394.4817	C	0.702130	-0.379780	-0.140847	420.4566	451.4037	479.8365	
	448.9022	534.473	C	1.607230	-1.586145	-0.099702	520.7606	543.1064	596.3355	
	605.4547	653.1584	C	-1.907154	-0.122101	0.037655	677.6653	704.9259	706.1561	
	711.5584	742.4686	C	-3.268231	0.009239	-0.038275	713.5148	835.1363	905.2282	
	814.2043	860.0492	C	-4.463744	0.126364	-0.107909	919.2097	977.3062	994.5182	
	993.0762	1015.085	C	-0.706393	-0.235046	0.101434	1016.423	1051.901	1122.354	
	1065.65	1170.296	C	1.784885	1.995151	-0.028847	1173.043	1206.433	1222.308	
	1350.858	1410.87	H	3.474076	-0.607082	0.683565	1244.701	1302.42	1347.508	
	1464.435	1485.224	H	3.343122	-0.538045	-1.089945	1412.291	1475.793	1479.38	
	1659.248	1683.041	H	0.759887	-0.466340	2.068286	1489.182	1654.72	2200.439	
	2372.416	3058.111	H	1.651383	-2.323014	0.702358	2396.795	3050.58	3067.122	
	3147.893	3161.895	H	1.419105	-2.086923	-1.051467	3088.154	3124.047	3125.037	
	3189.13	3252.661	H	-5.519960	0.230669	-0.170879	3148.946	3221.451	3484.402	
			H	2.275019	2.360838	-0.936645				
			H	2.377609	2.350065	0.822032				
			H	0.787849	2.434830	0.035529				
<b>i108 - p75</b>			<b>Vibrational frequencies</b>			<b>i110 - p76</b>				
<b>Cartesian coordinates</b>				-838.65	65.9409	81.5659	<b>Cartesian coordinates</b>			
C	2.686280	-0.518960	-0.397737	113.2635	175.5161	191.121	C	2.426589	-0.252139	-0.730028
C	1.709670	0.569297	-0.017926	235.6288	298.7372	329.9035	C	1.830135	0.620287	0.351692
C	0.751792	-0.440782	0.604269	421.5291	445.5755	456.5105	C	0.884486	-0.617929	0.655680
C	1.546253	-1.546600	-0.164081	504.1594	537.2936	571.0043	C	1.668360	-1.326232	-0.449149
C	-1.847718	-0.145910	0.162411	607.1872	681.3646	699.0406	C	-1.704674	-0.266126	0.183661
C	-3.189811	0.014961	-0.072564	711.64	802.7057	913.3328	C	-3.039415	-0.078608	-0.071951
C	-4.366562	0.157153	-0.276309	942.3374	976.2573	981.013	C	-4.209155	0.087422	-0.297457
C	-0.668507	-0.286917	0.368040	1061.768	1092.805	1114.03	C	-0.530400	-0.428097	0.403478
C	1.613369	1.875679	-0.243259	1182.727	1222.502	1232.185	C	1.178023	1.924966	-0.072584
H	3.491730	-0.620488	0.336630	1275.118	1348.738	1417.26	H	3.210323	-0.068266	-1.455118
H	3.123418	-0.466248	-1.395714	1463.238	1475.216	1479.594	H	2.516362	0.794512	1.188233
H	0.939965	-0.521013	1.681546	1499.417	1649.753	2200.119	H	1.027482	-1.038271	1.655017
H	1.783941	-2.447541	0.400706	2377.08	3036.425	3056.958	H	2.918377	-2.399166	0.734848
H	1.041718	-1.816217	-1.091954	3088.807	3098.177	3105.903	H	1.503096	-2.281066	-0.931336
H	-5.406737	0.284956	-0.455352	3139.478	3149.877	3487.391	H	-5.243281	0.234796	-0.495391
H	2.372122	2.403903	-0.809641				H	0.478760	1.766808	-0.896917
H	2.528710	2.694929	1.525184				H	1.939513	2.638723	-0.397993
H	0.716540	2.420191	0.031522				H	0.625687	2.370663	0.758604
<b>Vibrational frequencies</b>			<b>i110 - i108</b>			<b>Vibrational frequencies</b>				
	-492.497	63.4362	79.7071	<b>Cartesian coordinates</b>				-667.787	71.7436	78.3237
	125.1748	181.8838	190.4833	C	-2.453272	-0.393584	0.720915	152.8203	200.6673	236.9891
	224.4165	257.5028	343.9575	C	-1.739194	0.577586	-0.179498	248.9163	307.384	351.7692
	387.2036	438.4192	501.5934	C	-0.862610	-0.556550	-0.741194	359.4584	413.927	486.9381
	537.4634	592.5626	631.6637	C	-1.605373	-1.550338	0.225575	500.8982	541.659	598.3691
	693.9762	706.3578	713.4847	C	1.714951	-0.212446	-0.197576	704.8587	712.7371	729.8563
	776.1202	814.369	901.5501	C	3.041776	-0.020914	0.093818	804.7833	826.9839	878.9417
	918.7993	944.8986	952.5534	C	4.205298	0.146996	0.348891	901.0791	971.9648	991.8574
	980.032	1047.018	1091.595	C	0.550410	-0.388473	-0.457388	1040.345	1070.255	1098.212
	1192.152	1206.013	1217.255	C	-1.409400	2.015469	0.015915	1161.396	1183.986	1209.981
	1236.123	1257.418	1282.455	H	-2.938698	0.131006	-0.370391	1238.517	1310.05	1349.935
	1370.444	1433.431	1476.109	H	-2.942819	-0.222882	1.671819	1361.355	1419.994	1496.576
	1498.877	1730.877	2202.365	H	-0.995757	-0.762721	-1.807581	1503.67	1593.425	2200.483
	2400.536	3052.478	3063.014	H	-2.114602	-2.388575	-0.255029	2397.303	3051.244	3057.291
	3100.289	3129.456	3156.304	H	-0.927759	-1.939894	0.988538	3079.065	3128.199	3137.229
	3165.392	3249.027	3485.092	H	5.234074	0.296184	0.571550	3205.513	3234.671	3484.365
				H	-0.584478	2.133921	0.731752			
				H	-2.273111	2.554578	0.414476			
				H	-1.112369	2.491913	-0.921875			
<b>i108 - p74</b>			<b>Vibrational frequencies</b>			<b>i110 - p21</b>				
<b>Cartesian coordinates</b>				-1943.98	65.563	72.2146	<b>Cartesian coordinates</b>			
C	2.404294	-0.468496	-0.663754	142.0025	171.288	184.049	C	2.729603	-0.125883	-0.286647
C	1.704395	0.510581	-0.060107	243.9673	302.1581	340.2813	C	1.910010	0.371743	0.676733
C	0.768223	-0.462846	0.651707	440.7696	502.8359	533.3446	C	0.924454	-0.798265	0.544506
C	1.519722	-1.587156	-0.149922	587.5944	593.7656	686.5664	C	1.787988	-1.229533	-0.697038
C	-1.825179	-0.141764	0.175527	699.725	705.6258	709.454				
C	-3.162198	0.032938	-0.077861							
C	-4.334512	0.186175	-0.298900							
C	-0.650913	-0.298478	0.399609							
C	1.759054	1.989131	-0.004194							

C	-1.668327	-0.360819	0.170154	137.3691	162.5454	219.287
C	-3.005957	-0.133079	-0.032091	261.4148	280.9454	370.8193
C	-4.178461	0.068519	-0.209756	404.4164	481.8874	518.7108
C	-0.490086	-0.550548	0.341241	553.3421	566.0931	597.5446
C	0.795568	2.166851	-0.263668	689.5044	703.4794	709.9427
H	3.704120	0.168667	-0.653766	739.4368	811.9161	905.8259
H	2.080609	1.031838	1.517014	945.8546	985.3126	1030.867
H	1.045839	-1.512909	1.364611	1055.934	1067.296	1117.701
H	2.171558	-2.252651	-0.652539	1193.883	1219.619	1247.785
H	1.275358	-1.081727	-1.652139	1273.451	1358.475	1408.72
H	-5.214764	0.245615	-0.367548	1440.437	1474.737	1491.438
H	0.460281	1.744265	-1.202767	1539.208	2201.252	2399.884
H	1.612473	2.877577	-0.306357	3032.227	3047.906	3108.224
H	0.035773	2.325410	0.492896	3116.413	3128.995	3146.112
				3212.191	3233.244	3486.096

<b>Cartesian coordinates</b>			
C	2.869499	-0.199708	-0.002716
C	1.599137	0.546883	0.304074
C	0.679131	-0.485214	0.577946
C	2.162442	-1.413130	-0.598250
C	-1.908253	-0.232655	0.165990
C	-3.252017	-0.103730	-0.063033
C	-4.433071	0.012229	-0.263033
C	-0.722179	-0.342056	0.373585
C	1.280628	1.910852	-0.190671
H	3.449684	-0.472451	0.887253
H	3.541697	0.337295	-0.681607
H	0.943065	-1.241745	1.313819
H	2.453815	-2.419889	-0.304374
H	1.818087	-1.309883	-1.622743
H	-5.476532	0.116171	-0.438603
H	1.459026	1.996344	-1.272241
H	1.920002	2.658775	0.291249
H	0.239256	2.174563	0.003891

**Vibrational frequencies**

-477.034	66.5931	76.8315
131.3948	148.7541	173.2672
232.0016	242.952	342.2574
438.766	479.1476	499.7298
529.6501	550.1899	597.5299
652.6858	702.9212	717.3658
749.9413	805.6225	866.6986
908.6535	920.4754	943.3589
998.0047	1002.964	1083.205
1124.718	1181.023	1209.211
1238.04	1305.894	1351.633
1416.006	1420.698	1475.478
1514.284	2200.334	2398.007
3059.533	3074.092	3097.75
3111.911	3214.401	3238.632
3263.757	3270.84	3484.936

**i110 - i113**

**Cartesian coordinates**

C	2.748864	-0.167479	-0.184486
C	1.987511	0.839348	0.447134
C	0.797856	-0.886160	0.509343
C	1.736177	-1.164685	-0.674182
C	-1.739430	-0.361140	0.177011
C	-3.055480	-0.049701	-0.009370
C	-4.216499	0.228528	-0.176561
C	-0.575366	-0.672886	0.344432
C	1.032135	1.759254	-0.268427
H	3.683663	-0.504553	0.251511
H	2.409551	1.297682	1.344629
H	1.104225	-1.339772	1.446483
H	2.097861	-2.193464	-0.739743
H	1.258335	-0.914349	-1.625453
H	-5.241577	0.468129	-0.324334
H	0.639447	1.327416	-1.189415
H	1.567197	2.680635	-0.522836
H	0.186680	2.027808	0.369795

**Vibrational frequencies**

-871.613	67.3054	79.3009
184.0152	197.4987	265.7231
280.6275	313.597	395.8994
441.8627	476.422	508.2307
550.9535	594.0352	645.3997
660.6823	700.1934	756.0984
795.4902	875.4283	938.1019
966.2339	985.5366	1047.839
1069.318	1105.141	1163.366
1197.371	1235.063	1261.433
1371.355	1381.152	1421.634
1436.073	1485.915	1495.585
1511.75	2163.838	2276.193
3044.597	3068.764	3107.605
3113.627	3114.371	3152.627
3185.509	3189.856	3484.235

**Vibrational frequencies**

-867.184	67.4326	77.7385
89.4463	146.6918	198.8562
216.2929	320.4771	343.6242
442.7449	481.1052	497.8949
534.9783	568.9019	657.1892
698.8251	707.3474	708.6268
797.6857	829.4717	870.161
920.0131	984.5868	994.308
1002.168	1049.605	1188.49
1219.31	1223.803	1268.676
1360.773	1418.602	1452.425
1460.744	1477.784	1491.458
1511.642	2192.33	2357.948
3003.339	3026.681	3065.971
3067.944	3114.91	3132.349
3138.905	3227.411	3484.942

**i116 - p80**

**Cartesian coordinates**

C	-1.442143	-1.120072	-0.017233
C	-2.526316	-0.034703	0.292788
C	-1.369739	0.913368	0.507796
C	-0.419349	-0.049724	0.363488
C	2.181499	0.019598	0.021759
C	3.536516	0.053480	-0.174096
C	4.726776	0.085192	-0.346694
C	0.987446	-0.002394	0.198364
C	-3.507702	0.302420	-0.819648
H	-1.399706	-1.388213	-1.075722
H	-1.455299	-2.023854	0.592677
H	-3.065364	-0.253172	1.222143
H	-1.311421	1.975566	0.712558
H	-0.270946	-0.594024	2.199480
H	5.778751	0.114361	-0.498738
H	-4.100171	1.184987	-0.563223
H	-4.197677	-0.527840	-0.992931
H	-2.980092	0.509201	-1.755382

**Vibrational frequencies**

-905.073	58.7392	67.6896
140.5273	203.0967	237.7133
286.7959	319.8594	392.6981
418.4655	437.066	493.1172
498.566	521.1559	563.4911
574.2021	682.7977	707.1987
770.832	847.8055	892.1128
913.1247	927.9075	999.7466
1068.034	1080.23	1102.81
1177.606	1211.545	1228.873
1267.596	1287.253	1365.387
1417.734	1478.062	1497.423
1501.687	1585.884	2199.809
2379.036	3042.662	3050.758
3077.654	3118.589	3124.576
3140.329	3222.663	3483.213

**i110 - i81**

**Cartesian coordinates**

C	2.067867	-0.454378	-0.909720
C	1.882805	0.541402	0.208590
C	0.837011	-0.348646	0.930639
C	1.812106	-1.687913	-0.308263
C	-1.691099	-0.143471	0.278666
C	-3.008045	-0.042077	-0.071559
C	-4.169256	0.049046	-0.380425
C	-0.523525	-0.228337	0.599484
C	1.434946	1.938910	-0.191049
H	1.799310	-0.229205	-1.935875
H	2.772126	0.609560	0.846402
H	1.037991	-0.631029	1.961961
H	2.371977	-1.983560	0.575717
H	1.392853	-2.525652	-0.862445
H	-5.194437	0.131627	-0.649191
H	0.540619	1.896163	-0.817991
H	2.225481	2.447418	-0.748804
H	1.197231	2.537469	0.692045

**Vibrational frequencies**

-956.389	67.9261	74.1501
149.4657	196.5745	214.4943
229.2294	322.107	395.3633
416.2781	490.611	502.8381
527.8691	565.1158	651.0113
661.5129	687.692	689.9736
797.245	856.8469	899.0856
913.6935	968.9696	990.7165
1062.661	1136.567	1151.891
1227.129	1233.054	1247.022
1326.09	1363.212	1397.503
1419.157	1499.001	1500.264
1530.215	2175.001	2301.864
3040.398	3046.414	3116.545
3125.907	3128.275	3147.918
3187.459	3205.175	3485.794

**i102 - p67**

**Cartesian coordinates**

C	-3.362404	-0.118216	-0.531119
C	-2.274256	-0.769688	-0.124005
C	-0.966909	-0.166789	0.099785
C	-0.618137	1.249725	-0.097011
C	1.299006	0.137806	0.623464
C	2.449652	-0.265607	-0.185251
C	3.397077	-0.597518	-0.840028
C	0.674351	1.442024	0.183117
C	0.135221	-0.822069	0.534060
H	-4.303247	-0.635264	-0.676599
H	-3.355696	0.947734	-0.732185
H	-2.336365	-1.837927	0.066958
H	-1.311441	2.013578	-0.422747
H	1.625411	0.229050	1.668865
H	4.233230	-0.891686	-1.427124
H	1.227435	2.368895	1.026805
H	0.234710	-1.886699	0.692456
H	-0.415653	-0.845687	2.725494

**Vibrational frequencies**

-422.523	64.8582	124.2951
141.0136	209.015	226.6246
249.3202	284.0732	359.8859
435.9619	499.483	550.0352
588.5067	632.299	692.8597
716.1531	719.6899	765.9757
810.3434	877.1219	919.6809
929.8494	964.7352	977.2937
1028.49	1046.68	1050.822
1053.281	1116.762	1201.971
1232.126	1277.386	1308.649
1331.018	1418.369	1455.409
1594.368	1667.46	1725.659
2253.376	3037.644	3163.65
3178.367	3230.957	3247.751
3253.532	3257.497	3486.327

**i102 - p65**

**Cartesian coordinates**

C	-3.572523	-0.102635	0.079575
C	-2.410494	-0.736742	-0.086451
C	-1.092470	-0.120056	-0.069379
C	-0.761403	1.196784	-0.121258
C	1.254407	-0.118844	0.093392
C	2.640811	-0.176831	-0.001786
C	3.805935	-0.453796	-0.101492
C	0.666710	1.348114	-0.050397
C	0.172621	-0.928661	-0.007565
H	-4.513118	-0.638676	0.042316
H	-3.622626	0.965604	0.263986
H	-2.423908	-1.813789	-0.239329
H	-1.457557	2.020270	-0.212157
H	1.264326	0.143539	2.134792
H	4.839410	-0.689075	-0.184366
H	1.200147	2.287826	-0.094746

**Vibrational frequencies**

-788.033	56.1628	83.4037
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**i108 - i112**

H 0.306935 -1.499914 -0.935489  
H 0.184825 -1.645909 0.817152

2244.524 2945.16 3156.964  
3168.134 3226.974 3248.799  
3253.162 3256.947 3483.549

H -2.577703 -1.724651 -0.466127  
H -1.313584 -0.152070 -1.885830  
H -1.473068 2.115431 -0.488303  
H 0.756105 -0.293304 1.840852  
H 4.707379 -0.603870 0.413694  
H 1.001868 2.244354 0.403144  
H 0.344067 -1.895518 -0.737214

**Vibrational frequencies**

-760.592 59.4637 126.213  
131.9764 233.2761 245.3487  
330.1514 384.6213 401.618  
426.1884 482.6303 542.4632  
550.7124 570.1011 655.4283  
669.6571 681.2284 721.0858  
869.9698 888.7475 912.2013  
931.748 935.5829 956.0323  
1040.506 1044.117 1075.669  
1142.465 1160.495 1214.82  
1265.635 1323.564 1349.807  
1377.293 1421.634 1464.586  
1504.789 1634.405 1702.011  
2235.475 3055.077 3118.352  
3158.883 3168.337 3230.04  
3247.938 3253.802 3484.707

***i104 - p67***

**Cartesian coordinates**

C 3.419962 -0.078349 0.186018  
C 2.300603 -0.783985 0.057373  
C 0.944431 -0.218976 0.022601  
C 0.602365 1.211479 0.218822  
C -1.275383 0.150162 -0.670725  
C -2.493446 -0.250022 0.037420  
C -3.493295 -0.579490 0.610418  
C -0.660154 1.430364 -0.147396  
C -0.140417 -0.831620 -0.537572  
H 4.388614 -0.563258 0.178841  
H 3.412538 1.000232 0.300952  
H 2.357352 -1.862798 -0.059786  
H 0.653073 -0.709164 1.807603  
H 1.279328 1.944520 0.636113  
H -1.522901 0.274218 -1.735726  
H -4.375264 -0.871959 1.127168  
H -1.207850 2.360103 -0.085112  
H -0.212883 -1.869276 -0.831811

**Vibrational frequencies**

-1027.82 56.5409 128.2834  
136.954 186.6042 253.5313  
378.1634 405.6544 422.6604  
498.5071 532.7234 540.7962  
579.2733 646.5898 665.5093  
684.164 735.7034 746.0986  
780.2192 870.0612 904.0291  
925.8042 965.9859 975.3621  
1002.275 1028.617 1036.747  
1103.091 1111.087 1194.685  
1238.019 1272.114 1299.22  
1334.508 1379.656 1448.049  
1543.978 1667.293 1732.072  
2248.203 3007.389 3154.989  
3171.546 3231.283 3248.35  
3249.443 3256.585 3485.546

***i102 - p70***

**Cartesian coordinates**

C -3.616526 -0.522593 -0.004730  
C -2.342021 -0.271547 -0.117428  
C -1.076820 0.079061 0.009912  
C -0.509539 1.394627 -0.281052  
C 1.274975 0.121660 0.608882  
C 2.522864 -0.357266 0.016762  
C 3.544060 -0.752687 -0.471624  
C 0.788309 1.432942 0.023112  
C 0.070571 -0.838620 0.390840  
H -4.198066 -0.931205 -0.823237  
H -4.130782 -0.326260 0.932431  
H -1.984531 -1.156614 -2.008630  
H -1.094528 2.214897 -0.675172  
H 1.449237 0.261743 1.683387  
H 4.447380 -1.104761 -0.908178  
H 1.442061 2.288713 -0.084797  
H 0.282981 -1.519653 -0.437119  
H -0.148988 -1.440320 1.273274

**Vibrational frequencies**

-980.769 65.441 121.4948  
134.9608 226.3804 248.1691  
349.2514 385.5248 430.3761  
456.8882 517.4289 554.1515  
585.7879 625.3085 693.7927  
705.3656 707.9825 733.383  
782.5239 856.187 906.3941  
924.6849 951.2402 973.3557  
1023.618 1040.458 1049.638  
1051.144 1115.461 1203.316  
1238.057 1280.458 1300.376  
1326.394 1401.091 1449.989  
1552.826 1670.115 1728.613  
2252.247 3020.552 3164.33  
3178.392 3227.361 3246.955  
3254.806 3256.535 3485.973

***i83 - p56***

**Cartesian coordinates**

C -1.303119 -2.286704 0.116712  
C -2.194927 -1.387686 -0.202751  
C -1.532840 1.034832 0.074103  
C -0.685990 0.868237 1.083507  
C 1.333588 0.277813 -0.234920  
C 2.719324 -0.008766 -0.339923  
C 3.891156 -0.255806 -0.453505  
C 0.721609 0.550699 0.933807  
C -2.249969 1.539676 -0.889922  
H -1.460350 -3.348466 -0.080341  
H -0.361497 -2.012155 0.588450  
H -3.176244 -1.418381 -0.659751  
H -1.087238 0.911803 2.091885  
H 0.756519 0.261372 -1.155896  
H 4.927902 -0.469923 -0.551308  
H 1.309692 0.533381 1.846224  
H -2.209224 2.609137 -1.080146  
H -2.892545 0.939452 -1.521769

**Vibrational frequencies**

-334.602 45.4139 64.3195  
97.3814 102.6443 148.0536  
178.0526 197.5625 225.8082  
294.0987 301.2917 376.2332  
447.3447 517.8372 612.0493  
669.9833 706.5668 713.182  
764.0706 857.179 882.4376  
890.6922 912.2949 951.5936  
958.8657 992.7152 1002.338  
1057.805 1075.173 1144.846  
1298.783 1325.008 1383.437  
1390.726 1473.615 1645.131  
1670.048 1977.576 2223.159  
3090.768 3143.472 3171.97  
3176.579 3179.153 3192.045  
3232.005 3233.664 3483.486

**Vibrational frequencies**

-548.856 42.7059 99.3007  
136.864 165.7557 195.8821  
257.4955 380.0374 394.6072  
459.9111 503.875 520.6361  
585.8551 607.6581 649.895  
708.4058 715.1837 721.5836  
797.8567 858.4134 861.8361  
914.0636 973.8607 988.6922  
1021.135 1044.308 1062.23  
1121.938 1192.233 1214.785  
1248.117 1285.946 1303.726  
1348.318 1393.235 1478.832  
1486.691 1669.853 2028.213  
2252.223 3036.145 3082.872  
3137.857 3140.505 3228.125  
3229.736 3251.666 3486.737

***i104 - p69***

**Cartesian coordinates**

C -2.809099 0.217169 1.111085  
C -2.626317 -0.652851 0.149488  
C -0.727696 -0.425685 -1.155602  
C -0.546920 1.028556 -1.008321  
C 0.939038 -0.031134 0.444569  
C 2.396352 -0.144439 0.390306  
C 3.590754 -0.239527 0.352513  
C 0.396750 1.275781 -0.095343  
C 0.208472 -1.055667 -0.388839  
H -3.611734 0.109168 1.841778  
H -2.164428 1.088356 1.216107  
H -3.139405 -1.574063 -0.099331  
H -1.289684 -0.885956 -1.956459  
H -1.130500 1.768187 -1.540077  
H 0.624255 -0.136485 1.495484  
H 4.649630 -0.324761 0.310277  
H 0.744984 2.240323 0.246829  
H 0.388879 -2.117987 -0.313747

***i83 - p54***

**Cartesian coordinates**

C 3.389470 -0.808983 0.088187  
C 2.765596 0.366501 0.068095  
C 1.320275 0.569865 -0.110588  
C 0.494002 -0.605691 -0.486395  
C -1.855651 -0.749089 0.646069  
C -2.998931 -0.078377 0.132372  
C -3.977104 0.487355 -0.276507  
C -0.702559 -0.806130 -0.002744  
C 0.773019 1.779826 0.043555  
H 4.461926 -0.868611 0.230289  
H 2.859104 -1.749031 -0.021836  
H 3.344874 1.276363 0.205112  
H 0.914523 -1.311493 -1.195692  
H -1.962216 -1.279206 1.589162  
H -4.839605 0.987207 -0.646536  
H -0.287341 1.945432 -0.107144  
H 1.380675 2.633152 0.324864  
H -1.120639 -2.565458 -0.990478

**Vibrational frequencies**

-730.503 37.1547 57.6011  
104.0199 132.4537 145.5546  
187.7104 278.924 366.3232  
391.2994 405.5698 443.3919  
486.1371 555.1083 569.0221  
633.2683 671.8858 695.4964  
717.4806 793.8685 820.3105  
864.3631 924.7316 953.851

***i102 - i104***

**Cartesian coordinates**

C -3.490181 -0.018314 -0.211247  
C -2.369940 -0.736797 -0.080214  
C -1.013617 -0.215230 -0.102002  
C -0.616296 1.195995 -0.176043  
C 1.291926 0.061128 0.659300  
C 2.549583 -0.221792 -0.047296  
C 3.577654 -0.443228 -0.623703  
C 0.646137 1.370118 0.226234  
C 0.188159 -0.940376 0.408405  
H -4.461126 -0.497630 -0.199134  
H -3.474560 1.059897 -0.327712  
H -2.453029 -1.814286 0.045731  
H -1.267120 1.977427 -0.544796  
H 1.530112 0.098738 1.736421  
H 4.487298 -0.641958 -1.136981  
H 1.194861 2.302272 0.223559  
H -0.301075 -0.840983 -0.901898  
H 0.164088 -1.952512 0.784200

**Vibrational frequencies**

-403.756 52.1846 72.6796  
107.6677 136.829 185.4264  
233.0465 325.6515 364.0263  
468.577 526.1046 565.645  
683.638 691.2457 711.0674  
729.9513 796.6051 817.6094  
826.7235 898.1427 903.5357  
909.1173 948.0927 975.2159  
999.7542 1036.129 1050.82  
1095.034 1107.264 1125.229  
1224.044 1270.433 1305.096  
1386.778 1398.586 1497.188  
1653.967 1664.334 2252.494  
3003.136 3089.885 3173.169  
3223.57 3225.725 3233.682  
3252.732 3259.687 3487.005

**Vibrational frequencies**

-1893.89 63.2974 123.6407  
129.2052 224.3189 227.8439  
321.5072 412.9584 480.2481  
500.9238 561.3717 568.828  
632.5819 700.5368 708.1185  
721.1488 743.2194 816.9198  
880.5632 897.3984 901.5061  
962.9412 1020.965 1025.198  
1028.845 1050.517 1100.078  
1164.872 1208.85 1248.449  
1278.179 1307.228 1313.537  
1332 1420.916 1468.522  
1648.248 1681.064 2217.013

***i104 - p68***

**Cartesian coordinates**

C -2.916980 -0.230127 0.952330  
C -2.277729 -0.750702 -0.085839  
C -1.107444 -0.116195 -0.804346  
C -0.771732 1.296031 -0.407821  
C 1.085597 0.010211 0.027260  
C 2.483971 -0.243466 0.193087  
C 3.663907 -0.431043 0.305815  
C 0.480078 1.366974 0.046699  
C 0.182401 -0.845333 -0.539965  
H -3.734673 -0.761168 1.426315  
H -2.642795 0.732698 1.370150

964.8987	969.8495	992.5142	H	-3.139853	-1.830851	-0.055768	271.6591	369.5686	416.9287
1038.323	1065.258	1137.009	H	-0.358841	-0.942663	-1.020082	489.4319	528.201	568.9906
1265.7	1330.483	1339.701	H	-0.610058	2.380418	0.590990	608.8114	682.2767	688.8568
1432.947	1449.167	1471.91	H	-2.946773	-0.151037	1.707164	694.6869	702.3265	852.6286
1682.888	1737.013	2007.775	H	-3.698786	0.518446	0.253741	879.0737	915.3973	930.0001
2228.608	3157.029	3162.317	H	-2.890325	1.594588	1.406243	965.7554	1036.035	1067.75
3165.386	3175.681	3178.289	C	2.185018	0.506125	-0.517458	1115.425	1192.914	1281.25
3251.857	3252.486	3483.595	C	2.984417	-0.276944	0.266343	1291.828	1405.663	1429.671
			C	3.694206	-0.969038	0.950182	1484.611	1491.269	1564.066
			C	1.386062	1.185582	-1.130748	1706.828	2199.315	2383.722
			H	4.318731	-1.580224	1.555989	3043.753	3109.805	3116.496
			H	0.919963	1.790854	-1.872902	3141.23	3167.646	3186.184
							3234.123	3270.792	3483.945

**i81 - p50**

**Cartesian coordinates**

C	1.795882	-2.077228	-0.131084
C	2.667164	-1.106382	-0.062007
C	1.634563	1.109753	0.276475
C	0.631754	0.756941	1.119103
C	-1.791516	0.144136	0.327244
C	-3.055901	-0.178200	-0.083180
C	-4.168245	-0.462999	-0.445994
C	-0.671189	0.432332	0.688269
C	1.451723	1.411707	-1.179705
H	2.087949	-3.094806	-0.394616
H	0.739074	-1.908433	0.069256
H	3.736673	-1.029050	-0.211796
H	2.578463	1.399621	0.726936
H	0.833100	0.655813	2.180504
H	-5.151527	-0.712067	-0.764620
H	2.352875	1.179083	-1.748962
H	1.241511	2.479313	-1.310064
H	0.616463	0.850179	-1.601361

**Vibrational frequencies**

-272.219	47.5402	71.3881
74.3562	131.0712	141.9535
180.2645	204.5657	206.0029
309.8093	331.5037	372.2868
464.6793	529.3457	544.7935
590.0438	669.2279	680.6533
749.485	770.7961	776.7133
881.5197	928.1668	950.273
963.1041	1047.343	1081.282
1103.602	1189.101	1263.087
1398.553	1403.328	1442.976
1485.282	1486.368	1601.393
1671.101	2184.286	2330.147
3046.556	3090.78	3118.001
3150.808	3174.764	3184.73
3202.627	3232.257	3484.689

**i109 - i112**

**Cartesian coordinates**

C	-2.944858	-0.369387	-1.029583
C	-1.489771	0.123735	0.285239
C	-0.499366	-0.835340	0.371717
C	-2.927701	-0.256902	0.446907
C	2.042760	-0.315937	0.063129
C	3.372513	-0.046896	-0.092419
C	4.545947	0.191854	-0.230295
C	0.859618	-0.558417	0.198154
C	-1.149514	1.580754	1.122074
H	-3.142688	0.491034	-1.653708
H	-2.718857	-1.313523	-1.504196
H	-0.773125	-1.866497	0.576995
H	-3.551911	0.532303	0.863950
H	-3.082322	-1.196573	0.975033
H	5.581287	0.398696	-0.353590
H	-0.796570	1.979610	1.078947
H	-2.020240	2.163505	-0.183469
H	-0.353350	1.730660	-0.609501

**Vibrational frequencies**

-590.357	66.2089	68.9541
143.9107	178.7227	208.3629
230.4914	338.4417	368.8908
383.6142	452.9044	485.9433
521.5539	541.6576	560.302
637.7449	662.5998	704.731
789.7224	795.7804	811.9142
833.0878	997.8202	1049.365
1059.157	1100.295	1214.387
1223.544	1235.712	1265.687
1374.919	1429.24	1460.117
1475.664	1496.616	1504.026
1520.692	2169.081	2286.204
3045.72	3099.77	3115.426
3142.517	3167.736	3169.853
3183.983	3299.383	3483.913

**i37 - p55**

**Cartesian coordinates**

C	-2.173858	-1.868181	-0.547921
C	-1.314936	-0.850807	-0.514617
C	-1.545853	0.429020	0.175378
C	-0.647065	1.397539	0.138863
C	-2.845196	0.614020	0.931562
H	-1.930823	-2.783418	-1.074888

**Vibrational frequencies**

-327.957	19.7806	38.8766
93.6145	109.9501	163.4017
222.6612	238.4311	262.5031
300.9524	408.5398	422.1685
504.7884	538.5973	542.6455
663.2368	676.9245	692.3533
695.0619	728.7266	762.2317
788.5368	912.524	927.548
960.6666	993.4364	1043.708
1057.135	1086.217	1273.771
1336.697	1398.366	1453.361
1485.655	1495.323	1662.84
1721.199	2076.623	2255.178
3045.278	3112.26	3147.92
3163.521	3194.634	3235.403
3251.016	3451.446	3484.368

**i118 - p82**

**Cartesian coordinates**

C	0.730691	2.525391	-0.223846
C	1.748552	-1.021118	-0.015226
C	1.794766	0.306372	0.047087
C	0.612449	1.199038	0.076981
C	-1.776612	0.069751	0.021556
C	-3.012299	-0.522133	-0.016388
C	-4.095749	-1.043446	-0.049630
C	-0.691590	0.594348	0.058285
C	2.950106	-1.909177	-0.066976
H	1.709985	2.978685	-0.320596
H	-0.141058	3.159798	-0.312296
H	0.777597	-1.511867	-0.028116
H	2.753238	0.819513	0.062565
H	-5.053473	-1.504487	-0.079401
H	2.946009	-2.514067	-0.979361
H	2.951090	-2.607452	0.775983
H	3.879432	-1.336047	-0.039378
H	0.615294	1.321762	1.926846

**Vibrational frequencies**

-1081.02	61.5583	91.1639
115.049	178.2452	188.1949
201.2396	252.8396	307.1251
375.4288	417.8214	432.2538
477.6075	533.1257	548.7632
599.4047	643.3201	654.672
674.3549	682.8316	720.0843
834.8579	889.8578	920.6452
996.0998	1006.226	1074.24
1077.933	1134.199	1308.977
1345.097	1351.66	1417.428
1428.965	1484.045	1493.804
1566.433	1756.61	2202.921
2390.851	3040.345	3101.394
3129.114	3168.935	3172.183
3175.487	3276.224	3485.85

**i118 - p17**

**Cartesian coordinates**

C	0.685726	2.232329	-0.488494
C	2.613941	-0.404909	-0.126695
C	1.482101	-0.463057	0.527996
C	0.152999	1.422485	0.464754
C	-2.081102	0.075395	0.091558
C	-3.250405	-0.615538	-0.091064
C	-4.278019	-1.221033	-0.249611
C	-1.054930	0.691107	0.248502
C	3.626904	-1.516519	-0.219136
H	0.320717	2.213660	-1.507911
H	1.522655	2.878599	-0.254644
H	2.856143	0.516644	-0.658846
H	0.976005	-1.221807	1.111466
H	0.446438	1.553799	1.501498
H	-5.188230	-1.752233	-0.389929
H	4.587026	-1.194563	0.195411
H	3.797465	-1.789432	-1.264812
H	3.298488	-2.406222	0.320905

**Vibrational frequencies**

-391.327	30.235	64.0587
108.3565	119.5285	129.7415
174.3987	203.0949	244.0704

**i81 - p5**

**Cartesian coordinates**

C	1.589458	1.052642	0.019210
C	1.571023	-0.247528	-0.649066
C	0.416840	-0.890509	-1.018309
C	2.669351	1.828612	0.090149
C	-1.981408	-0.197387	-0.234503
C	-3.237947	0.158310	0.168902
C	-4.345010	0.472170	0.525002
C	-0.866293	-0.511285	-0.594096
H	0.651432	1.386839	0.454533
H	2.493056	-0.563499	-1.126164
H	0.482867	-1.782964	-1.632264
H	3.618292	1.519927	-0.338916
H	2.637955	2.797059	0.574591
H	-5.323363	0.747410	0.837238
C	2.266342	-1.537735	1.218958
H	1.471773	-1.250654	1.896020
H	3.235112	-1.075219	1.361654
H	2.238747	-2.542633	0.815829

**Vibrational frequencies**

-429.616	53.8567	57.8755
105.9181	124.53	145.0776
175.7946	183.8665	300.7774
307.1807	410.4871	437.3264
484.0978	496.4558	539.4609
542.6925	639.3103	665.3839
679.1679	697.4146	757.5493
771.4558	825.073	926.171
956.4858	965.3201	1048.549
1125.081	1202.672	1257.97
1320.603	1395.505	1413.907
1421.826	1460.139	1525.686
1711.886	2178.438	2310.071
3103.599	3154.607	3177.559
3182.285	3199.457	3251.468
3275.042	3280.635	3483.981

**i83 - p58**

**Cartesian coordinates**

C	1.474240	-1.811246	-0.886762
C	2.090180	-0.894513	-0.189822
H	1.923720	-2.786783	-1.079918
H	0.481332	-1.639286	-1.297620
H	3.052007	-0.828374	0.303175
C	0.783277	1.180932	0.296368
C	0.219565	1.309639	-0.901870
C	-1.919969	-0.020651	-0.678789
C	-1.723623	-0.603820	0.598157
C	1.498339	-1.141622	1.666472
C	-1.062425	0.794437	-1.329836
C	1.190686	1.391941	1.514954
H	0.811693	1.811802	-1.662821
H	-2.849666	-0.281262	-1.174834
H	-1.462609	-1.604547	2.613530
H	-1.366385	1.114457	-2.321928
H	0.853038	2.280370	2.041409
H	1.835317	0.703041	2.045766

**Vibrational frequencies**

-362.091	50.0211	56.4921
88.1033	121.0659	143.7126
172.504	189.2191	

C	-1.789151	0.263403	0.019309
C	-0.699123	1.051266	-0.006664
C	-2.904292	-1.926953	-0.160231
C	1.734145	0.045988	-0.017007
C	3.002980	-0.469807	-0.019089
C	4.116551	-0.925504	-0.020749
C	0.610588	0.490705	-0.015163
C	-0.781889	2.555828	-0.016206
H	-0.810282	-1.680339	-0.083628
H	-2.765192	0.741549	0.038782
H	-3.883628	-1.459808	-0.164284
H	-2.864640	-3.004934	-0.254331
H	5.099789	-1.330352	-0.021209
H	-0.276920	2.973845	0.858907
H	-1.821792	2.886454	-0.010266
H	-0.290139	2.963417	-0.903551
H	-1.454888	-1.419109	1.897364

**Vibrational frequencies**

-879.01	57.984	75.8331
121.7683	158.8638	175.1201
205.4794	241.4873	299.0434
368.5405	406.5629	412.27
449.7955	518.5272	532.8825
598.9668	620.9896	651.2982
671.5088	675.942	699.0599
894.0642	913.865	944.7848
1038.81	1055.192	1058.859
1075.649	1178.702	1257.785
1304.755	1378.732	1420.565
1454.059	1479.936	1502.061
1609.803	1702.476	2196.466
2374.599	3053.635	3122.787
3144.605	3161.769	3175.954
3182.854	3260.172	3483.85

***i12 - p11***

**Cartesian coordinates**

C	3.830421	0.190925	-0.256782
C	1.357838	-0.024545	0.029787
C	0.340331	-0.923695	-0.024562
C	2.736181	-0.560685	-0.005022
C	-2.207593	-0.295658	-0.025159
C	-3.539529	0.021939	-0.028031
C	-4.709677	0.302866	-0.030975
C	-1.030494	-0.570911	-0.021825
C	1.150317	1.438278	0.114082
H	4.804514	-0.269888	-0.362973
H	3.784406	1.271978	-0.316985
H	0.558063	-1.987137	-0.075205
H	2.832778	-1.642856	-0.039891
H	2.877175	-0.749007	1.914202
H	-5.744249	0.548106	-0.033563
H	1.547586	1.933967	-0.777099
H	1.679841	1.845615	0.980620
H	0.093121	1.686137	0.201805

**Vibrational frequencies**

-863.719	58.9396	66.3713
114.6793	175.0788	206.0426
208.1124	288.4678	327.127
373.2919	407.2847	438.839
447.3277	478.4582	543.9763
580.2517	598.7232	669.4168
675.2884	700.2246	797.285
830.207	879.7514	918.9641
994.5405	1034.973	1064.596
1092.917	1223.167	1238.46
1317.496	1384.835	1434.696
1451.925	1490.09	1496.387
1617.979	1697.607	2197.375
2372.434	3052.915	3114.402
3163.004	3164.735	3172.573
3174.99	3261.411	3486.253

***i12 - p83***

**Cartesian coordinates**

C	-4.189203	0.183605	0.015850
C	-1.133879	0.080252	-0.004521
C	-0.205477	-0.864911	-0.001898
C	-3.288187	-0.818036	-0.009168
C	2.367179	-0.305064	0.001025
C	3.704373	-0.006892	0.002548
C	4.878571	0.256594	0.003893
C	1.188250	-0.570177	-0.000334
C	-1.132548	1.548842	-0.006521
H	-4.546767	0.599966	0.951157
H	-4.558124	0.636135	-0.898006
H	-0.488835	-1.915703	-0.000990
H	-3.008233	-1.335369	0.901866
H	-3.019213	-1.299654	-0.942822
H	5.916192	0.487930	0.005083
H	-1.664513	1.929881	0.870029
H	-1.654652	1.927536	-0.890026
H	-0.110321	1.943997	-0.001538

**Vibrational frequencies**

-301.737	17.8391	48.6404
53.3513	120.9807	124.7566
153.7995	190.6828	223.5428
301.8775	317.4962	366.2642
456.181	502.1097	553.5813
563.5198	681.8469	698.6639
758.0849	815.6092	834.694
885.9762	913.2206	957.283
1029.947	1046.669	1060.584
1202.08	1241.528	1321.83
1328.208	1399.98	1462.578
1467.041	1468.41	1607.832
1720.467	2193.952	2372.009
3026.036	3105.07	3111.601
3140.507	3143.574	3156.124
3227.55	3252.452	3487.285

***i83 - i105***

**Cartesian coordinates**

C	-0.094425	-1.450682	-0.486632
C	1.151970	-1.263358	0.063562
C	1.842857	0.023417	-0.030138
C	1.001329	1.208441	-0.291558
C	-1.116077	0.170991	0.531770
C	-2.491530	0.085133	0.224051
C	-3.654612	-0.024226	-0.079268
C	-0.318787	1.265059	-0.054095
C	3.164235	0.143713	0.167566
H	-0.631359	-2.373465	-0.293543
H	-0.386150	-0.923605	-1.386816
H	1.560946	-2.007566	0.740246
H	1.498209	2.085725	-0.693500
H	-0.843086	-0.170337	1.524845
H	-4.684266	-0.111563	-0.329213
H	-0.862517	2.163581	-0.333535
H	3.781713	-0.722169	0.380024
H	3.656754	-1.108477	0.119944

**Vibrational frequencies**

-732.696	63.0822	120.0496
163.7865	278.596	336.2558
346.6825	375.2372	448.1264
487.1314	510.7611	596.1395
617.5724	654.0455	692.57
722.574	745.3521	777.3594
792.0564	834.7392	919.9988
943.7053	952.0716	984.2426
998.2728	1025.921	1071.602
1108.193	1232.079	1263.034
1317.875	1332.437	1395.332
1428.962	1464.953	1549.04
1642.076	1697.376	2160.936
3156.473	3157.807	3165.94
3177.902	3180.16	3199.044
3246.803	3249.517	3480.799

***i118 - i120***

**Cartesian coordinates**

C	0.732534	2.121743	-0.134112
C	2.684916	-0.217250	-0.180829
C	1.422798	-0.342798	0.238025
C	0.397014	0.710989	0.192346
C	-2.114096	-0.058038	0.024502
C	-3.420075	-0.458385	-0.054427
C	-4.569907	-0.809606	-0.123317
C	-0.958645	0.296517	0.088008
C	3.713636	-1.300050	-0.088222
H	1.764621	2.437432	-0.133187
H	-0.059429	2.808328	-0.392769
H	0.479397	1.524557	1.117240
H	3.008576	0.716234	-0.634806
H	1.088720	-1.287187	0.659573
H	-5.584950	-1.119352	-0.186369
H	4.557566	-0.987267	0.535874
H	4.120904	-1.537206	-1.076149
H	3.295542	-2.214271	0.338755

**Vibrational frequencies**

-1835.98	56.2619	76.7184
128.3715	170.7355	192.6894
201.5051	249.2758	311.037
364.1853	400.3431	432.1293
501.7702	517.7588	552.3868
602.353	653.328	657.1007
689.4975	705.9233	828.0004
901.7969	974.058	999.1286
1026.706	1066.915	1132.873
1179.311	1290.29	1310.97
1329.788	1376.052	1421.115
1432.669	1485.843	1495.355
1713.967	2188.233	2241.699
2341.015	3037.618	3096.787
3128.734	3169.497	3174.451

3195.426 3322.151 3485.921

***i38 - i112***

**Cartesian coordinates**

C	-3.910877	0.241144	-0.123864
C	-1.348114	-0.090673	0.013711
C	-0.300821	-0.971300	-0.007456
C	-2.695577	-0.590067	0.026431
C	2.228397	-0.297704	-0.008089
C	3.551702	0.045191	-0.010393
C	4.717590	0.349419	-0.012710
C	1.053037	-0.598627	-0.004557
C	-1.142783	1.395383	0.031856
H	-4.864464	-0.248027	-0.254422
H	-3.841057	1.317728	-0.179292
H	-3.310996	-0.233515	1.040165
H	-0.507469	-2.037750	-0.035027
H	-2.837710	-1.659959	-0.088571
H	5.746929	0.614563	-0.015031
H	-1.654191	1.852150	0.886483
H	-1.561009	1.847876	-0.873831
H	-0.085362	1.650327	0.089957

**Vibrational frequencies**

-1872.05	62.7416	65.3202
145.112	198.0314	204.9514
223.8791	269.3778	361.6941
368.1441	411.6498	450.5596
535.9273	537.8757	550.2244
584.3693	621.6784	642.9636
691.968	790.1076	795.1206
826.429	882.9618	969.4757
1058.063	1066.865	1142.264
1230.146	1231.623	1269.746
1382.982	1430.368	1440.99
1465.842	1489.343	1494.966
1596.344	2179.227	2251.499
2317.637	3038.264	3094.66
3159.092	3170.833	3184.319
3189.139	3310.463	3488.346

***i115 - i120***

**Cartesian coordinates**

C	-2.774974	-0.188904	0.022616
C	-1.363918	-0.426369	0.004179
C	-0.409182	0.549551	-0.005603
C	-3.792213	-1.257046	-0.090244
C	2.136253	-0.086674	-0.004467
C	3.465976	-0.405645	-0.002294
C	4.637713	-0.685688	-0.000316
C	0.955540	0.189160	-0.003262
C	-0.750034	2.022047	-0.015311
H	-3.134611	0.823902	-0.126892
H	-1.033676	-1.461609	0.018733
H	-4.829153	-0.992084	-0.232003
H	-3.297510	-0.615890	1.056038
H	-3.487366	-2.294748	-0.097824
H	5.672031	-0.930742	0.001502
H	-1.323426	2.296884	0.876257
H	-1.351362	2.282237	-0.892521
H	0.154112	2.629458	-0.035075

**Vibrational frequencies**

-1904.75	48.0736	64.302
88.1305	129.295	182.0064
193.3824	250.4349	339.9339
360.9936	402.2687	475.0886
496.4189	511.558	551.4639
602.0775	610.5749	645.515
695.3088	724.2628	859.3446
896.1598	907.0331	985.1239
1043.208	1053.225	1131.229
1228.689	1247.303	1285.179
1362.4	1407.703	1421.298
1443.281	1494.469	1497.815
1606.652	2180.453	2252.087
2322.908	3033.185	3

H	-1.277631	-1.081909	1.506300
H	4.962050	1.441799	0.085486
H	-0.558566	1.130315	0.627857
H	-1.385523	2.640972	1.063698
H	-0.696451	2.443262	-0.545099

**Vibrational frequencies**

-201.171	33.5987	47.0581
92.55	114.884	148.3986
164.7983	194.5531	229.4203
261.8916	361.2452	457.2658
496.804	536.9378	566.7742
620.581	673.448	692.9862
702.0484	718.7064	850.1763
867.0593	913.0629	948.7944
972.4013	1048.812	1068.285
1130.24	1210.452	1282.525
1301.954	1414.039	1440.185
1490.603	1494.598	1609.474
1709.497	2191.243	2350.949
3046.569	3055.54	3106.402
3165.633	3176.267	3186.472
3244.228	3275.8	3484.367

**i113 - p78**

**Cartesian coordinates**

C	-2.364668	-0.802412	-0.049469
C	-3.490848	-0.083711	-0.108001
C	0.088421	-1.067897	-0.002966
C	-1.012124	-0.270794	0.051276
C	2.541606	-0.152356	-0.021386
C	3.822866	0.326771	-0.034196
C	4.949483	0.750794	-0.046098
C	1.405466	-0.569575	-0.013113
C	-3.625827	1.404386	-0.043248
H	-2.442980	-1.885836	-0.091186
H	-4.425333	-0.630883	-0.204815
H	-0.030226	-2.148240	-0.021228
H	-0.865642	0.802393	-0.007394
H	5.944061	1.126680	-0.056702
H	-2.674659	1.917564	0.099103
H	-4.286364	1.686156	0.782747
H	-4.085617	1.787311	-0.959981
H	-1.019491	0.133621	2.062666

**Vibrational frequencies**

-742.107	54.6814	74.0382
82.7903	123.1846	166.0353
193.3392	273.4232	299.9744
343.6379	364.7964	395.0257
465.8502	480.4862	550.0262
567.555	631.6451	670.8059
686.02	744.3506	784.5661
859.8626	942.9557	977.9247
1020.883	1057.439	1069.109
1169.54	1222.755	1274.296
1318.703	1326.118	1419.577
1448.902	1486.894	1501.609
1606.786	1732.494	2189.933
2344.309	3049.055	3103.763
3149.706	3162.887	3171.253
3183.44	3204.81	3482.6

**i113 - p71**

**Cartesian coordinates**

C	1.421546	-0.505185	-0.026059
C	2.606939	-1.124336	-0.032594
C	-0.007608	1.530179	-0.120198
C	1.215051	0.936266	-0.040673
C	-2.296050	0.258145	-0.033633
C	-3.495834	-0.397040	0.013319
C	-4.551524	-0.974078	0.055682
C	-1.232645	0.835605	-0.072179
C	3.966106	-0.500530	-0.010162
H	0.520426	-1.111344	-0.021378
H	2.596622	-2.211572	-0.046093
H	-0.067985	2.610552	-0.201687
H	2.079108	1.579486	-0.163498
H	-5.485126	-1.481453	0.094518
H	3.941791	0.586036	0.076025
H	4.520647	-0.759148	-0.918133
H	4.542718	-0.890300	0.834378
H	1.595911	1.323585	1.944840

**Vibrational frequencies**

-725.4	24.5197	55.5404
91.2941	118.6147	178.5083
228.7769	233.9713	301.3597
348.9075	359.879	394.2258
517.0412	526.5767	559.3951
572.8901	658.8391	677.7802
709.341	760.361	767.0043
807.0138	942.2062	992.0697
1018.937	1028.082	1064.216
1148.958	1191.11	1252.882

1300.296	1377	1424.228
1469.119	1482.408	1494.503
1577.453	1732.274	2188.478
2340.15	3047.369	3103.642
3147.8	3167.533	3185.115
3188.212	3215.642	3483.851

**i34 - p14**

**Cartesian coordinates**

C	3.701796	-1.259943	-0.166797
C	2.856043	-0.240535	-0.019959
C	0.471327	0.563805	-0.004525
C	1.411615	-0.419816	0.079923
C	-2.076969	-0.077843	-0.022071
C	-3.407305	-0.399360	-0.033651
C	-4.577328	-0.681175	-0.043986
C	-0.899083	0.197140	-0.013634
C	0.753185	2.042426	-0.035653
H	4.769514	-1.099720	-0.255036
H	3.349958	-2.286489	-0.203032
H	3.251611	0.769064	0.019952
H	1.058231	-1.446674	0.047986
H	1.353879	-0.636851	2.128909
H	-5.611341	-0.928773	-0.052951
H	1.816020	2.261380	-0.124446
H	0.378186	2.512664	0.878347
H	0.234254	2.507203	-0.877616

**Vibrational frequencies**

-705.749	63.8602	74.3832
85.6748	107.0759	171.9344
200.332	248.2787	267.0405
332.6908	375.2522	382.8755
420.6106	510.1219	525.0949
602.7578	609.8719	677.2708
684.6189	699.4577	735.6968
906.6197	941.5918	964.9414
1005.938	1026.395	1062.313
1072.488	1197.845	1280.653
1332.268	1370.647	1429.179
1453.248	1482.509	1497.673
1605.93	1711.637	2191.962
2352.397	3056.841	3118.68
3156.855	3168.568	3181.143
3200.684	3253.035	3485.962

**i105 - p66**

**Cartesian coordinates**

C	-0.267185	1.235323	-0.295996
C	1.060321	1.221532	-0.080887
C	1.811637	-0.016716	0.091453
C	1.028643	-1.256441	0.050894
C	-1.047639	-0.028274	-0.589057
C	-2.378336	-0.027170	0.028023
C	-3.473735	-0.040457	0.514642
C	-0.270468	-1.275383	-0.237985
C	3.137118	-0.019800	0.297033
H	-0.789899	2.172517	-0.450598
H	-0.864477	1.440135	1.691287
H	1.595090	2.159157	0.030502
H	1.547168	-2.184311	0.270664
H	-1.216803	-0.045299	-1.678305
H	-4.438957	-0.046104	0.960554
H	-0.821138	-2.209314	-0.258387
H	3.703738	0.903938	0.331748
H	3.683132	-0.946405	0.433822

**Vibrational frequencies**

-636.871	64.5167	141.5172
196.3698	219.0551	338.9245
364.0619	372.625	419.2155
419.6185	521.6839	538.597
611.8371	664.4432	694.5239
703.0303	712.1444	789.3771
799.1683	824.7791	887.9881
924.112	953.2183	974.0634
1012.443	1016.779	1064.436
1070.667	1180.03	1223.431
1302.84	1309.244	1344.603
1396.095	1439.616	1474.058
1642.007	1674.674	1752.871
2252.221	2987.255	3161.442
3186.468	3190.674	3210.431
3213.228	3253.258	3486.345

**i105 - i107**

**Cartesian coordinates**

C	0.350003	1.274304	0.215847
C	-1.110318	1.234687	-0.060486
C	-1.827879	-0.021580	-0.105606
C	-1.001336	-1.236342	-0.047923
C	1.091217	0.013944	0.580087
C	2.428968	-0.025939	-0.026886
C	3.521035	-0.064667	-0.520207
C	0.300375	-1.234143	0.234317

C	-3.170141	-0.103860	-0.212615
H	0.806969	2.234354	0.412349
H	-0.262618	1.306145	-0.992493
H	-1.659541	2.166139	0.010811
H	-1.500441	-2.180818	-0.240828
H	1.243177	0.002053	1.673932
H	4.486927	-0.098089	-0.963379
H	0.852983	-2.166886	0.267839
H	-3.791412	0.783922	-0.246084
H	-3.667586	-1.065255	-0.261314

**Vibrational frequencies**

-1944.35	51.0993	139.7577
191.7121	281.5793	326.0065
369.4449	405.8445	466.8485
512.2626	578.0786	622.5753
643.2837	677.1229	701.1447
713.087	767.5369	782.5217
825.8408	864.6322	873.5058
936.7644	949.9214	1015.826
1040.405	1057.131	1137.571
1214.038	1241.805	1288.816
1303.823	1319.868	1358.951
1388.925	1446.784	1468.347
1631.582	1740.526	2221.964
2250.378	2946.843	3158.776
3183.033	3200.451	3206.876
3229.677	3251.826	3486.001

**i111 - i122**

**Cartesian coordinates**

C	-1.654415	-1.515091	-0.605907
C	-1.876199	-0.056046	-0.395601
C	-0.895779	0.873753	-0.127650
C	-2.006668	-1.674178	0.824045
C	1.630310	0.177710	-0.036654
C	2.948387	-0.180435	0.014276
C	4.109749	-0.497910	0.059087
C	0.459643	0.494191	-0.089687
C	-1.225883	2.310078	0.188872
H	-2.351216	-1.972057	-1.306431
H	-0.624378	-1.768577	-0.851561
H	-2.901604	0.292855	-0.457868
H	-3.031954	-1.827205	1.133286
H	-1.238177	-1.585135	1.579219
H	5.135245	-0.775251	0.099033
H	-0.980573	2.546424	1.229374
H	-2.289070	2.504735	0.035521
H	-0.653141	2.991780	-0.445261

**Vibrational frequencies**

-564.139	61.8875	95.0222
141.7804	163.3355	195.0019
215.7964	274.2867	322.8529
426.1887	499.96	505.6034
538.9299	582.2956	611.5294
629.3825	654.0513	654.8385
688.6914	821.1443	862.463
913.2801	1042.26	1059.18
1072.217	1110.149	1164.093
1232.805	1237.105	1266.853
1382.102	1423.674	1457.843
1486.168	1488.751	1501.327
1524.27	2174.92	2302.647
3040.121	3098.659	3106.59
3139.272	3166.749	3176.598
3198.457	3294.173	3487.072

**i116 - i117**

**Cartesian coordinates**

C	1.621114	-0.763838	1.160334
C	2.311585	0.604961	-0.354673
C	1.760164	-0.483965	-1.028993
C	0.797177	-1.162447	-0.074915
C	-1.734568	-0.333867	-0.053693
C	-3.040065	0.088457	-0.038849
C	-4.185091	0.456541	-0.023859
C	-0.5		



676.9864	683.4338	705.4205
766.4635	861.0195	882.6274
958.9157	983.0185	999.5332
1053.096	1067.199	1103.807
1198.595	1222.447	1227.656
1330.282	1381.336	1428.804
1440.283	1466.116	1499.449
1527.02	2201.468	2399.731
3042.174	3048.456	3094.324
3114.751	3117.526	3159.978
3202.168	3237.832	3486.841

**i122 – p84**

**Cartesian coordinates**

C	-1.361350	-2.124506	-0.557384
C	-2.091480	0.124865	-0.234384
C	-1.161729	1.045784	-0.032189
C	-0.947873	-2.523824	0.657348
C	1.405754	0.441354	-0.044874
C	2.741022	0.133449	-0.043924
C	3.912963	-0.139079	-0.042505
C	0.225516	0.697022	-0.045200
C	-1.481036	2.507110	0.221820
H	-2.345702	-2.385860	-0.930297
H	-0.660758	-1.716255	-1.277249
H	-3.171079	0.214163	-0.234664
H	-1.621525	-3.011463	1.353453
H	0.061323	-2.322894	0.998961
H	4.949192	-0.377138	-0.041652
H	-1.068609	2.821664	1.184098
H	-2.559416	2.671137	0.229612
H	-1.034154	3.133590	-0.554516

**Vibrational frequencies**

-278.269	44.3921	59.493
86.9455	107.4164	139.5964
154.3098	212.4601	241.3898
289.8474	330.4724	374.7873
507.0186	512.2854	589.448
607.074	620.9415	676.2288
698.3041	730.3555	838.9479
883.1035	928.2944	974.3256
988.7084	1043.983	1046.028
1067.413	1241.058	1279.246
1340.685	1403.294	1466.297
1476.131	1489.842	1620.2
1665.891	2197.392	2379.415
3053.396	3126.128	3150.526
3151.7	3163.526	3225.303
3235.662	3260.841	3486.021

**i120 – p82**

**Cartesian coordinates**

C	-0.744066	2.491629	-0.166762
C	-1.738477	-1.063939	0.016967
C	-1.786325	0.264746	-0.073346
C	-0.616129	1.152059	-0.105383
C	1.778083	0.052321	-0.026666
C	3.019626	-0.526220	0.008971
C	4.108562	-1.036619	0.038836
C	0.686215	0.565751	-0.060437
C	-2.936860	-1.955923	0.053577
H	-1.724913	2.948503	-0.231057
H	0.120837	3.140405	-0.213002
H	-0.766512	-1.550043	0.071665
H	-2.749017	0.768311	-0.125833
H	5.070791	-1.488332	0.066124
H	-2.958848	-2.534111	0.983041
H	-2.907525	-2.679077	-0.767578
H	-3.867423	-1.389005	-0.019941
H	-0.841176	3.120524	2.122035

**Vibrational frequencies**

-399.806	62.258	92.2794
106.424	137.8541	175.1502
181.3573	201.5189	215.3375
256.8425	326.638	378.5343
431.8368	540.0057	541.0862
633.9615	638.7572	659.662
681.9979	716.0132	753.934
852.9976	924.6795	939.416
1000.801	1011.741	1076.129
1084.015	1136.116	1319.423
1353.106	1366.859	1421.201
1442.484	1483.046	1495.674
1641.817	1748.905	2200.952
2383.855	3041.836	3102.269
3130.901	3166.677	3169.591
3170.692	3269.786	3485.83

**i120 – p14**

**Cartesian coordinates**

C	0.668492	2.068069	-0.058575
C	2.807546	-0.168558	0.094608
C	1.374940	-0.374579	0.077182

C	0.424540	0.582044	0.010406
C	-2.118780	-0.098538	-0.000486
C	-3.445830	-0.436922	-0.007764
C	-4.612088	-0.733111	-0.014490
C	-0.945282	0.190283	0.006220
C	3.687356	-1.178912	0.167525
H	0.210240	2.482245	-0.960437
H	0.205090	2.563409	0.798865
H	1.728848	2.315699	-0.066985
H	3.186292	0.846750	0.035947
H	1.042347	-1.408129	0.124233
H	-5.642995	-0.993313	-0.020791
H	3.357327	-2.209065	0.257321
H	4.753983	-0.996900	0.214853
H	4.113490	-1.699339	-2.030757

**Vibrational frequencies**

-430.41	61.8482	75.5678
97.1424	103.3732	153.4177
191.1362	220.2519	248.2006
262.4558	350.3005	373.6545
415.873	509.9443	513.1341
592.751	607.1612	678.7055
697.1528	704.7887	733.9133
911.1986	932.65	958.0669
1005.936	1022.902	1065.875
1068.289	1202.652	1277.62
1316.886	1369.206	1427.818
1455.882	1481.228	1497.389
1649.031	1684.888	2196.661
2371.335	3059.269	3122.098
3160.212	3163.252	3177.195
3195.29	3258.094	3487.061

**i120 – p13**

**Cartesian coordinates**

C	-0.664048	2.581903	-0.046198
C	-1.798680	-1.118017	0.115352
C	-1.754049	0.327513	0.058367
C	-0.633072	1.076294	0.007996
C	1.770660	0.003744	-0.002546
C	3.026128	-0.543267	-0.010561
C	4.128315	-1.025983	-0.018048
C	0.657836	0.475185	0.003945
C	-2.943041	-1.815830	0.163543
H	-1.691534	2.949202	-0.045626
H	-0.139591	3.008580	0.813239
H	-0.162890	2.945114	-0.947550
H	-0.848270	-1.644306	0.108543
H	-2.709785	0.846364	0.056752
H	5.101581	-1.454193	-0.025325
H	-3.907448	-1.319058	0.202753
H	-2.941749	-2.896072	0.242361
H	-3.440608	-2.204887	-2.036244

**Vibrational frequencies**

-430.439	59.7534	79.3186
122.2701	140.8898	161.8233
179.3636	229.4103	241.9144
275.2853	302.702	379.2776
435.0273	517.4747	533.6864
607.7158	622.0783	651.7686
674.9033	708.4935	719.3289
912.9254	948.3364	955.4832
1030.839	1042.395	1056.212
1072.605	1189.431	1259.711
1327.509	1382.361	1418.107
1458.031	1478.124	1501.211
1652.753	1686.321	2196.667
2372.562	3053.257	3120.61
3147.161	3159.258	3174.19
3189.118	3255.438	3485.085

**i107 – p64**

**Cartesian coordinates**

C	-0.345424	-1.222465	0.014987
C	1.133031	-1.256009	0.238226
C	1.828739	0.055518	-0.059693
C	1.025183	1.264303	0.126839
C	-1.043185	-0.060161	0.156261
C	-2.448639	-0.005688	-0.137660
C	-3.616469	0.067407	-0.403983
C	-0.305724	1.219686	0.247525
C	3.107341	0.115676	-0.437752
H	-0.873620	-2.152431	-0.157519
H	1.591877	-2.074147	-0.321652
H	1.295371	-1.488500	1.304250
H	1.538431	2.220318	0.125763
H	-1.315614	-0.112739	2.034867
H	-4.653230	0.126712	-0.632188
H	-0.889189	2.123842	0.370601
H	3.693136	-0.781332	-0.607185
H	3.603720	1.068680	-0.585433

**Vibrational frequencies**

-430.41	61.8482	75.5678
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-953.521	64.7668	146.2635
169.0523	258.7266	345.5738
379.477	399.5186	411.0277
463.6035	506.8372	531.7004
587.5171	630.6155	679.6948
703.1791	714.6344	736.9544
778.9822	804.1848	828.0297
925.3831	951.9577	961.0536
985.4616	1004.261	1063.979
1174.746	1197.167	1230.206
1308.074	1348.8	1353.638
1425.446	1451.143	1470.477
1577.41	1685.382	1732.676
2244.97	2978.079	3101.699
3155.828	3196.03	3216.282
3227.807	3244.666	3485.195

**i107 – p66**

**Cartesian coordinates**

C	-0.298935	-1.187849	0.563734
C	0.968169	-1.215903	0.102119
C	1.738654	0.019521	-0.127811
C	0.986582	1.271698	-0.021244
C	-1.096847	0.084909	0.682729
C	-2.323739	0.006792	-0.119954
C	-3.322935	-0.060374	-0.778651
C	-0.295666	1.315207	0.332952
C	3.046110	-0.004498	-0.405655
H	-0.816410	-2.110325	0.801952
H	0.631732	-1.604220	-1.761723
H	1.515828	-2.152703	0.106160
H	1.515798	2.192502	-0.245557
H	-1.419002	0.182931	1.735467
H	-4.205645	-0.119181	-1.368529
H	-0.822228	2.261743	0.388553
H	3.587932	-0.939806	-0.490441
H	3.603647	0.912033	-0.562489

**Vibrational frequencies**

-867.239	48.411	138.11
173.9257	272.5591	311.8032
369.4411	386.5765	422.1314
446.7559	541.9213	544.0685
603.2564	667.8193	689.614
715.9531	720.9832	783.0347
798.0684	810.5567	896.9864
930.7129	954.095	970.4637
1015.762	1018.631	1045.551
1070.692	1182.951	1223.335
1278.423	1324.029	1346.089
1397.568	1436.664	1474.029
1626.506	1695.406	1762.853
2249.517	3000.129	3162.777
3184.826	3188.642	3208.556
3211.265	3253.615	3486.18

**i117 – p17**

**Cartesian coordinates**

C	-1.524482	1.873739	0.863238
C	-1.908936	-1.496551	-0.416585
C	-1.899805	-0.361639	-1.074272
C	-0.847518	1.509828	-0.261999
C	1.572458	0.472532	-0.141404
C	2.825120	-0.077586	-0.068482
C	3.923573	-0.564169	-0.001977
C	0.463555	0.944949	-0.200514
C	-1.275696	-1.784578	0.913153
H	-1.182590	1.574829	1.846418
H	-2.458923	2.415189	0.790092
H	-2.422026	-2.341648	-0.887217
H	-2.335103	-0.085402	-2.026125
H	-1.125012	1.951490	-1.213356
H	4.893547	-0.995345	0.057728
H	-0.507008	-2.556078	0.807549
H	-2.022598	-2.164032	1.616889
H	-0.809897		

***ii17 - p72***

**Cartesian coordinates**

C	-1.403899	-2.299087	0.118196
C	-1.999678	1.352711	-0.297713
C	-2.069609	0.024796	-0.391303
C	-1.071196	-0.976239	0.066527
C	1.496964	-0.356955	-0.015095
C	2.827138	-0.034348	-0.079456
C	3.994608	0.249966	-0.136984
C	0.323982	-0.629778	0.046423
C	-0.930444	2.173759	0.355688
H	-0.660411	-3.056017	0.329571
H	-2.435741	-2.608174	-0.000738
H	-2.827359	1.908462	-0.730996
H	-2.947009	-0.413828	-0.857120
H	-1.210042	-0.548546	1.888844
H	5.027236	0.498094	-0.189356
H	-1.359241	3.091962	0.763275
H	-0.160132	2.462838	-0.366880
H	-0.434486	1.636250	1.165691

**Vibrational frequencies**

-1033.75	61.0348	64.1119
112.7052	135.4104	215.6387
275.0332	280.5957	338.1528
380.1866	441.9487	471.5581
500.5322	533.3354	568.4662
582.8014	626.1135	665.7559
684.2	702.0227	711.938
776.9278	891.8141	904.9064
982.2284	1006.176	1071.493
1073.653	1116.26	1275.318
1343.831	1392.795	1414.534
1454.49	1484.523	1514.268
1561.386	1739.62	2201.221
2386.649	3049.364	3114.996
3137.391	3166.358	3171.704
3191.26	3277.476	3485.884

***ii19 - ii17***

**Cartesian coordinates**

C	1.335835	-2.362638	0.311607
C	2.129132	1.323936	-0.104634
C	2.114033	-0.005797	-0.234738
C	1.001734	-0.965040	-0.106589
C	-1.543029	-0.312233	-0.052298
C	-2.871115	0.013622	-0.037763
C	-4.040295	0.302608	-0.023613
C	-0.360472	-0.572916	-0.054436
C	1.014565	2.258684	0.252638
H	0.535179	-3.055460	0.521592
H	2.369218	-2.621145	0.491047
H	3.091263	1.800235	-0.278273
H	3.060170	-0.488569	-0.471079
H	-5.072819	0.555496	-0.010725
H	0.656162	2.789704	-0.636054
H	1.376372	3.016634	0.952981
H	0.162942	1.753242	0.703517
H	1.139183	-1.831485	-0.974047

**Vibrational frequencies**

-1845.98	34.7283	59.1795
93.7039	109.4709	211.2633
250.0364	272.3838	306.6404
377.6125	445.9567	474.3298
515.5122	548.9626	566.8881
600.6452	642.1671	649.2323
702.1192	704.3522	775.3783
885.9258	967.7442	1008.217
1037.634	1069.663	1118.419
1183.214	1226.873	1304.693
1391.01	1415.59	1426.161
1461.551	1490.802	1503.485
1736.179	2185.412	2239.298
2334.315	3046.679	3101.985
3146.364	3167.684	3178.52
3186.961	3320.16	3486.623

***ii19 - p72***

**Cartesian coordinates**

C	-1.332551	-2.256579	-0.277824
C	-2.085646	1.363532	0.117147
C	-2.115753	0.027762	0.102339
C	-1.036774	-0.952596	-0.099847
C	1.521496	-0.324168	-0.019484
C	2.854221	-0.011637	0.027831
C	4.024426	0.264684	0.069037
C	0.342385	-0.579377	-0.064019
C	-0.945602	2.309817	-0.093917
H	-0.557065	-2.993778	-0.440460
H	-2.364026	-2.587635	-0.319188
H	-3.042040	1.847681	0.303846
H	-3.083435	-0.442561	0.255915
H	5.059524	0.505118	0.107063
H	-0.686961	2.805617	0.847890

H	-1.247690	3.095388	-0.792612
H	-0.050106	1.830331	-0.481205
H	-1.385414	-3.108784	1.951160

**Vibrational frequencies**

-396.837	39.2533	64.3259
104.0296	116.631	139.8448
180.3268	220.9709	271.5772
292.6142	332.6836	385.4982
488.8626	544.3987	574.1876
610.5564	631.3713	684.8999
701.6111	716.8439	741.0959
808.5056	901.2764	938.2443
981.7025	1023.216	1074.466
1078.588	1125.959	1305.602
1372.817	1415.352	1425.086
1470.044	1490.647	1508.211
1628.468	1744.681	2199.163
2379.417	3052.367	3106.402
3147.712	3167.138	3173.416
3194.642	3267.56	3485.459

***ii19 - p14***

**Cartesian coordinates**

C	-0.992350	1.631287	-0.066048
C	-2.699149	-1.009877	-0.119209
C	-1.247511	-0.902469	-0.104917
C	-0.484838	0.211936	-0.063833
C	2.136957	-0.027336	-0.002167
C	3.501373	-0.139813	0.035148
C	4.700155	-0.238711	0.068609
C	0.931970	0.059817	-0.031804
C	-3.592533	-0.161229	0.412842
H	-1.128722	1.997352	0.956782
H	-1.950033	1.705403	-0.584073
H	-0.272456	2.288223	-0.555999
H	-3.081070	-1.914637	-0.586219
H	-0.718502	-1.849365	-0.162670
H	5.759202	-0.328001	0.099809
H	-4.650773	-0.392229	0.385427
H	-4.183128	1.235063	-1.299692
H	-3.298964	0.716553	0.974908

**Vibrational frequencies**

-424.775	55.0114	70.3355
105.0798	183.4856	192.1754
220.9299	239.6911	264.694
304.3367	318.345	380.1815
499.9352	510.3131	535.2861
574.9169	599.5255	673.0174
674.7981	702.0395	776.4384
902.1433	931.9405	963.3322
1023.93	1051.656	1054.626
1071.017	1119.586	1301.114
1338.837	1393.044	1422.289
1461.19	1493.687	1511.359
1651.169	1689.77	2195.912
2372.14	3051.51	3122.845
3152.935	3162.541	3171.997
3186.494	3260.213	3485.204

***ii19 - p13***

**Cartesian coordinates**

C	1.366660	-2.375147	-0.020924
C	2.019238	1.471001	0.071159
C	2.084850	0.017256	0.038632
C	1.087521	-0.891296	-0.000651
C	-1.479585	-0.325063	0.001123
C	-2.819545	-0.045400	0.002217
C	-3.996843	0.203622	0.002703
C	-0.289827	-0.540566	-0.002829
C	0.995004	2.261817	-0.282309
H	0.900281	-2.864871	0.838300
H	2.440088	-2.569015	0.004899
H	0.949802	-2.831898	-0.922704
H	2.931157	1.950899	0.417606
H	3.090969	-0.392236	0.083023
H	-5.037519	0.421841	0.004890
H	1.098544	3.339184	-0.229389
H	-0.253659	2.415334	1.648886
H	0.075501	1.873425	-0.700247

**Vibrational frequencies**

-396.293	60.3037	66.0037
112.7486	139.565	159.4028
208.4492	216.4418	256.8739
271.0752	307.0127	340.4972
484.1327	521.9531	564.3436
599.4329	614.4651	674.4583
678.9894	701.4159	708.4764
909.1196	963.399	973.3759
1013.942	1034.871	1075.323
1076.29	1143.887	1246.003
1349.783	1418.398	1425.421
1467.613	1477.969	1504.115

1649.478	1697.015	2194.188
2366.318	3051.743	3118.905
3147.438	3161.684	3173.557
3182.716	3270.654	3484.154

***ii8 - p61***

**Cartesian coordinates**

C	0.194056	-1.112742	-0.042448
C	-1.081607	-0.691996	0.007331
C	-1.052342	0.795996	0.059762
C	-2.091227	1.618588	-0.211251
C	1.103159	0.047972	0.001487
C	2.520840	-0.050440	-0.029168
C	3.716945	-0.159752	-0.058228
C	0.369580	1.180379	0.078225
C	-2.332708	-1.504947	-0.012993
H	0.532498	-2.138538	-0.102339
H	-1.089139	0.685169	1.984524
H	-1.953362	2.691142	-0.282248
H	-3.096328	1.231532	-0.335635
H	4.776002	-0.250445	-0.083201
H	0.737807	2.194698	0.119022
H	-2.955863	-1.252451	-0.877098
H	-2.930302	-1.329558	0.886515
H	-2.101486	-2.569900	-0.065838

**Vibrational frequencies**

-897.875	98.8438	121.1883
137.6519	208.3251	245.1895
273.6231	300.7931	388.0341
429.6665	434.1399	506.6923
564.7575	611.7634	627.2981
647.6905	662.8107	700.9319
716.0202	767.6012	829.6459
876.3638	932.8551	945.8922
970.5591	1018.742	1064.387
1137.755	1185.23	1209.215
1340.463	1354.699	1424.107
1445.062	1486.065	1493.927
1611.302	1641.014	1694.417
2242.536	3042.212	3102.523
3140.978	3161.802	3237.793
3258.123	3260.194	3484.719

***ii9 - p10***

**Cartesian coordinates**

C	-3.347258	-0.701320	-0.245775
C	-2.060933	-0.412408	-0.025380
C	-1.669383	1.005141	0.004786
C	-0.429346	1.559008	-0.066229
C	1.925588	0.414648	-0.048015
C	3.161176	-0.171281	-0.039082
C	4.247207	-0.690710	-0.030531
C	0.818033	0.902692	-0.054324
C	-1.034210	-1.488774	0.190094
H	-3.695701	-1.727119	-0.289679
H	-4.088935	0.077539	-0.388563
H	-1.922870	1.241188	2.039670
H	-2.496620	1.703604	-0.083613
H	-0.370359	2.642764	-0.113503
H	5.206759	-1.148848	-0.022384
H	-0.499347	-1.331848	1.130669
H	-0.286396	-1.490147	-0.606041
H	-1.511777	-2.469111	0.220182

**Vibrational frequencies**

-712.668	56.0789	67.0478
122.2308	192.2798	213.7011
226.2827	276.7457	292.1202
366.675	397.8455	406.9507
447.0207	538.7176	546.0702
594.8472	656.5894	673.4046
711.1428	724.4474	752.8436
801.7414	858.1443	942.5454
989.9284	1007.048	1054.624
1079.308	1167.73	1259.74

H	0.713417	1.631013	-1.336399	824.2193	850.578	921.3639
H	0.828729	-2.046196	-0.669287	1001.041	1042.014	1063.358
H	2.213558	1.437714	1.387316	1073.314	1222.539	1256.371
H	0.441600	1.265439	1.129293	1308.977	1730.915	1418.922
H	-5.410584	0.559357	0.179934	1452.249	1480.866	1500.02
H	3.284439	-1.254037	1.099962	1612.683	1695.66	2196.762
H	3.794180	-0.002087	-0.031525	2373.265	3044.618	3106.331
H	3.196070	-1.551142	-0.642679	3148.913	3170.627	3178.572
				3189.764	3264.36	3483.841

C	-3.022703	-0.464989	-0.008829			
C	-4.133747	-0.932385	-0.039057			
C	-0.641257	0.527437	0.049800			
C	0.867321	2.532637	-0.151831			
H	2.775211	-3.130644	-0.181603			
H	3.881152	-1.647482	-0.089669			
H	0.801911	-1.714068	-0.017287			
H	1.269175	0.646529	1.176277			
H	2.797619	0.673977	-0.001347			
H	-5.112335	-1.346673	-0.067735			
H	1.798213	2.877316	0.306559			
H	0.045489	3.128042	0.246682			
H	0.938376	2.715655	-1.229288			

**Vibrational frequencies**

-592.59	60.6903	73.0014
158.0919	191.4419	205.8316
256.5202	338.7997	364.3049
384.3611	450.3509	477.4624
533.6018	540.8016	562.7273
647.8809	660.0426	689.8086
768.5045	793.0349	812.6257
836.9312	998.3189	1051.117
1068.127	1103.276	1213.203
1228.294	1236.92	1270.739
1358.425	1426.644	1454.825
1483.805	1501.291	1504.837
1530.997	2172.953	2295.12
3043.148	3098.284	3112.124
3138.811	3168.737	3181.006
3181.82	3297.898	3486.12

**i36 - p12**

**Cartesian coordinates**

C	-0.771407	1.980764	-0.291499
C	-1.761189	1.170883	0.110740
C	-1.819266	-0.288881	0.014398
C	-0.755914	-1.118315	-0.057733
C	1.796337	-0.520274	-0.010349
C	3.132103	-0.223518	0.013511
C	4.306223	0.040462	0.034228
C	0.610517	-0.757919	-0.031489
C	-3.209473	-0.867372	0.035111
H	0.573298	2.139262	1.493681
H	-0.879632	3.055315	-0.202457
H	0.113156	1.612407	-0.794901
H	-2.649960	1.629067	0.540093
H	-0.943049	-2.186781	-0.123947
H	5.343972	0.270785	0.054956
H	-3.807220	-0.462453	-0.787216
H	-3.718861	-0.597824	0.966191
H	-3.199297	-1.954755	-0.047919

**Vibrational frequencies**

-1881.23	55.7838	86.1748
132.0248	152.1655	172.81
196.1523	240.171	300.0111
360.3345	417.1032	485.1432
525.5235	555.454	608.3163
613.8644	624.8125	656.5326
708.9591	798.1155	875.8028
917.7261	1003.416	1027.827
1043.396	1063.665	1155.298
1230.794	1245.53	1317.586
1361.324	1397.526	1420.332
1482.256	1493.946	1502.058
1634.641	2142.905	2171.374
2286.302	3042.262	3109.495
3152.141	3157.965	3176.459
3197.327	3255.621	3484.199

**i121 - p79**

**Cartesian coordinates**

C	0.981123	2.198906	-0.555941
C	1.765603	-0.612812	0.094191
C	0.718036	-1.373885	-0.183728
C	1.256795	1.617296	0.626675
C	-1.786887	-0.588087	-0.038572
C	-3.092516	-0.179193	0.034019
C	-4.238368	0.182840	0.099280
C	-0.632734	-0.939598	-0.099205
C	3.217941	-0.840419	0.035161
H	1.753150	2.684731	-1.142820
H	-0.012958	2.147498	-0.985600
H	0.873972	-2.407768	-0.504098
H	2.228470	1.738338	1.094503
H	0.462067	1.226041	1.251900
H	-5.251115	0.500882	0.158364
H	3.678439	-0.688030	1.015984
H	3.683748	-0.133076	-0.657892
H	3.450262	-1.858909	-0.301616

**Vibrational frequencies**

-319.575	35.8921	62.3443
73.6589	125.6408	138.8206
177.678	206.3082	216.6907
283.2741	308.4891	362.8287
416.3141	466.8003	552.2703
553.9832	674.4181	681.7387
766.1161	794.3184	830.1275
905.2039	934.4586	968.3505
1043.607	1043.832	1077.843
1210.604	1241.058	1295.208
1332.202	1403.148	1460.755
1462.854	1481.347	1610.503
1728.953	2198.077	2379.13
3015.74	3085.798	3091.398
3105.468	3145.251	3159.538
3233.106	3257.661	3486.243

**Vibrational frequencies**

-474.072	58.8137	65.1434
91.4474	158.6406	189.1002
209.9622	221.1326	255.6073
292.5058	353.7519	396.1681
437.5864	477.5008	546.6886
555.5074	570.4091	672.5784
699.07	737.4866	802.8534
835.4065	845.7728	982.7015
1019.749	1031.906	1062.94
1107.694	1187.338	1235.991
1349.586	1380.195	1415.308
1465.292	1483.455	1495.606
1641.337	1700.62	2194.612
2364.961	3046.382	3108.451
3146.926	3157.082	3171.985
3176.303	3270.753	3485.564

**i22 - i23**

**Cartesian coordinates**

C	0.756893	-1.337264	-0.000167
C	1.748427	-0.449748	-0.000038
C	1.559994	0.999248	-0.000074
C	0.430454	1.740245	-0.000023
C	-1.410182	0.066233	-0.000082
C	-2.733561	-0.395668	0.000011
C	-3.841784	-0.869973	0.000077
C	-0.957684	1.328803	0.000061
C	3.192245	-0.911065	0.000153
H	0.808318	-2.420264	-0.000129
H	2.490116	1.562950	-0.000105
H	0.575492	2.816676	-0.000024
H	-0.521319	-0.787633	-0.000258
H	-4.825494	-1.273454	0.000150
H	-1.689588	2.133739	0.000246
H	3.712712	-0.528886	0.883497
H	3.712899	-0.529062	-0.883156
H	3.268041	-1.998931	0.000271

**Vibrational frequencies**

-1231.78	60.3041	129.2851
134.5868	159.6686	244.6739
300.5066	337.6527	379.5353
438.8113	469.0316	524.907
611.37	619.9001	656.9975
674.2221	677.1063	737.0728
777.1582	898.6072	919.8385
969.527	987.7982	1010.126
1012.343	1052.914	1053.411
1110.374	1238.8	1307.117
1341.093	1409.424	1468.911
1481.771	1483.961	1497.552
1632.586	1691.385	1726.703
2201.551	3048.387	3115.701
3148.13	3156.711	3163.514
3189.165	3213.545	3481.743

**i121 - p12**

**Cartesian coordinates**

C	-2.446669	1.868478	-0.179475
C	-1.529188	-0.444668	0.003907
C	-0.428108	-1.220625	-0.039676
C	2.046541	-0.345191	-0.024152
C	3.340352	0.103295	-0.016615
C	4.476461	0.500040	-0.010348
C	0.902464	-0.735325	-0.032255
C	-2.896662	-1.060653	0.004683
H	-0.540627	-2.300111	-0.079819
H	5.480354	0.850311	-0.004064
H	-3.460284	-0.761882	-0.884615
H	-3.465109	-0.729277	0.879158
H	-2.838796	-2.149332	0.021468
C	-1.418655	1.022518	0.048220
H	-2.281129	2.937821	-0.222501
H	-3.468472	1.522815	-0.285911
H	-0.409065	1.422181	0.064390
H	-1.296082	1.080260	1.986155

**Vibrational frequencies**

-855.536	58.2014	64.8345
105.9954	183.9043	191.7673
224.0024	299.5582	311.8237
361.1925	413.2123	425.1865
441.2601	465.6357	541.1028
566.4603	591.7904	673.4965
682.3321	699.995	783.6922

**i38 - p12**

**Cartesian coordinates**

C	-2.473419	1.797113	0.184999
C	-1.415948	0.976357	0.108720
C	-1.495453	-0.477720	0.028274
C	-0.375966	-1.232810	-0.033962
C	2.086130	-0.324650	-0.016263
C	3.374338	0.138960	-0.008192
C	4.505774	0.549081	-0.001192
C	0.945997	-0.727001	-0.023341
C	-2.847512	-1.130462	0.007684
H	-2.337881	2.868665	0.267147
H	-3.491244	1.428264	0.246582
H	-3.007815	2.165548	-1.997530
H	-0.418310	1.404572	0.088349
H	-0.468239	-2.313247	-0.097762
H	5.505318	0.911626	0.004853
H	-3.404390	-0.899399	0.920907
H	-2.761679	-2.214212	-0.075873
H	-3.439399	-0.765017	-0.837033

**Vibrational frequencies**

-431.738	58.7848	66.771
107.6918	159.5092	182.8392
192.0319	223.9798	259.261
310.4744	365.4114	412.7873
432.3164	459.8014	541.4581
565.0709	596.2	672.3928
683.5847	747.9234	787.8588
829.6574	855.8893	961.3941
1007.431	1026.876	1066.132
1081.841	1223.57	1261.86
1334.547	1382.192	1422.26
1463.984	1484.18	1502.124
1653.918	1677.065	2195.498
2369.26	3047.65	3110.528
3146.241	3167.639	3175.328
3193.22	3258.473	3483.108

**i77 - p13**

**Cartesian coordinates**

C	2.892059	-2.004087	-0.063555
C	1.788591	-1.251931	0.012935
C	0.720556	1.004519	0.065768
C	1.812681	0.189537	-0.031044
C	-1.727283	0.026459	0.020392
C	-3.002584	-0.471837	-0.019235
C	-4.121655	-0.912129	-0.056222
C	-0.599161	0.455745	0.055796
C	0.820719	2.496940	-0.163569
H			

222.4777	239.2758	297.908
375.6986	381.0319	427.1068
448.933	523.0145	536.89
596.4357	627.7729	653.2444
680.04	683.0845	695.8258
900.7163	949.7509	955.1154
1036.9	1043.669	1055.576
1068.628	1188.841	1253.906
1328.856	1381.388	1417.83
1454.777	1488.347	1501.772
1588.282	1678.218	2196.649
2373.57	3053.108	3129.515
3152.278	3158.546	3170.434
3179.687	3250.743	3483.426

**i77 - p5**

**Cartesian coordinates**

C	3.013653	-1.771042	-0.418815
C	1.876120	-1.104090	-0.173241
C	0.678544	0.842468	0.820839
C	1.816991	0.108497	0.595535
C	-1.733758	-0.046166	0.258947
C	-2.992629	-0.505137	-0.025336
C	-4.098546	-0.908465	-0.275241
C	-0.623367	0.356259	0.513056
C	0.674337	2.500895	-0.867156
H	3.018954	-2.686786	-0.997457
H	3.967982	-1.417537	-0.040155
H	0.936703	-1.486936	-0.564511
H	0.719821	1.667721	1.522722
H	2.751760	0.500692	0.986044
H	-5.075896	-1.265869	-0.493255
H	1.625722	2.984883	-0.682624
H	-0.226052	3.035070	-0.588371
H	0.612941	1.829443	-1.713919

**Vibrational frequencies**

-446.962	57.7509	78.4893
87.1003	128.5987	158.6206
171.0598	183.8749	291.7805
306.6214	410.2559	446.7723
494.3556	505.8738	544.2976
550.2397	635.5628	649.6495
670.5605	696.0913	759.6873
802.4797	848.9222	927.5613
945.1672	947.3347	1041.222
1121.272	1196.77	1251.587
1320.517	1393.898	1415.963
1421.819	1467.695	1521.364
1648.069	2196.185	2370.855
3102.427	3149.609	3166.82
3174.481	3200.842	3247.539
3272.627	3279.667	3485.503

**i77 - i79**

**Cartesian coordinates**

C	3.075455	1.686809	-0.305593
C	1.940344	1.294649	0.262748
C	0.742746	-0.929939	-0.309829
C	1.612388	-0.097929	0.599029
C	-1.764360	-0.017921	-0.126325
C	-3.043236	0.467413	-0.017529
C	-4.163486	0.894906	0.077333
C	-0.640770	-0.443698	-0.227603
C	0.825580	-2.426386	0.020470
H	3.257055	2.730733	-0.536362
H	3.859660	0.978048	-0.552798
H	1.180089	2.045529	0.492155
H	1.078024	-0.772052	-1.343173
H	1.724179	-0.436788	1.626442
H	-5.152552	1.275458	0.162524
H	1.857256	-2.770831	-0.079484
H	0.193098	-3.009092	-0.651468
H	0.495225	-2.608426	1.045958

**Vibrational frequencies**

-194.784	36.993	81.7814
102.8853	188.8029	225.3927
235.0605	255.4581	302.5981
378.973	427.0681	493.508
544.1109	562.1278	601.0905
660.5436	685.9707	697.1523
719.5373	908.1153	977.5731
983.4682	1019.809	1029.33
1097.791	1107.475	1141.099
1192.855	1264.753	1318.736
1325.201	1370.098	1414.537
1460.488	1497.646	1504.061
1718.347	2197.77	2392.531
3037.059	3058.138	3098.393
3140.662	3146.314	3153.62
3167.685	3243.599	3484.468

**i79 - i91**

**Cartesian coordinates**

C	3.013653	-1.771042	-0.418815
C	1.876120	-1.104090	-0.173241
C	0.678544	0.842468	0.820839
C	1.816991	0.108497	0.595535
C	-1.733758	-0.046166	0.258947
C	-2.992629	-0.505137	-0.025336
C	-4.098546	-0.908465	-0.275241
C	-0.623367	0.356259	0.513056
C	0.674337	2.500895	-0.867156
H	3.018954	-2.686786	-0.997457
H	3.967982	-1.417537	-0.040155
H	0.936703	-1.486936	-0.564511
H	0.719821	1.667721	1.522722
H	2.751760	0.500692	0.986044
H	-5.075896	-1.265869	-0.493255
H	1.625722	2.984883	-0.682624
H	-0.226052	3.035070	-0.588371
H	0.612941	1.829443	-1.713919

C	-0.310373	1.434530	0.693447
C	0.879542	1.727580	-0.074356
C	1.502909	-0.689598	-0.478574
C	1.739742	0.810226	-0.548134
C	-1.050717	-0.427786	-0.221711
C	-2.429119	-0.409466	-0.108770
C	-3.624662	-0.352912	0.012498
C	0.049156	-0.929670	-0.502882
C	2.153524	-1.331684	0.761702
H	-1.120533	2.157052	0.677918
H	-0.226233	0.871535	1.615199
H	1.050035	2.769262	-0.339129
H	1.955367	-1.139719	-1.368476
H	2.614823	1.132160	-1.103807
H	-4.682472	-0.316993	0.112553
H	3.230424	-1.148349	0.755983
H	1.981876	-2.410308	0.775169
H	1.736702	-0.901966	1.674893

**Vibrational frequencies**

-686.581	90.1467	104.6256
129.956	241.592	265.747
272.2447	345.7843	433.0615
470.2593	486.0405	513.703
543.4618	644.0014	669.7264
685.8364	691.8613	694.2934
758.4433	866.4902	891.2687
957.6821	982.7237	1022.602
1067.341	1090.234	1120.428
1178.283	1247.698	1320.942
1345.871	1397.847	1414.385
1492.614	1497.89	1507.063
1645.514	2029.459	2258.073
3056.696	3063.461	3140.263
3143.421	3146.667	3154.069
3188.741	3241.73	3485.676

**i91 - i97**

**Cartesian coordinates**

C	-0.658749	1.350973	0.572818
C	0.577689	1.776273	-0.185847
C	1.398000	-0.511670	-0.142790
C	1.529627	0.908471	-0.537329
C	-0.957059	-0.106329	0.258340
C	-2.277719	-0.498877	-0.049598
C	-3.415764	-0.792864	-0.318945
C	0.109717	-0.968002	0.224317
C	2.646795	-1.283805	0.201450
H	-1.513783	1.972427	0.294096
H	-0.505301	1.514947	1.648998
H	0.683116	2.828639	-0.432829
H	0.725984	-1.311329	-0.925741
H	2.415329	1.228005	-1.077046
H	-4.415866	-1.066451	-0.552993
H	3.403789	-1.197953	-0.582759
H	2.416661	-2.336750	0.371206
H	3.074855	-0.876555	1.122577

**Vibrational frequencies**

-1579.64	100.593	128.0893
186.4628	242.6862	295.6837
309.6779	392.7384	449.3778
470.0614	543.5788	571.816
613.0017	628.5085	670.3153
700.5994	746.3372	846.0654
890.4583	934.4498	950.8755
991.0965	1005.279	1030.097
1140.635	1166.514	1190.687
1208.524	1241.092	1316.971
1371.109	1409.575	1425.118
1470.503	1487.424	1492.448
1512.642	1693.752	2118.604
2185.178	3009.409	3046.185
3091.111	3113.215	3147.252
3177.497	3200.272	3486.204

**i97 - i94**

**Cartesian coordinates**

C	-0.399773	1.553205	-0.061868
C	1.068062	1.677153	0.257438
C	1.551683	-0.640284	-0.436001
C	1.951002	0.693729	0.114412
C	-0.834010	0.107739	-0.247029
C	-2.197857	-0.220653	-0.006967
C	-3.356329	-0.456478	0.214301
C	0.081641	-0.805967	-0.609507
C	1.458834	-1.850325	0.499557
H	-0.641638	2.148044	-0.951891
H	-0.987078	1.990879	0.752587
H	1.397446	2.641765	0.633027
H	2.125411	-0.887152	-1.334106
H	2.994707	0.852458	0.368747
H	-4.379320	-0.676226	0.401733
H	2.002541	-2.756059	0.240319
H	0.203760	-2.026801	-0.014432

H	1.344649	-1.635616	1.557999
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**Vibrational frequencies**

-1905.04	95.704	105.4988
163.257	265.0107	288.9055
414.5088	464.5971	476.4254
518.5756	546.8748	578.0603
665.1448	670.7069	707.8105
723.2548	755.7468	855.8849
895.9871	950.7953	966.6941
1001.867	1017.569	1053.933
1070.725	1136.416	1170.431
1197.267	1222.528	1240.182
1254.764	1357.302	1359.964
1417.808	1430.951	1472.782
1627.366	1742.9	1953.812
2225.98	3031.841	3067.826
3074.225	3117.37	3169.72
3194.171	3236.178	3485.667

**i21 - i22**

**Cartesian coordinates**

C	-1.115833	1.271619	0.339255
C	-2.066802	0.252739	0.146487
C	-1.638227	-1.085200	0.210830
C	-0.306882	-1.422635	0.070930
C	1.982663	-0.333615	-0.042082
C	3.225886	0.160562	-0.077500
C	4.376890	0.563488	-0.076530
C	0.708163	-0.454423	-0.127046
C	-3.448168	0.581405	-0.351729
H	-1.361312	2.275181	-0.005053
H	-0.508192	1.257567	1.240184
H	-2.376341	-1.879235	0.162427
H	-0.042335	-2.463476	-0.083370
H	5.376841	0.924135	-0.084276
H	0.022862	0.640810	-0.340268
H	-3.393488	1.306243	-1.170143
H	-4.050271	1.038292	0.439925
H	-3.973900	-0.303161	-0.715112

**Vibrational frequencies**

-1702.89	60.8787	64.1678
72.8072	160.4948	252.4724
278.1995	379.7606	408.4408
419.5843	447.7413	492.7737
499.4845	552.6229	575.5063
630.1652	670.7656	771.203
800.4663	855.7067	941.6476
973.7846	1006.19	1027.285
1046.271	1064.188	1167.75
1223.63	1265.557	1288.868
1401.284	1422.1	1464.917
1486.161	1492.084	1500.371
1529.188	1589.765	1873.518
2054.915	3043.555	3104.723
3116.009	3140.105	3186.407
3194.656	3204.766	3474.771

3121.073	3135.456	3165.65	H	0.806868	2.813431	-0.091025	1192.768	1204.569	1280.856
3184.255	3203.321	3477.301	H	-4.690343	-1.215576	0.352520	1285.876	1330.053	1413.426
			H	-1.460177	2.222664	0.197378	1417.494	1450.239	1549.62
			H	-0.387779	-0.776705	-0.316539	1650.413	2196.161	2370.132
			H	0.717452	-2.341201	-0.541387	3104.448	3152.153	3161.742
			H	0.646366	-1.036523	-1.804136	3175.736	3182.602	3255.312
							3276.155	3281.271	3484.188
<b>i79 - p4</b>									
<b>Cartesian coordinates</b>									
C	-3.606509	-0.187920	-0.487711						
C	-2.833543	-0.907694	0.338522						
C	-0.578431	-0.104479	-0.373975						
C	-1.394798	-0.823969	0.457698						
C	2.040458	-0.184311	-0.161613						
C	3.404978	-0.227063	-0.051691						
C	4.603795	-0.265008	0.046681						
C	0.836438	-0.151878	-0.256006						
C	-0.817525	2.157098	0.368522						
H	-4.680795	-0.325371	-0.505612						
H	-3.198715	0.553839	-1.166654						
H	-3.317709	-1.614557	1.006873						
H	-0.964143	0.277229	-1.313551						
H	-0.936567	-1.335765	1.297672						
H	5.662729	-0.300722	0.134902						
H	-1.899347	2.207536	0.379174						
H	-0.287033	2.657802	-0.432197						
H	-0.307596	2.051355	1.316831						
<b>Vibrational frequencies</b>									
	-422.19	62.0216	72.0153						
	97.0894	127.8711	134.2174						
	197.9519	212.2755	268.3504						
	278.7959	426.0589	456.6343						
	484.5616	500.4323	545.2904						
	557.515	561.2549	631.8788						
	671.8263	699.9766	769.3781						
	806.4032	859.6587	935.8085						
	940.8811	1011.471	1035.811						
	1078.294	1221.665	1278.902						
	1323.83	1342.617	1408.479						
	1423.35	1455.419	1548.835						
	1668.221	2196.499	2369.428						
	3104.762	3159.367	3174.019						
	3181.196	3196.954	3251.699						
	3275.813	3285.174	3485.711						
<b>i26 - i24</b>									
<b>Cartesian coordinates</b>									
C	-2.502322	-1.399791	-0.409521						
C	-1.591881	-0.568570	0.125028						
C	-1.763157	0.894702	0.015604						
C	-0.749052	1.789740	0.036323						
C	1.056700	0.189881	-0.430568						
C	2.384226	-0.289691	-0.233923						
C	3.494273	-0.717168	-0.059490						
C	0.639018	1.411596	0.063940						
C	-0.397707	-1.072123	0.796791						
H	-2.388193	-2.476045	-0.344344						
H	-3.384114	-1.019521	-0.913941						
H	-2.783052	1.259537	-0.059624						
H	-0.989104	2.848448	0.072299						
H	0.508769	-0.264536	-1.248652						
H	4.477744	-1.091968	0.091254						
H	1.346414	2.038653	0.597402						
H	-0.118531	-2.109981	0.650688						
H	-0.090519	-0.616049	1.729818						
<b>Vibrational frequencies</b>									
	-611.155	94.7097	120.4762						
	140.2697	254.9356	307.9184						
	356.5719	413.8491	458.8066						
	481.8045	549.4475	574.2354						
	600.0942	675.9926	681.2004						
	704.2891	735.7797	763.5581						
	791.0228	835.3628	882.1208						
	915.9817	929.2884	969.3114						
	987.3883	1022.898	1035.699						
	1076.05	1198.782	1259.357						
	1303.305	1324.768	1406.977						
	1450.558	1478.206	1523.201						
	1613.12	1670.417	2226.123						
	3156.062	3159.005	3170.607						
	3183.009	3190.792	3198.215						
	3250.427	3260.575	3483.739						
<b>i22 - i24</b>									
<b>Cartesian coordinates</b>									
C	2.783322	-1.110792	0.625056						
C	1.789709	-0.510120	-0.043810						
C	1.724304	0.962771	-0.088058						
C	0.628703	1.742053	-0.082829						
C	-1.320793	0.161895	-0.009070						
C	-2.624770	-0.296677	0.136971						
C	-3.719134	-0.795889	0.247902						
C	-0.785584	1.383127	0.033602						
C	0.737594	-1.271449	-0.742904						
H	2.842966	-2.190988	0.699033						
H	3.559291	-0.535028	1.118534						
H	2.685245	1.470407	-0.075533						
<b>i77 - p14</b>									
<b>Cartesian coordinates</b>									
C	3.719732	-1.286233	-0.083028						
C	2.851459	-0.267932	-0.069631						
C	0.490093	0.540353	0.104205						
C	1.426773	-0.453958	0.059044						
C	-2.067083	-0.094482	0.021305						
C	-3.399182	-0.407053	-0.040730						
C	-4.569662	-0.679924	-0.097910						
C	-0.891278	0.175390	0.076217						
C	0.786207	2.003744	-0.150240						
H	4.784795	-1.120395	-0.190529						
H	3.384929	-2.314753	0.101469						
H	3.230807	0.744443	-0.168904						
H	1.075334	-1.477496	0.153044						
H	-5.604467	-0.918783	-0.149548						
H	1.766560	2.291188	0.228729						
H	0.037905	2.632054	0.332648						
H	0.753126	2.203325	-1.225681						
H	0.488652	0.780989	2.094383						
<b>Vibrational frequencies</b>									
	-820.889	63.3925	84.506						
	100.024	136.1196	198.4972						
	201.6075	275.3836	315.7792						
	374.645	394.4141	414.2574						
	429.4845	510.9269	525.2222						
	590.3989	607.557	674.3856						
	682.4671	701.8718	731.2946						
	911.8284	917.0498	962.1125						
	1006.078	1034.499	1054.712						
	1071.466	1208.986	1273.363						
	1330.488	1358.925	1420.113						
	1452.852	1480.949	1506.199						
	1590.065	1671.668	1671.668						
	2373.046	3061.579	3140.355						
	3158.628	3168.186	3184.363						
	3193.837	3255.075	3485.665						
<b>i97 - i94</b>									
<b>Cartesian coordinates</b>									
C	-0.684388	1.469997	-0.018165						
C	0.774538	1.814823	0.048605						
C	1.463821	-0.531741	-0.094012						
C	1.747098	0.902021	0.010574						
C	-0.937709	-0.021247	-0.019944						
C	-2.297396	-0.443443	0.014395						
C	-3.458722	-0.756761	0.044584						
C	0.067594	-0.921683	-0.050728						
C	2.543976	-1.528614	0.136556						
H	-1.134200	1.914793	-0.917202						
H	-1.219380	1.929807	0.823026						
H	1.027853	2.866330	0.136724						
H	2.020192	-1.033664	-1.076726						
H	2.786816	1.209590	0.067694						
H	-4.481589	-1.045002	0.072666						
H	-0.169719	-1.980833	-0.043913						
H	2.295492	-2.574143	0.248467						
H	3.561667	-1.186997	0.258079						
<b>Vibrational frequencies</b>									
	-1887.11	86.3967							

C	0.068194	-0.943578	-0.051101	555.4251	603.6087	664.19	C	-0.965489	0.765957	-0.828703
C	2.527181	-1.514851	0.136245	700.5398	724.7974	736.3477	C	-2.043304	-0.078888	-0.724441
H	-1.094914	1.951421	-0.875239	814.8535	911.1796	927.6562	C	1.545913	0.169826	-0.331032
H	-1.139187	1.959861	0.867539	967.8636	1007.438	1016.065	C	2.857692	-0.130301	-0.077959
H	1.104782	2.829890	0.100582	1024.363	1070.443	1113.645	C	4.009935	-0.394419	0.147642
H	0.872682	-0.856428	-1.192235	1181.708	1199.246	1277.3	C	0.382960	0.420200	-0.543555
H	2.831243	1.152659	-0.006904	1303.591	1344.856	1418.74	C	-1.175811	2.189261	1.069689
H	-4.485773	-0.996243	0.056901	1456.981	1492.221	1500.558	H	-1.445987	-2.877025	1.229908
H	-0.175191	-1.999340	0.002364	1525.683	1620.374	1665.035	H	-0.287335	-1.455460	1.000781
H	2.322883	-2.574934	0.220430	2238.598	3051.67	3116.897	H	-3.079203	-1.874894	-0.204906
H	3.558583	-1.189021	0.126887	3142.849	3187.876	3202.014	H	-1.081817	1.648325	-1.449413
				3210.234	3224.013	3483.713	H	-2.963612	0.285207	-1.170698

**Vibrational frequencies**

-1898.27	77.3598	139.1369
147.7745	302.1956	333.1432
371.1081	431.9254	493.6498
502.6867	523.9527	551.3991
571.7634	588.7679	663.1174
685.9302	707.168	774.0358
876.3583	885.3924	929.5635
959.9421	970.6145	1006.562
1016.332	1102.467	1179.882
1204.274	1237.911	1306.08
1325.822	1370.471	1398.774
1442.792	1487.511	1508.331
1576.231	1744.095	1762.419
2174.975	3009.019	3035.313
3170.922	3177.417	3200.463
3202.229	3272.872	3485.338

**i94 - i100**

**Cartesian coordinates**

C	-0.656630	1.472527	0.007941
C	0.802985	1.807242	0.086223
C	1.493293	-0.600951	-0.066615
C	1.786282	0.851933	-0.007268
C	-0.914601	-0.022476	-0.014690
C	-2.286138	-0.422222	0.011835
C	-3.452242	-0.711606	0.037114
C	0.060212	-0.940799	-0.077533
C	2.443824	-1.594111	0.136939
H	-1.111648	1.915060	-0.890975
H	-1.203638	1.916640	0.849747
H	1.084817	2.851577	0.138595
H	1.760924	0.118298	-1.183047
H	2.831644	1.125394	0.092893
H	-4.480925	-0.979615	0.060764
H	-0.195547	-1.994134	-0.101228
H	2.161215	-2.636699	0.078628
H	3.491252	-1.353736	0.270947

**Vibrational frequencies**

-1919.04	80.2905	139.7058
146.6145	298.5027	329.9005
374.2942	436.5574	508.8032
516.3418	535.8379	550.8361
593.0593	656.2675	667.7194
680.2148	707.4476	719.0246
871.4752	896.364	905.9258
928.3652	967.977	975.1549
1005.115	1105.216	1150.088
1184.576	1230.54	1308.974
1329.778	1354.352	1407.805
1433.217	1487.992	1512.362
1558.457	1644.278	1719.345
2235.314	2995.947	3030.715
3171.621	3193.761	3202.367
3214.128	3272.039	3486.435

**i97 - p2**

**Cartesian coordinates**

C	-0.673937	1.394816	-0.015274
C	0.658621	1.826054	-0.105104
C	1.437320	-0.464696	-0.006205
C	1.691679	0.910844	-0.080436
C	-0.945059	0.010491	-0.025823
C	-2.295537	-0.453757	-0.038279
C	-3.432982	-0.839793	-0.045634
C	0.115037	-0.896541	0.006533
C	2.576291	-1.446626	0.052769
H	-1.486958	2.093877	-0.167705
H	-0.975134	1.752938	1.813829
H	0.869854	2.887024	-0.167098
H	2.718731	1.258766	-0.128746
H	-4.439449	-1.182678	-0.052822
H	-0.105807	-1.958100	0.029695
H	3.337329	-1.210834	-0.695480
H	2.232444	-2.467754	-0.120650
H	3.060390	-1.417992	1.033686

**Vibrational frequencies**

-877.858	102.6893	129.6876
137.4349	188.0444	325.6699
335.6733	361.8482	403.6095
461.0204	485.0203	535.2655

**i93 - i97**

**Cartesian coordinates**

C	-0.686744	1.390047	-0.032807
C	0.686923	1.828167	-0.031757
C	1.414619	-0.496313	-0.004725
C	1.730965	0.897839	-0.060708
C	-0.993756	0.021776	-0.031848
C	-2.337138	-0.415166	-0.011317
C	-3.481225	-0.797690	-0.003634
C	0.111466	-0.909695	0.015454
C	2.545796	-1.484905	0.013484
H	-1.468702	2.133444	-0.140879
H	0.874482	2.888660	-0.164026
H	2.759142	1.233749	-0.038906
H	-4.489177	-1.134469	0.000005
H	-0.118482	-1.968671	0.048606
H	3.147310	-1.392104	-0.896408
H	2.182789	-2.511474	0.082108
H	3.211046	-1.296057	0.861709
H	-0.043844	1.842574	1.134939

**Vibrational frequencies**

-2000.18	84.9884	125.9566
136.5815	181.3814	321.0156
336.2794	450.2981	468.7558
515.2595	520.4602	543.7288
553.1405	649.9499	671.5683
702.464	708.5254	807.2525
842.8474	903.5906	972.3227
1017.303	1052.884	1064.962
1084.38	1100.253	1168.944
1206.918	1255.787	1310.984
1376.36	1407.594	1436.009
1476.719	1481.986	1484.699
1499.444	1527.076	1673.328
2190.328	3043.531	3105.066
3142.43	3194.582	3203.189
3208.988	3223.687	3484.248

**i97 - p7**

**Cartesian coordinates**

C	-0.689532	1.460646	-0.047060
C	0.762762	1.822114	-0.028862
C	1.467864	-0.518468	0.106269
C	1.739880	0.918876	0.041207
C	-0.938201	-0.025767	0.012924
C	-2.302114	-0.448432	-0.008022
C	-3.461419	-0.764105	-0.029001
C	0.063755	-0.916606	0.083099
C	2.454377	-1.430168	0.174940
H	-1.165929	1.869015	-0.947815
H	-1.206399	1.945188	0.791764
H	1.003323	2.879491	-0.076834
H	2.778472	1.233845	0.050572
H	-4.483858	-1.055565	-0.047660
H	-0.163401	-1.976598	0.124658
H	3.495387	-1.130620	0.214788
H	2.918717	-1.862947	-2.185513
H	2.239458	-2.490349	0.243086

**Vibrational frequencies**

-328.872	101.2231	115.2748
133.6466	146.628	173.7453
312.6377	362.7808	369.8765
442.8722	526.7235	529.3999
551.008	604.5996	667.5049
696.5531	706.4517	717.6623
801.2873	896.8165	906.059
932.6394	935.4994	965.116
981.8752	1013.56	1020.917
1159.228	1203.066	1232.804
1318.765	1360.622	1401.375
1434.953	1465.258	1467.385
1657.78	1693.524	1753.538
2236.834	3028.402	3052.14
3162.76	3177.817	3198.954
3200.962	3254.925	3486.429

**i99 - p5**

**Cartesian coordinates**

C	-1.238544	-1.917718	0.770344
C	-2.141533	-1.348693	-0.043837

**Vibrational frequencies**

-443.358	64.1921	67.1262
86.3107	116.4482	126.3732
178.2861	207.7035	302.2255
319.1254	429.4235	459.3585
481.6787	522.7503	551.1657
554.7263	622.1648	651.6143
702.9509	706.522	761.6534
813.5841	839.6706	944.3317
950.3008	954.7329	1038.35
1103.66	1166.456	1260.038
1347.158	1411.557	1422.437
1434.269	1472.582	1512.55
1667.047	2195.416	2367.142
3105.812	3162.144	3175.036
3183.09	3197.476	3268.819
3276.698	3283.505	3486.351

**i79 - p14**

**Cartesian coordinates**

C	3.631394	-0.100567	-0.466060
C	2.769150	-0.974361	0.066180
C	0.540317	0.241820	0.203498
C	1.321760	-0.880099	0.134227
C	-2.075883	-0.035548	0.008604
C	-3.434029	-0.168785	-0.110568
C	-4.626686	-0.286401	-0.216811
C	-0.877922	0.071819	0.113396
C	1.038792	1.662979	0.067731
H	4.694727	-0.310372	-0.463071
H	3.317523	0.816377	-0.947696
H	3.176311	-1.900725	0.465503
H	0.491047	0.364835	2.166712
H	0.799264	-1.828636	0.211359
H	-5.680304	-0.392151	-0.312638
H	1.997754	1.791272	0.571186
H	0.318352	2.358597	0.497567
H	1.163969	1.915663	-0.990114

**Vibrational frequencies**

-891.709	62.6036	74.182
120.2439	199.1538	213.4114
247.9015	289.3994	322.0259
357.2246	415.4293	448.8714
501.7317	509.8839	546.8593
581.5493	597.9896	639.5451
697.0979	712.7122	765.3201
894.0324	913.8208	961.8986
1027.391	1051.056	1058.108
1070.216	1120.565	1295.346
1344.776	1387.831	1425.253
1462.061	1495.835	1514.597
1586.584	1687.425	2199.604
2376.688	3052.982	3128.712
3153.192	3158.388	3177.96
3189.35	3268.986	3488.894

**i79 - p13**

**Cartesian coordinates**

C	-1.010415	2.308041	0.219590
C	-1.988310	1.515781	-0.233283
C	-1.062697	-0.839631	0.051409
C	-2.060295	0.068695	-0.162145
C	1.506978	-0.267991	-0.012746
C	2.847051	0.0	

**Vibrational frequencies**

-832.992	62.5922	63.7763
115.1468	172.0852	195.2385
223.4784	251.7398	294.8433
328.1297	371.4867	426.9996
483.1567	524.1693	563.397
582.579	624.2797	653.524
690.7584	695.5853	697.48
894.107	959.9348	964.9321
1009.645	1034.483	1063.147
1076.005	1139.368	1235.629
1346.15	1409.139	1418.805
1460.564	1484.369	1500.624
1586.818	1686.949	2194.732
2369.441	3051.013	3126.493
3151.022	3155.288	3168.738
3177.398	3263.217	3486.299

**i28 - p7****Cartesian coordinates**

C	0.590665	1.477186	0.018065
C	-0.875687	1.780477	0.010916
C	-1.500439	-0.589280	-0.033633
C	-1.819148	0.840896	-0.017907
C	0.899962	0.003558	-0.017448
C	2.272275	-0.367994	-0.058864
C	3.441855	-0.645804	-0.090940
C	-0.075753	-0.937226	0.040380
C	-2.445770	-1.532639	-0.123073
H	1.060279	1.918168	0.907827
H	1.079071	1.967775	-0.833700
H	-1.155452	2.829150	0.024756
H	-2.868334	1.118202	-0.033519
H	4.473516	-0.901702	-0.121758
H	-0.020394	-1.263171	2.052221
H	0.193218	-1.984686	-0.042506
H	-2.193791	-2.587105	-0.127744
H	-3.495865	-1.271673	-0.190561

**Vibrational frequencies**

-731.363	98.9859	126.5902
143.8952	235.9301	297.2774
361.4435	368.3134	387.4239
443.1453	526.0761	552.0015
559.0409	601.718	662.3507
697.3686	704.3439	711.7927
796.0647	893.5226	914.9668
933.5323	952.8724	967.3752
978.7211	1012.061	1020.785
1162.366	1202.852	1233.615
1311.892	1358.943	1402.337
1429.052	1464.188	1467.607
1616.899	1690.534	1760.224
2222.088	3026.489	3050.109
3160.176	3175.014	3196.785
3203.082	3250.743	3484.623

**i28 - p8****Cartesian coordinates**

C	0.559291	1.378876	-0.129584
C	-0.848599	1.759315	-0.095899
C	-1.516640	-0.591767	0.031053
C	-1.820180	0.836561	-0.035196
C	0.929680	0.081158	0.009041
C	2.285064	-0.325578	-0.099264
C	3.423654	-0.705931	-0.178490
C	-0.093994	-0.963151	0.389705
C	-2.455683	-1.516037	-0.186991
H	1.020024	2.074500	1.819264
H	1.296786	2.119825	-0.413617
H	-1.093717	2.812156	-0.172331
H	-2.863072	1.131659	-0.088238
H	4.433140	-1.031198	-0.255258
H	-0.031571	-1.087465	1.481223
H	0.173797	-1.929414	-0.042628
H	-2.225396	-2.575887	-0.175776
H	-3.485549	-1.234862	-0.378881

**Vibrational frequencies**

-574.029	79.7916	132.0117
144.436	231.9519	264.3735
315.9275	380.0378	404.8572
450.5978	489.8044	550.6698
568.386	590.2827	668.189
688.0288	694.4795	729.2722
814.0084	868.965	915.1841
935.2307	946.6981	968.3254
984.5118	1005.417	1054.819
1169.792	1197.222	1236.506
1315.407	1339.013	1369.87
1426.133	1459.342	1470.47
1594.622	1678.141	1725.145
2217.173	3006.336	3114.106
3155.253	3188.975	3211.766
3223.804	3243.858	3482.461

**i100 - p7****Cartesian coordinates**

C	0.608594	1.447088	-0.060838
C	-0.854280	1.740476	-0.117698
C	-1.455479	-0.646709	-0.023973
C	-1.801787	0.786300	-0.003931
C	0.926265	-0.027163	-0.009974
C	2.310015	-0.379166	0.019240
C	3.484738	-0.631120	0.043796
C	-0.030766	-0.967485	0.000642
C	-2.391047	-1.602144	-0.076188
H	1.052208	1.939989	0.815505
H	1.115291	1.895842	-0.924869
H	-1.146721	2.782383	-0.194988
H	-2.151199	0.905516	1.901416
H	-2.848096	1.046586	-0.124438
H	4.521566	-0.865877	0.066994
H	0.249615	-2.015188	0.025550
H	-2.122976	-2.652203	-0.103419
H	-3.447205	-1.357508	-0.088203

**Vibrational frequencies**

-829.291	96.501	132.8881
144.5538	256.104	304.4565
368.7126	371.9952	436.7827
454.6309	526.4318	533.5698
552.862	642.5088	664.2999
691.5882	704.2036	718.2557
789.7481	890.3451	908.6023
933.1132	934.7966	969.2769
982.021	1018.761	1026.319
1159.014	1193.077	1230.22
1314.873	1357.364	1399.412
1435.114	1461.139	1465.386
1629.307	1686.942	1745.262
2236.242	3023.38	3049.999
3158.833	3188.25	3195.297
3206.648	3249.449	3484.471

**i100 - p62****Cartesian coordinates**

C	0.553753	1.378022	-0.210510
C	-0.736671	1.766010	-0.199754
C	-1.476216	-0.635872	0.036607
C	-1.830634	0.826814	0.207851
C	0.907033	-0.043750	-0.024830
C	2.290358	-0.396841	-0.008114
C	3.461498	-0.663919	0.003175
C	-0.058991	-0.978992	0.075973
C	-2.408605	-1.580934	-0.117453
H	1.141665	1.957816	1.612728
H	1.335154	2.051065	-0.542081
H	-0.994348	2.799803	-0.400265
H	-2.037751	1.006557	1.274731
H	-2.759296	1.058775	-0.319727
H	4.496745	-0.905944	0.017865
H	0.211706	-2.026993	0.144195
H	-2.140135	-2.629720	-0.182470
H	-3.462892	-1.334576	-0.182648

**Vibrational frequencies**

-719.931	87.264	124.5657
144.5709	246.0274	288.1934
361.4358	377.71	424.1192
441.8341	513.4865	552.7996
554.2133	638.662	663.2016
679.2255	709.6471	719.0355
768.6852	866.8007	912.6186
922.0705	952.8439	971.7504
981.5004	1011.945	1034.206
1174.816	1198.377	1231.703
1311.078	1349.974	1366.825
1433.298	1454.544	1465.597
1610.005	1679.271	1717.485
2240.105	2994.024	3097.918
3157.218	3196.649	3204.391
3219.657	3246.207	3485.745

**i26 - i28****Cartesian coordinates**

C	2.440243	-1.507262	0.252095
C	1.516403	-0.582409	-0.037842
C	1.831266	0.834429	-0.113491
C	0.862739	1.787747	-0.069026
C	-0.941926	0.036553	0.059589
C	-2.310464	-0.299246	0.048941
C	-3.477081	-0.606637	0.041276
C	-0.518054	1.457463	0.101975
C	0.087445	-0.987442	-0.354164
H	2.191380	-2.561139	0.311166
H	3.472751	-1.230406	0.436180
H	2.876220	1.122337	-0.148649
H	1.128246	2.838224	-0.087794
H	-0.672056	0.756324	1.164766

H	-4.505808	-0.874348	0.031787
H	-1.291670	2.214095	0.073435
H	-0.142465	-1.958924	0.087696
H	-0.000033	-1.105335	-1.444704

**Vibrational frequencies**

-1869.79	87.8584	135.8246
144.4033	259.4268	380.4382
390.5913	431.6339	486.2977
512.1206	540.2528	561.3102
585.7113	668.1494	709.5388
720.435	768.5914	833.1654
864.5703	904.4751	928.4881
945.8976	970.2164	979.1909
1071.93	1155.78	1168.541
1238.5	1247.383	1277.447
1318.465	1338.592	1397.916
1456.032	1476.072	1492.696
1565.947	1686.811	2145.567
2181.135	2996.719	3110.632
3155.812	3189.274	3207.666
3227.517	3244.697	3484.628

**i26 - p8****Cartesian coordinates**

C	2.437631	-1.497002	0.210664
C	1.506134	-0.575822	-0.057248
C	1.822375	0.847807	-0.084867
C	0.852644	1.783705	-0.050873
C	-0.924921	0.115556	0.015496
C	-2.302543	-0.256648	0.036583
C	-3.452799	-0.603777	0.023328
C	-0.539239	1.419420	0.063172
C	0.079171	-0.944957	-0.388362
H	2.193992	-2.552037	0.269511
H	3.471227	-1.216054	0.381721
H	2.867845	1.138543	-0.078979
H	1.111456	2.836284	-0.042229
H	-0.568306	-0.262224	2.045659
H	-4.473738	-0.900872	0.022438
H	-1.280623	2.191574	0.229830
H	-0.185411	-1.910402	0.044596
H	-0.007159	-1.054508	-1.479905

**Vibrational frequencies**

-674.806	98.591	140.3414
143.4248	273.3043	331.7143
371.9229	390.5634	413.0704
449.0619	501.1232	547.6688
552.5602	592.5663	663.0716
677.9309	706.1539	731.6008
802.331	870.1431	911.1282
917.4671	942.8658	972.3178
987.3821	994.9606	1066.9
1167.084	1193.528	1237.146
1317.537	1337.088	1368.098
1428.425	1463.743	1473.421
1545.111	1665.058	1708.838
2233.393	3005.466	3128.426
3158.235	3183.801	3202.52
3215.239	3247.812	3486.589

**i24 - p35****Cartesian coordinates**

C	-2.356861	-1.216371	-1.068294
C	-1.917773	-0.917320	0.127809
C	-1.531952	1.350369	-0.120551
C	-0.362817	1.950984	0.005866
C	1.266265	0.098447	-0.338337
C	2.548876	-0.493846	-0.168635
C	3.622957	-1.017388	-0.036188
C	0.949621	1.313025	0.132529
C	-1.561073	-1.057877	1.398921
H	-2.619574	-2.246088	-1.291918
H	-2.464924	-0.478967	-1.852851
H	-2.526706	1.771907	-0.191342
H	-0.355295	3.043859	0.043194
H	0.527752	-0.480300	-0.885562
H	4.575049	-1.475120	0.082794
H	1.719879	1.891491	0.635077
H	-0.517442	-1.181991	





C	1.017978	0.074391	0.140204
C	2.342422	-0.390720	-0.026061
C	3.471078	-0.798856	-0.142718
C	0.660160	1.480461	0.014413
C	-2.581443	-1.438625	-0.088769
H	0.102247	-1.962385	0.027385
H	-2.739665	1.278635	-0.102512
H	-0.860537	2.926747	-0.128613
H	0.470413	-0.425631	1.180851
H	4.465896	-1.155191	-0.256745
H	1.468090	2.199857	-0.041283
H	-3.560428	-0.958218	-0.060451
H	-2.523858	-2.158678	0.732269
H	-2.503410	-2.001984	-1.023771

**Vibrational frequencies**

-2203.98	95.0343	113.6001
135.1152	198.8575	276.9776
337.2256	435.9572	442.081
514.8255	536.456	539.3913
563.6041	626.3902	688.8924
714.2761	741.2577	752.7866
822.9034	872.6349	973.1661
991.573	1003.86	1052.53
1064.795	1130.012	1170.117
1206.985	1234.54	1281.282
1312.744	1386.5	1419.497
1448.799	1483.686	1502.5
1577.588	1665.45	2189.386
2192.84	3049.799	3113.783
3147.435	3197.174	3211.593
3225.342	3230.936	3482.118

**i97 - i27**

**Cartesian coordinates**

C	-0.134878	-0.918745	0.083723
C	-1.415914	-0.499207	0.008276
C	-1.715420	0.927940	-0.063463
C	-0.711923	1.848798	-0.077575
C	0.992930	0.007306	0.134200
C	2.328007	-0.424684	-0.022938
C	3.473058	-0.787711	-0.133650
C	0.652439	1.481817	0.042099
C	-2.567450	-1.460009	-0.037795
H	0.098697	-1.977668	0.093240
H	-2.749656	1.242367	-0.139374
H	-0.942528	2.903577	-0.182227
H	0.872815	0.812417	1.137466
H	4.479430	-1.111433	-0.243448
H	1.462846	2.180681	-0.108433
H	-3.134886	-1.332099	-0.965577
H	-3.259650	-1.274139	0.790197
H	-2.232157	-2.496725	0.020902

**Vibrational frequencies**

-2226.81	108.5743	130.3199
153.1693	178.102	328.3382
332.3838	400.6954	440.931
507.5792	528.3755	536.6962
551.6485	620.1056	686.8636
710.9899	711.9181	771.8869
851.5061	862.5123	966.2729
969.8179	1022.257	1063.046
1071.467	1125.952	1166.231
1188.879	1235.972	1287.318
1325.732	1386.761	1413.511
1474.844	1480.138	1495.142
1539.829	1690.856	2178.922
2186.989	3039.757	3099.252
3140.008	3195.118	3199.414
3214.24	3242.86	3482.39

**i81 - p12**

**Cartesian coordinates**

C	2.431250	1.907205	-0.087448
C	1.416480	1.060907	0.076171
C	1.535644	-0.404293	0.065263
C	0.421859	-1.189442	-0.053911
C	-2.051585	-0.331071	-0.030777
C	-3.346976	0.107888	-0.020724
C	-4.486357	0.496396	-0.011435
C	-0.902960	-0.713972	-0.040698
C	2.898506	-1.020150	-0.114657
H	2.264427	2.977701	-0.087933
H	3.453350	1.572315	-0.226954
H	0.412391	1.451958	0.209922
H	1.576078	-0.533665	2.064483
H	0.544357	-2.265307	-0.136849
H	-5.493115	0.838194	-0.002941
H	3.273075	-0.797245	-1.119178
H	2.858148	-2.103275	0.004235
H	3.616127	-0.621479	0.604508

**Vibrational frequencies**

-834.284	63.3184	77.5197
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135.4284	194.3447	202.002
229.3976	308.1573	329.9629
375.4342	407.8302	425.8662
452.5019	458.1036	544.6623
565.6435	598.365	684.7034
698.8189	729.6093	783.6628
821.728	842.8841	966.3436
1005.876	1042.184	1058.755
1076.4	1227.701	1255.568
1338.83	1377.488	1421.422
1461.188	1486.673	1503.102
1581.481	1714.682	2186.188
2335.764	3048.135	3120.499
3149.461	3161.716	3175.097
3185.949	3250.626	3485.763

**i101 - i107**

**Cartesian coordinates**

C	-0.336603	-1.245437	0.000507
C	1.135787	-1.253007	0.275404
C	1.826157	0.063107	-0.053717
C	1.043952	1.262666	0.094856
C	-1.067163	-0.064344	0.131476
C	-2.480523	-0.019516	-0.109567
C	-3.662570	0.028150	-0.310755
C	-0.329922	1.230762	0.222232
C	3.124277	0.091769	-0.406633
H	-0.860710	-2.178504	-0.156765
H	1.617843	-2.075941	-0.258738
H	1.301234	-1.456337	1.347933
H	1.545953	2.222901	0.080239
H	-0.824737	0.513690	1.296995
H	-4.709151	0.066476	-0.494498
H	-0.929229	2.132070	0.232867
H	3.699204	-0.820183	-0.524335
H	3.636548	1.030929	-0.586518

**Vibrational frequencies**

-1937.47	73.5741	143.2752
152.7795	249.5374	377.5195
395.5243	414.9839	482.5047
521.1207	589.2305	613.1289
648.3553	673.2503	681.8851
721.5955	731.6642	770.9318
783.7496	876.5492	902.6545
926.1867	958.6711	983.4244
1054.906	1112.724	1164.688
1197.282	1237.997	1290.052
1334.896	1340.461	1397.035
1446.554	1473.261	1501.292
1540.504	1635.615	1794.88
2246.945	2954.027	3086.082
3156.81	3206.659	3224.672
3230.091	3247.826	3483.376

**Products**

**p1 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p1 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>4</sub>H**

**Cartesian coordinates**

C	-0.119132	-1.207129	0.000149
C	-1.506056	-1.203155	-0.000033
C	-2.202394	-0.000058	-0.000037
C	-1.506328	1.203124	-0.000004
C	0.586783	-0.000013	0.000051
C	2.019228	0.000048	-0.000004
C	3.219987	0.000088	-0.000046
C	-0.119329	1.207103	0.000021
H	0.428652	-2.141832	-0.000257
H	-2.045047	-2.143573	-0.000099
H	-3.286444	-0.000185	-0.000104
H	-2.045401	2.143499	-0.000018
H	4.283296	0.000145	-0.000094
H	0.428390	2.141893	-0.000008

**Vibrational frequencies**

137.2745	155.4812	366.7227
412.9701	474.7877	541.5413
555.6264	639.4061	663.8127
703.3922	711.5259	781.6306
782.0688	868.2194	948.2836
1002.296	1019.549	1023.236
1060.86	1112.24	1188.054
1211.568	1234.385	1320.032
1357.334	1488.024	1539.473
1648.272	1679.345	2244.399
3196.38	3205.343	3214.876
3222.268	3227.896	3483.02

**p2 + H**

**Cartesian coordinates**

C	-0.093758	-0.863922	-0.006412
C	-1.421860	-0.444566	-0.007011
C	-1.685643	0.923345	-0.004259
C	-0.649614	1.850446	0.001450

C	0.954960	0.057837	-0.000241
C	2.313154	-0.398221	0.000211
C	3.451092	-0.781638	0.001316
C	0.669197	1.427021	0.003988
C	-2.538587	-1.455617	0.005862
H	0.138019	-1.923800	-0.011769
H	-2.714595	1.268449	-0.007928
H	-0.873846	2.911059	0.002257
H	4.458572	-1.121447	0.002330
H	1.482049	2.142860	0.007126
H	-3.503485	-0.982736	-0.186045
H	-2.598729	-1.955694	0.977024
H	-2.381633	-2.226805	-0.752418

**Vibrational frequencies**

100.2684	132.0827	140.3079
213.1518	342.3365	370.5312
454.8882	475.1953	537.2177
555.5959	597.4935	665.5339
700.0257	715.1578	732.0887
805.1614	909.7547	927.0631
940.0639	1003.216	1020.135
1032.914	1074.52	1129.2
1182.854	1202.438	1283.369
1313.513	1347.383	1428.012
1462.334	1495.058	1510.904
1536	1656.531	1680.967
2244.755	3049.307	3115.428
3136.76	3186.69	3195.739
3205.942	3226.776	3484.471

**p3 + H**

**Cartesian coordinates**

C	-0.388002	1.203090	-0.003931
C	0.997850	1.196372	-0.010341
C	1.714553	0.000001	-0.011185
C	0.997850	-1.196371	-0.010341
C	-1.099343	0.000000	0.000265
C	-2.531166	0.000000	0.004602
C	-3.732127	0.000000	0.008940
C	-0.388002	-1.203090	-0.003931
C	3.219851	0.000000	0.015999
H	-0.930424	2.141102	-0.005183
H	1.533832	-2.140091	-0.016813
H	1.533833	-2.140090	-0.016812
H	-4.795352	-0.000001	0.012924
H	-0.930423	-2.141102	-0.005183
H	3.626405	0.884802	-0.478331
H	3.626404	-0.884754	-0.478419
H	3.586941	-0.000051	1.047356

**Vibrational frequencies**

40.1003	97.1158	144.0103
239.7333	345.8306	415.5648
421.8661	429.0543	543.1074
554.8194	657.2005	663.6753
703.1983	703.2224	738.0337
840.0936	845.5815	861.3044
981.7195	997.0826	1016.445
1045.594	1066.44	1149.71
1215.191	1239.104	1248.623
1314.823	1344.783	1419.554
1451.421	1497.328	1499.904
1561.544	1635.825	1691.698
2243.207	3051.406	3118.535
3142.983	3191.415	3191.929
3218.677	3220.471	3483.322

**p4 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p4 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>4</sub>H**

**Cartesian coordinates**

C	3.967542	-0.675382	0.000041
C	2.981453	0.221625	0.000035
C	1.573221	-0.135655	-0.000068
C	0.580674	0.768434	-0.000025
C	-1.970093	0.150682	-0.000037
C	-3		

1342.937	1457.151	1680.829	794.987	895.1136	904.344	C	-1.076620	-1.474437	0.000266
1734.668	2199.087	2377.408	931.3438	935.6056	967.4538	H	-3.781526	-1.653556	-0.000307
3154.116	3164.853	3166.634	982.6561	1011.914	1022.045	H	-4.149319	0.158744	-0.000433
3178.193	3249.461	3486.149	1159.161	1203.061	1235.751	H	-2.506625	1.744784	-0.000039
			1316.716	1361.74	1403.15	H	-0.378579	2.658789	0.000076
			1436.199	1467.065	1468.82	H	5.182321	-1.153320	-0.000271
			1682.535	1703.42	1770.481	H	-0.429217	-1.413250	0.878458
			2236.24	3030.23	3052.853	H	-0.428453	-1.413047	-0.877343
			3156.753	3173.043	3192.856	H	-1.569351	-2.447866	-0.000043
			3195.69	3247.038	3485.7				
<b>p5 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p5 + CH<sub>3</sub> for C<sub>3</sub>H<sub>8</sub>+C<sub>4</sub>H</b>									
<b>Cartesian coordinates</b>									
C	-3.213372	-1.286990	0.000049						
C	-2.030902	-0.671451	-0.000076						
C	-1.890410	0.774811	0.000032						
C	-0.721885	1.439458	0.000010						
C	1.645520	0.302812	-0.000060						
C	2.882678	-0.284244	-0.000011						
C	3.968980	-0.801880	0.000071						
C	0.551055	0.815293	-0.000061						
H	-3.289438	-2.367817	-0.000067						
H	-4.143834	-0.726859	0.000248						
H	-1.113804	-1.254393	-0.000262						
H	-2.808188	1.356640	0.000130						
H	-0.723583	2.524855	0.000097						
H	4.928859	-1.259279	0.000133						
<b>Vibrational frequencies</b>									
	65.4365	112.2861	140.0314						
	186.8957	285.2683	309.8054						
	415.3092	448.2982	540.9786						
	548.9506	633.186	673.4727						
	693.8402	713.8642	776.1019						
	808.197	945.2111	962.5078						
	1003.176	1052.711	1136.439						
	1201.272	1271.622	1324.527						
	1400.174	1474.248	1664.292						
	1730.807	2199.196	2377.847						
	3155.062	3172.744	3181.155						
	3197.452	3249.907	3485.948						
<b>p6 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p6 + CH<sub>3</sub> for C<sub>3</sub>H<sub>8</sub>+C<sub>4</sub>H</b>									
<b>Cartesian coordinates</b>									
C	-1.725736	1.895825	0.000004						
C	-2.163439	0.640744	-0.000006						
C	-1.304703	-0.557270	-0.000003						
C	-1.823932	-1.793011	0.000003						
C	1.306784	-0.189267	0.000002						
C	2.662507	0.011902	0.000001						
C	3.851894	0.191312	-0.000001						
C	0.114184	-0.372091	-0.000001						
H	-2.420847	2.726713	0.000006						
H	-0.665903	2.128220	0.000008						
H	-3.230998	0.437595	-0.000011						
H	-1.192628	-2.672345	0.000006						
H	-2.898341	-1.938913	0.000004						
H	4.903359	0.349874	-0.000007						
<b>Vibrational frequencies</b>									
	75.9086	99.2378	126.1788						
	214.8756	285.9187	303.1816						
	449.0971	479.9479	529.581						
	559.4795	605.0739	653.1668						
	676.8704	713.8159	720.8604						
	782.2363	902.5195	951.396						
	969.1704	1020.22	1058.053						
	1106.378	1336.852	1357.346						
	1433.734	1463.203	1672.855						
	1735.224	2200.101	2388.791						
	3161.275	3167.557	3180.7						
	3257.436	3265.083	3482.301						
<b>p7 + H</b>									
<b>Cartesian coordinates</b>									
C	-0.589898	1.454659	0.000347						
C	0.875474	1.761534	-0.000159						
C	1.497041	-0.608716	-0.000011						
C	1.819449	0.822045	-0.000254						
C	-0.892433	-0.023429	0.000072						
C	-2.272231	-0.393125	-0.000003						
C	-3.443687	-0.661180	-0.000126						
C	0.075645	-0.952282	-0.000010						
C	2.446142	-1.554485	0.000128						
H	-1.070399	1.919691	-0.870300						
H	-1.069570	1.919090	0.871792						
H	1.154422	2.810656	-0.000422						
H	2.869060	1.098601	-0.000581						
H	-4.477530	-0.909629	-0.000641						
H	-0.191050	-2.003957	-0.000132						
H	3.499111	-1.295847	0.000095						
H	2.192942	-2.608724	0.000284						
<b>Vibrational frequencies</b>									
	102.7726	134.098	144.1735						
	307.0424	359.9408	369.0903						
	443.3595	527.5033	528.6802						
	552.4073	601.1244	662.5223						
	694.9364	697.008	714.0365						
<b>p8 + H</b>									
<b>Cartesian coordinates</b>									
C	0.064247	-0.959762	0.326436						
C	1.497918	-0.579329	0.025044						
C	1.815859	0.847338	0.055193						
C	0.851109	1.779183	0.011455						
C	-0.943862	0.130264	0.032083						
C	-2.314054	-0.251235	-0.050725						
C	-3.458295	-0.614977	-0.112784						
C	-0.554169	1.411579	-0.078378						
C	2.434310	-1.496260	-0.232935						
H	-0.018911	-1.190518	1.398360						
H	-0.209080	-1.876481	-0.201092						
H	2.862305	1.134747	0.055710						
H	1.108174	2.832240	-0.003852						
H	-4.474057	-0.923461	-0.173125						
H	-1.292292	2.187397	-0.244404						
H	3.470004	-1.212425	-0.385732						
H	2.195482	-2.552303	-0.298197						
<b>Vibrational frequencies</b>									
	77.3561	137.5664	144.6094						
	279.9149	378.3471	403.0227						
	445.5934	491.8687	542.405						
	552.993	591.0382	667.0719						
	684.8337	697.8013	729.7476						
	808.9972	870.3167	918.4813						
	928.7735	943.7596	969.9554						
	985.3606	1000.389	1059.33						
	1167.986	1199.533	1238.686						
	1319.492	1342.51	1375.303						
	1430.629	1460.948	1471.714						
	1652.559	1698.256	1737.945						
	2232.576	3016.022	3106.421						
	3157.667	3182.467	3200.933						
	3213.447	3246.052	3484.856						
<b>p9 + H</b>									
<b>Cartesian coordinates</b>									
C	-3.354151	1.297763	0.000058						
C	-2.548753	0.230606	-0.000013						
C	-1.099782	0.430418	-0.000093						
C	-0.184984	-0.552433	-0.000034						
C	2.406051	-0.130580	0.000001						
C	3.759070	0.080901	0.000026						
C	4.947997	0.266921	0.000041						
C	1.211383	-0.311937	-0.000035						
C	-3.086850	-1.174091	0.000024						
H	-4.433482	1.193714	0.000167						
H	-2.953624	2.306011	0.000007						
H	-0.753502	1.460411	-0.000194						
H	-0.491177	-1.594674	0.000072						
H	5.998552	0.430606	0.000017						
H	-2.744550	-1.723747	0.882199						
H	-2.744777	-1.723692	-0.882277						
H	-4.177322	-1.174036	0.000164						
<b>Vibrational frequencies</b>									
	58.8391	64.0943	144.1668						
	190.5245	191.2799	217.1604						
	262.8032	385.7763	386.491						
	491.3231	502.6815	514.2702						
	566.3862	567.4062	668.5738						
	705.8933	709.9744	789.7764						
	870.8784	878.1916	936.9139						
	991.9218	1000.504	1045.815						
	1069.958	1221.096	1295.321						
	1335.025	1349.317	1416.472						
	1453.994	1486.218	1504.766						
	1687.203	1726.449	2197.252						
	2376.975	3047.422	3109.48						
	3149.013	3159.58	3177.684						
	3183.486	3249.433	3482.831						
<b>p10 + H</b>									
<b>Cartesian coordinates</b>									
C	-3.409638	-0.634936	-0.000266						
C	-2.097837	-0.370368	-0.000018						
C	-1.683691	1.035004	0.000014						
C	-0.452067	1.574660	0.000074						
C	1.902960	0.416468	0.000043						
C	3.138495	-0.172956	-0.000052						
C	4.223466	-0.693821	-0.000160						
C	0.798389	0.906838	0.000082						
<b>Vibrational frequencies</b>									
	59.3075	65.5971	122.0355						
	184.4683	191.1507	223.8815						
	301.3124	364.8094	384.8834						

1462.166	1480.471	1502.167	267.7569	377.6264	481.9922	917.6913	944.0256	1039.296
1672.625	1724.7	2196.76	499.8837	575.5649	614.764	1041.171	1102.117	1178.211
2373.875	3045.817	3107.493	634.148	678.3496	897.5154	1215.484	1230.719	1278.926
3148.008	3163.844	3177.537	985.3654	1184.886	1445.861	1307.507	1459.926	1484.176
3190.559	3253.147	3484.544	1870.239	1992.18	2135.699	1692.948	2200.042	2379.916
			3113.837	3193.342	3475.249	3061.495	3073.259	3108.8
						3131.063	3225.866	3483.783

**p13 + H**

**Cartesian coordinates**

C	2.926147	-1.960428	-0.000219
C	1.812977	-1.226291	0.000286
C	0.727424	1.015615	0.000064
C	1.818678	0.226429	0.000017
C	-1.714992	0.031708	0.000083
C	-2.989874	-0.469082	-0.000027
C	-4.109005	-0.911175	-0.000160
C	-0.585569	0.461480	0.000146
C	0.811600	2.520556	-0.000074
H	2.888902	-3.043255	0.000076
H	3.909140	-1.498878	-0.000994
H	0.842834	-1.715752	0.001010
H	2.792904	0.709842	-0.000224
H	-5.097189	-1.303717	-0.000250
H	0.313412	2.934447	0.880895
H	0.313784	2.934286	-0.881331
H	1.851893	2.850155	0.000112

**Vibrational frequencies**

58.0956	84.9051	131.6158
164.0951	175.3371	218.2121
240.3065	300.2229	379.528
432.4656	516.1173	531.9993
597.9112	621.7892	651.8174
673.6836	692.7904	693.5834
909.2055	949.716	951.842
1035.574	1042.392	1057.367
1075.098	1187.402	1261.399
1329.594	1386.416	1420.251
1460.607	1479.877	1502.735
1676.593	1733.317	2195.975
2375.179	3052.892	3121.613
3143.766	3158.26	3174.322
3187.672	3252.648	3483.361

**p14 + H**

**Cartesian coordinates**

C	2.875935	-0.249925	0.000085
C	1.433821	-0.427794	0.000004
C	0.501249	0.545255	-0.000015
C	3.731089	-1.273863	-0.000044
C	-2.055062	-0.089067	0.000009
C	-3.388408	-0.402834	0.000009
C	-4.560019	-0.677169	0.000006
C	-0.876526	0.177651	0.000004
C	0.769434	2.029168	-0.000043
H	3.271545	0.760897	0.000330
H	1.083681	-1.456709	-0.000024
H	3.381715	-2.301985	-0.000267
H	4.803004	-1.116211	0.000060
H	-5.595603	-0.917991	0.000004
H	0.315758	2.492231	-0.880305
H	1.833824	2.259152	-0.000820
H	0.316992	2.492084	0.880933

**Vibrational frequencies**

65.0133	76.434	92.6233
115.8714	195.6417	196.18
264.8212	340.137	373.6622
417.5593	510.24	512.5337
591.2502	607.3807	673.603
675.5994	700.0816	734.7264
911.403	929.0883	956.7683
1009.804	1023.954	1067.889
1074.044	1204.499	1279.931
1335.335	1373.463	1433.04
1461.452	1481.409	1501.34
1677.131	1732.223	2197.047
2375.977	3060.334	3122.625
3155.518	3163.839	3176.802
3199.499	3252.04	3486.246

**p15 + C<sub>2</sub>H<sub>4</sub> for C<sub>4</sub>H<sub>6</sub>+C<sub>2</sub>H<sub>4</sub> and p15 + C<sub>2</sub>H<sub>6</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	1.837346	-0.000287	-0.000035
C	3.142449	0.000454	0.000102
C	-0.709121	-0.000464	-0.000130
C	-2.053644	-0.000077	0.000042
C	-3.266622	0.000380	0.000105
C	0.535046	-0.000432	-0.000156
H	3.709239	-0.927963	0.000180
H	3.708158	0.929530	0.000178
H	-4.330125	0.000989	0.000076

**Vibrational frequencies**

90.0988	106.5706	183.2606
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**p16 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	0.000000	0.000000	-1.970927
C	0.000000	0.000000	-3.174012
C	0.000000	0.000000	0.604352
C	0.000000	0.000000	1.970926
C	0.000000	0.000000	3.174013
C	0.000000	0.000000	-0.604353
H	0.000000	0.000000	-4.237603
H	0.000000	0.000000	4.237604

**Vibrational frequencies**

112.6457	112.6458	273.6364
273.6365	497.2868	497.2868
631.4301	642.2422	642.2425
709.2776	709.2776	709.9626
709.9626	1195.706	2151.819
2264.468	2391.428	3484.538
3484.623		

**p17 + C<sub>2</sub>H<sub>3</sub> for C<sub>4</sub>H<sub>6</sub>+C<sub>2</sub>H<sub>3</sub> and p17 + C<sub>2</sub>H<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>2</sub>H<sub>3</sub>**

**Cartesian coordinates**

C	1.923257	-0.462888	0.000108
C	2.809197	0.533180	0.000139
C	-0.684885	-0.130762	-0.000349
C	-2.045103	0.033319	-0.000135
C	-3.239495	0.177114	0.000337
C	0.514583	-0.267933	-0.000346
H	2.262077	-1.495267	0.000671
H	2.494843	1.570430	-0.000447
H	3.872869	0.327834	0.000726
H	-4.295112	0.304818	0.000532

**Vibrational frequencies**

106.4483	123.7463	254.2653
318.9346	492.307	536.8749
562.874	674.8498	692.2592
698.7706	708.2178	967.4467
1009.4	1050.575	1204.264
1318.907	1450.706	1700.351
2199.801	2384.991	3164.643
3176.839	3263.937	3483.021

**p18 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	2.869259	0.566455	0.000029
C	2.027174	-0.445795	0.000002
C	-0.587322	-0.132128	-0.000025
C	-1.947516	0.030569	-0.000008
C	-3.141940	0.173694	0.000019
C	0.611728	-0.272396	-0.000024
H	2.809553	1.646067	-0.000063
H	2.399858	-1.469241	0.000058
H	-4.197703	0.300775	0.000055

**Vibrational frequencies**

100.7183	132.864	242.192
338.4086	465.6437	542.5644
553.6478	675.0254	685.9507
712.2801	716.2686	870.9187
912.1698	1192.043	1258.966
1643.876	2197.696	2378.108
3142.02	3258.874	3482.56

**p19 + H**

**Cartesian coordinates**

C	-3.074198	-0.074497	0.000501
C	-1.912064	-1.039400	-0.000124
C	-0.979482	-0.074629	-0.000353
C	-1.995747	1.057096	-0.000072
C	1.639053	-0.029619	-0.000284
C	3.007951	0.006203	0.000027
C	4.210805	0.037466	0.000371
C	0.431445	-0.068670	-0.000440
H	-3.709164	-0.102429	0.890126
H	-3.710498	-0.102364	-0.888165
H	-1.850181	-2.120751	-0.000005
H	-1.984887	1.687964	0.891400
H	-1.985595	1.687616	-0.891799
H	5.273740	0.066262	0.000680

**Vibrational frequencies**

76.206	78.3417	197.6573
225.9842	316.0761	447.1011
478.7047	485.8405	573.3762
576.4318	677.7347	686.3529
773.4199	881.1629	886.3121

**p20 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>2</sub>H and p20 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>2</sub>H**

**Cartesian coordinates**

C	-3.526462	-0.994452	-0.337897
C	-2.706475	-0.099767	0.552069
C	-1.636044	0.534233	0.180413
C	-0.561199	1.181363	-0.206198
C	1.875551	0.205457	-0.057696
C	3.148868	-0.295704	0.011755
C	4.266942	-0.736129	0.071383
C	0.750241	0.637719	-0.116326
H	-4.541223	-0.599985	-0.442081
H	-3.604504	-1.994024	0.098081
H	-3.081951	-1.080668	-1.329659
H	-3.036160	0.023168	1.582340
H	-0.658694	2.182686	-0.619279
H	5.253994	-1.127499	0.125572

**Vibrational frequencies**

55.5917	112.9094	153.4871
173.3995	207.203	251.1286
346.0934	425.6661	500.6801
547.16	558.2001	586.7604
681.7068	693.2663	761.1761
783.4934	898.9836	906.2988
1067.897	1092.154	1132.244
1213.692	1306.142	1415.162
1459.126	1493.216	1509.767
2080.994	2200.602	2386.898
3050.151	3116.969	3145.13
3153.99	3159.884	3484.689

**p21 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>2</sub>H and p21 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>2</sub>H**

**Cartesian coordinates**

C	1.947946	-1.049391	-0.0005820
C	2.696648	-0.169894	-0.668047
C	1.981978	1.045588	-0.121192
C	1.109625	0.015691	0.692541
C	-1.498807	0.003766	0.182670
C	-2.842084	-0.007672	-0.093304
C	-4.020167	-0.018773	-0.335710
C	-0.316306	0.014460	0.420329
H	1.910675	-2.129855	0.051360
H	3.527215	-0.270391	-1.355844
H	1.410557	1.627309	-0.847251
H	2.575501	1.721008	0.500388
H	1.280329	0.078491	1.771847
H	-5.061599	-0.029203	-0.549298

**Vibrational frequencies**

79.6809	91.92	193.43
233.3231	331.8157	448.6493
480.0062	545.07	596.1144
629.0397	679.9738	699.0323
804.6733	865.6652	907.3545
931.9426	963.9569	1010.092
1015.949	1104.072	1138.236
1172.964	1209.605	1241.846
1314.174	1352.661	1485.427
1671.854	2201.067	2398.542
3072.19	3076.396	3133.024
3210.391	3242.968	3485.183

**p22 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>2</sub>H and p22 + CH<sub>3</sub> for C<sub>3</sub>H**

676.6952	712.6673	762.1836			3181.823	3224.647	3235.092	
876.8927	893.5398	923.4031	3469.146		3255.267	3267.445	3481.016	
947.796	1022.882	1136.867						
1188.382	1236.742	1326.935						
1380.397	1461.313	1489.064						
2097.51	2206.697	2412.726						
3042.87	3074.272	3150.168						
3175.817	3234.661	3486.923						
<b>p23 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p23 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>4</sub>H</b>			<b>p26 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p26 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>4</sub>H</b>			<b>p29 + H</b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C	-3.265609	0.013186	0.000000	C	-0.109229	1.355569	-0.000001	
C	-1.818993	-0.193371	0.000019	C	1.225140	1.210228	0.000001	
C	-0.801566	-1.041762	-0.000003	C	1.529651	-0.230083	0.000000	
C	-2.278231	1.191216	-0.000006	C	2.740017	-0.795517	0.000001	
C	1.710959	-0.268873	0.000000	C	-0.737741	0.015378	-0.000002	
C	3.022055	0.128874	0.000000	C	-2.141106	-0.207354	-0.000001	
C	4.173333	0.478824	0.000001	C	-3.331170	-0.372974	0.000002	
C	0.553801	-0.614264	-0.000001	C	0.237015	-0.922522	-0.000001	
H	-3.815715	-0.185243	-0.914315	H	-0.668932	2.280530	0.000000	
H	-3.815728	-0.185237	0.914308	H	1.970635	1.992562	0.000004	
H	-0.985290	-2.112279	-0.000025	H	2.859742	-1.873487	0.000000	
H	-2.174384	1.766611	0.914225	H	3.642480	-0.193761	0.000003	
H	-2.174362	1.766574	-0.914257	H	-4.383098	-0.527718	0.000007	
H	5.190978	0.786597	0.000003	H	0.103711	-1.994478	-0.000001	
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
63.1377	88.2248	183.9845	116.6594	149.1345	229.7303	66.8372	81.1905	
195.7355	298.0719	337.3678	343.7997	416.0533	526.7586	183.8862	211.4077	
448.6898	459.0613	547.3477	544.8538	605.0084	657.4958	394.6758	426.7696	
558.8284	674.7956	684.4258	665.9892	695.8014	702.7416	516.6623	626.1735	
750.0536	775.7657	785.551	724.8243	792.1076	858.5924	668.2503	697.1516	
795.873	941.145	1018.496	928.1479	943.8537	957.073	833.4303	902.6747	
1049.913	1075.245	1092.807	974.3599	979.0245	1106.955	1006.461	1012.858	
1101.583	1169.005	1217.744	1185.262	1237.736	1339.712	1185.648	1251.117	
1363.968	1443.964	1474.312	1371.266	1456.932	1587.628	1347.14	1355.332	
1852.553	2200.177	2383.703	1663.974	1741.775	2241.05	1727.023	2235.395	
3130.755	3136.122	3178.236	3157.738	3238.67	3249.757	3173.383	3173.858	
3212.47	3225.336	3487.716	3256.721	3263.069	3482.199	3188.382	3484.166	
<b>p24 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p24 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>4</sub>H</b>			<b>p27 + H for C<sub>4</sub>H<sub>6</sub>+C<sub>4</sub>H and p27 + CH<sub>3</sub> for C<sub>3</sub>H<sub>5</sub>+C<sub>4</sub>H</b>			<b>p30 + H</b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C	2.639032	1.425045	0.080948	C	-2.835350	-1.568470	0.000012	
C	2.075722	0.239449	0.040815	C	-1.981591	-0.590937	-0.000004	
C	1.044836	-0.607555	-0.601306	C	-1.130489	0.409057	-0.000010	
C	1.934966	-1.113108	0.562897	C	-1.574327	1.856581	0.000015	
C	-1.515109	-0.123654	-0.171486	C	1.469049	-0.015332	-0.000026	
C	-2.843854	0.128954	0.055375	C	2.824970	-0.212426	-0.000003	
C	-4.009515	0.349767	0.254159	C	4.015983	-0.382757	0.000023	
C	-0.346545	-0.345923	-0.367705	C	0.273009	0.147646	-0.000035	
H	2.325028	2.214344	-0.592809	H	-3.201266	-1.993879	-0.929449	
H	3.427808	1.645760	0.791831	H	-3.201211	-1.993900	0.929485	
H	1.279840	-1.012283	-1.581729	H	-1.185756	2.368674	-0.883703	
H	1.451018	-1.249622	1.524120	H	-1.185408	2.368731	0.883547	
H	2.679013	-1.860014	0.306831	H	-2.662274	1.924249	0.000239	
H	-5.039903	0.543961	0.429573	H	5.068394	-0.534053	0.000043	
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
72.6683	103.9842	178.123	70.1724	99.2797	153.2636	54.5995	99.8415	
236.919	324.4048	341.8165	175.2717	232.7988	239.0947	237.8384	300.5094	
446.2523	505.2718	542.4959	349.415	452.6067	511.728	381.4678	446.6744	
575.494	615.6847	699.4504	511.9846	553.9265	570.2154	636.8368	691.5593	
717.5671	718.4596	789.2496	655.8606	666.6256	666.9657	697.9775	698.58	
907.1206	937.207	952.3354	712.4474	903.545	919.1365	779.0591	822.0264	
1017.43	1064.934	1087.334	1014.152	1059.783	1065.36	976.8145	1007.656	
1105.08	1133.094	1212.273	1247.444	1332.428	1411.684	1124.729	1242.343	
1358.751	1444.548	1475.984	1471.324	1480.349	1506.783	1387.319	1465.998	
1873.53	2202.375	2397.774	2077.207	2198.498	2384.163	1715.891	2231.791	
3135.595	3157.508	3160.869	3059.509	3131.675	3138.929	3184.669	3186.788	
3226.969	3248.41	3484.945	3160.228	3220.606	3482.982	3210.702	3482.474	
<b>p25 + C<sub>2</sub>H<sub>2</sub></b>			<b>p28 + H</b>			<b>p31 + H</b>		
<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>			<b>Cartesian coordinates</b>		
C	0.000000	0.000000	-2.542029	C	0.506515	1.063206	-0.000015	
C	0.000000	0.000000	-0.000002	C	1.849226	1.151954	0.000000	
C	0.000000	0.000000	1.307906	C	2.424414	-0.204765	0.000015	
C	0.000000	0.000000	2.542029	C	1.424510	-1.104969	-0.000001	
C	0.000000	0.000000	-1.307904	C	-1.073915	-0.907240	-0.000013	
H	0.000000	0.000000	-3.605608	C	-2.277830	-0.154760	0.000002	
H	0.000000	0.000000	3.605614	C	-3.310045	0.461130	0.000016	
<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
126.1772	126.1772	400.5175	0.156199	-0.362542	-0.000016	2.819769	-1.659849	
400.5175	466.592	466.592	H	-0.213869	1.867748	-0.000020	H	0.516028
502.7307	502.7307	507.4123	H	2.430614	2.064202	0.000007	H	-1.864202
507.4123	762.1091	1573.721	H	3.484116	-0.421805	0.000050	H	-4.501559
1661.122	1969.552	3461.402	H	1.505635	-2.182663	0.000018	H	-0.105135
			H	-1.179333	-1.988619	-0.000007		
			H	-4.221603	1.009046	0.000028		
			<b>Vibrational frequencies</b>			<b>Vibrational frequencies</b>		
			112.3331	123.6842	227.5084	77.9834	115.9391	
			330.8642	443.6743	486.8553	168.6747	284.2158	
			574.7805	635.2798	693.6114	393.6278	432.8814	
			707.924	730.8762	746.991	570.333	665.2838	
			797.4083	818.0277	900.2392	699.4643	701.2131	
			915.1362	945.5701	966.651	781.6142	888.2317	
			999.1586	1043.892	1110.997	982.4754	1019.863	
			1113.455	1197.022	1312.787	1148.52	1251.212	
			1371.332	1411.916	1569.219	1336.756	1441.052	
			1652.346	1723.85	2233.918	1719.651	2231.893	
						3164.805	3174.678	
						3203.143	3481.164	
						129.4743		
						314.2218		
						546.5185		
						690.5173		
						708.8687		
						948.4869		
						1040.225		
						1298.483		
						1666.346		
						2237.309		
						3193.269		
						3483.125		

**p32 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C	-1.177648	-0.314304	0.000000
C	-0.043214	-1.182129	0.000000
C	1.153899	-0.388357	0.000000
C	0.771942	0.918263	0.000000
C	-0.704860	0.967262	0.000000
H	-2.211148	-0.626219	0.000000
H	-0.078687	-2.264383	0.000000
H	2.162698	-0.773205	0.000000
H	1.419420	1.784385	0.000000
H	-1.292996	1.875016	0.000000

**Vibrational frequencies**

133.8883	498.4348	523.0012
683.7653	728.0541	820.6602
848.4568	906.2099	920.552
927.0305	955.3665	1062.965
1074.895	1150.439	1219.122
1290.885	1396.038	1517.556
1555.915	3225.55	3226.765
3238.247	3257.544	3266.28

**p33 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C	0.380047	0.331991	0.465998
C	-0.379980	-0.331943	-0.465892
C	-1.045039	-0.913118	-1.281191
C	1.044973	0.913031	1.281111
H	-1.633466	-1.427308	-2.002548
H	1.633460	1.427540	2.002390

**Vibrational frequencies**

228.6549	246.6393	533.8018
667.2128	692.1275	697.7692
706.2012	911.657	2144.077
2336.388	3483.639	3484.782

**p34 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C	2.622239	-0.563082	0.000074
C	1.317301	-0.404338	0.000060
C	-0.683864	1.058796	-0.000034
C	-1.628915	-0.006010	-0.000019
C	-2.443379	-0.890358	-0.000010
C	0.647821	0.890661	0.000058
H	3.318404	-1.389420	-0.000800
H	0.671843	-1.288192	0.000309
H	-1.093821	2.063329	-0.000160
H	-3.166449	-1.670011	-0.000024
H	1.282806	1.770274	-0.000100

**Vibrational frequencies**

133.1093	147.3766	270.326
311.5474	433.5967	493.9573
679.7631	698.7953	713.4466
724.6605	792.6721	798.566
891.0499	946.4702	1011.07
1126.951	1238.521	1262.56
1415.811	1646.064	1696.93
2232.786	3078.276	3186.495
3205.855	3264.725	3484.755

**p35 + C<sub>2</sub>H<sub>2</sub> for C<sub>2</sub>H<sub>6</sub>+C<sub>2</sub>H and p35 + C<sub>2</sub>H<sub>4</sub> for C<sub>2</sub>H<sub>6</sub>+C<sub>2</sub>H**

**Cartesian coordinates**

C	-2.937478	-0.467605	0.000264
C	-1.853012	0.275349	-0.000148
C	0.589300	0.556525	0.000072
C	1.926363	0.072404	0.000027
C	3.064179	-0.314816	0.000003
C	-0.489322	-0.239935	-0.000077
H	-4.006262	-0.310833	-0.000388
H	-1.962952	1.365289	-0.000306
H	0.463935	1.636570	0.000256
H	4.068240	-0.664750	-0.000058
H	-0.363136	-1.317805	-0.000354

**Vibrational frequencies**

121.9087	133.3967	198.3831
308.2878	451.3278	462.9673
549.982	654.4084	661.6942
695.1149	819.8158	834.4385
892.9028	986.591	1036.168
1155.321	1237.365	1317.646
1337.704	1653.47	1706.575
2236.295	3067.247	3169.683
3200.233	3265.884	3483.135

**p36 + H**

**Cartesian coordinates**

C	-0.499820	-0.455153	0.761175
C	-1.370153	-1.275557	-0.179384
C	-2.122525	-0.238527	-0.549633
C	-1.379383	0.764464	0.328629
C	0.662147	0.308089	0.120621
C	2.021278	-0.043859	-0.057725
C	3.170255	-0.372423	-0.186687
C	-0.097107	1.351513	-0.241612
H	-0.404485	-0.750246	1.805363
H	-1.330206	-2.317098	-0.472524
H	-2.929123	-0.114301	-1.261679
H	-1.942817	1.344996	1.058787
H	4.188463	-0.653824	-0.308030
H	0.110021	2.259198	-0.794221

**Vibrational frequencies**

117.5605	157.5216	327.4926
366.1672	446.1596	518.0029
600.6824	623.905	686.7014
695.5428	788.4767	835.0016
865.7291	890.0411	921.8124
955.904	974.7211	981.2306
1003.406	1060.864	1134.543
1160.694	1193.419	1213.442
1223.431	1261.891	1301.665
1641.99	1681.105	2240.181
3135.935	3146.865	3205.375
3227.755	3238.052	3483.839

**p37 + H**

**Cartesian coordinates**

C	-2.965041	0.438213	0.000018
C	-2.981308	-0.878281	-0.000039
C	-1.700692	-0.240599	0.000032
C	-0.364176	-0.255877	0.000023
C	1.757938	1.041728	-0.000019
C	2.620079	-0.089778	-0.000005
C	3.357418	-1.040924	0.000006
C	0.413825	0.959664	-0.000006
H	-3.523615	1.359018	0.000032
H	-3.560835	-1.786145	-0.000089
H	0.154164	-1.207911	0.000038
H	2.234825	2.015645	-0.000042
H	4.011376	-1.878686	0.000014
H	-0.144168	1.893207	-0.000018

**Vibrational frequencies**

76.5897	96.7041	176.433
191.1211	337.8596	359.0185
450.2157	485.716	576.3861
637.7269	681.2443	705.8666
711.8995	762.7698	850.6595
861.7857	936.2936	939.7396
958.1269	998.6393	1047.691
1123.008	1148.567	1261.966
1327.15	1449.866	1607.646
1681.516	1834.154	2224.586
3160.744	3193.336	3198.269
3270.971	3312.172	3488.878

**p38 + H**

**Cartesian coordinates**

C	-2.745982	1.060291	0.000051
C	-3.388185	-0.088855	0.000066
C	-1.958311	-0.138967	-0.000022
C	-0.787605	-0.783336	-0.000107
C	1.683721	-0.673184	0.000092
C	2.907486	0.050229	0.000045
C	3.954067	0.644141	0.000016
C	0.475589	-0.083047	-0.000138
H	-2.795066	2.136064	0.000080
H	-4.330454	-0.610580	0.000116
H	-0.786190	-1.868255	-0.000146
H	1.757066	-1.757577	0.000323
H	4.876038	1.172659	-0.000013
H	0.433929	1.004065	-0.000375

**Vibrational frequencies**

87.3304	105.4867	148.6189
207.0715	300.0317	362.2017
443.5306	443.9025	507.1983
602.245	629.8202	707.1709
711.4876	817.8696	855.6705
869.9125	935.6477	944.3597
1000.502	1011.801	1063.276
1122.702	1186.664	1263.295
1329.459	1386.732	1608.662
1699.771	1836.705	2225.572
3160.402	3166.058	3183.741
3271.969	3313.36	3487.943

**p39 + H**

**Cartesian coordinates**

C	1.885657	1.030585	0.000000
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C	2.990956	0.288795	-0.000003
C	2.151675	-1.009475	0.000001
C	1.020841	-0.286850	0.000003
C	-1.312647	0.406400	0.000000
C	-2.709103	0.151606	-0.000001
C	-3.895867	-0.043018	-0.000002
C	-0.376287	-0.562579	0.000002
H	1.673032	2.090129	0.000005
H	4.050846	0.501352	-0.000005
H	2.375345	-2.067384	-0.000006
H	-1.007014	1.448908	0.000002
H	-4.944264	-0.219912	-0.000001
H	-0.679296	-1.605873	0.000001

**Vibrational frequencies**

87.6094	108.6489	166.9918
220.2759	294.7074	452.4591
463.8609	500.1729	569.7566
605.6637	645.3592	720.2188
724.1691	773.6156	825.8977
870.4598	900.4426	946.6609
975.3573	1037.83	1080.82
1166.377	1244.3	1288.398
1303.093	1317.951	1646.807
1654.018	1720.371	2230.065
3173.498	3181.33	3229.504
3245.509	3267.332	3482.015

**p40 + H**

**Cartesian coordinates**

C	2.189626	0.555202	0.000005
C	2.322091	-0.985754	0.000000
C	0.998201	-1.117128	-0.000005
C	0.851017	0.452553	-0.000001
C	-1.537199	1.123195	-0.000002
C	-2.117044	-0.174486	0.000000
C	-2.663413	-1.246125	0.000004
C	-0.216974	1.397662	-0.000002
H	2.884505	1.384531	0.000010
H	3.157243	-1.671520	0.000001
H	0.298785	-1.939182	-0.000011
H	-2.240769	1.949485	-0.000003
H	-3.140652	-2.196179	0.000007
H	0.083059	2.442147	-0.000002

**Vibrational frequencies**

79.0792	128.4733	177.971
232.6787	337.2897	413.6664
503.1269	590.9295	616.3277
649.7562	659.9129	708.5203
733.0337	761.0305	835.5014
839.8161	921.2547	938.6721
963.1651	996.6241	1080.063
1163.413	1212.633	1248.718
1319.759	1428.818	1641.053
1648.375	1714.013	2224.935
3169.105	3189.878	3229.087
3242.451	3277.729	3485.283

**p41 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	1.787533	0.549942	-0.000173
C	2.787314	-0.562785	0.000218
C	-0.770727	0.162555	-0.000353
C	-2.108841	-0.044975	-0.000938
C	-3.303994	-0.232056	0.0002407
C	0.446711	0.353750	-0.002265
H	2.153968	1.572587	0.012027
H	3.390561	-0.538264	0.914922
H	3.481163	-0.460776	-0.840947
H	2.300836	-1.536179	-0.065820
H	-4.354498	-0.395952	0.005874

**Vibrational frequencies**

64.6793	105.5026	134.0108
243.51	376.1539	480.8512
494.0885	560.0406	605.7504
621.0332	692.7526	707.7419
985.7091	1012.442	1118.493
1251.198	1409.119	1437.467
1479.787	1509.641	2046.647
2152.93	3032.093	3088.81

H	1.909135	-2.637053	0.000010
H	0.173867	-1.989436	0.000028
H	2.284524	2.143982	0.000011
H	0.525892	2.724329	0.000010
H	-5.376971	-0.476938	-0.000011
H	3.488611	0.312907	-0.882652
H	3.757477	-1.196677	-0.000070
H	3.488649	0.312821	0.882663

**Vibrational frequencies**

	47.892	71.8052	115.7005
	224.5828	224.927	277.1914
	324.2144	375.3811	394.469
	456.2356	517.464	541.5167
	593.7978	616.4813	670.6009
	676.6133	710.5014	721.5159
	793.3948	835.7667	950.36
	956.6396	978.9573	1029.856
	1072.662	1079.332	1232.439
	1385.977	1420.29	1443.309
	1458.149	1487.428	1507.545
	1672.37	1734.248	2199.924
	2388.649	3042.139	3102.838
	3146.946	3166.061	3181.075
	3257.017	3275.458	3483.094

**p43 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C	-1.506682	-0.934790	-0.000005
C	-0.468798	-0.095838	0.000000
C	0.905915	-0.625145	0.000006
C	2.003407	0.095197	-0.000006
C	-0.631986	1.397996	0.000002
H	-2.527761	-0.569582	-0.000009
H	-1.364971	-2.010547	0.000000
H	0.999441	-1.716432	0.000023
H	3.069156	-0.080521	-0.000012
H	-0.150594	1.835741	-0.879549
H	-0.150703	1.835724	0.879622
H	-1.685699	1.681095	-0.000059

**Vibrational frequencies**

	139.9676	194.6897	260.528
	430.7047	432.1952	539.7518
	633.6071	744.1209	765.0388
	860.8482	882.623	925.5955
	992.3672	1051.158	1074.827
	1257.239	1331.109	1418.713
	1450.726	1481.531	1501.413
	1660.496	1726.846	3049.067
	3066.871	3113.86	3139.991
	3156.346	3244.734	3265.109

**p44 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	2.702594	0.719827	-0.015428
C	1.909157	-0.545616	0.010819
C	-0.725462	-0.159464	0.001285
C	-2.083419	0.041464	-0.002933
C	-3.273144	0.216771	-0.006585
C	0.465269	-0.338809	0.003999
H	2.229799	1.678056	0.148684
H	3.776402	0.668366	-0.141221
H	2.179136	-1.181235	-0.844059
H	2.169648	-1.142196	0.899745
H	-4.324956	0.371968	-0.010090

**Vibrational frequencies**

	106.1982	133.982	151.8071
	246.4161	324.3032	452.1658
	478.0011	546.93	570.7661
	673.3448	674.1422	710.5773
	864.7691	981.0399	1096.591
	1178.518	1207.252	1361.864
	1446.026	1459.955	2203.258
	2407.604	2982.328	3023.964
	3169.884	3289.226	3483.37

**p45 + H**

**Cartesian coordinates**

C	2.967909	1.316333	-0.465261
C	2.302456	0.007171	-0.119889
C	1.202066	-0.034295	0.572926
C	0.094341	-0.075777	1.277335
C	-2.315313	-0.014359	0.224991
C	-3.574103	0.018266	-0.315150
C	-4.679479	0.047022	-0.789703
C	-1.202243	-0.041801	0.691311
C	2.971577	-1.251115	-0.614606
H	3.060441	1.413947	-1.551435
H	3.978698	1.345572	-0.045902
H	2.406819	2.169416	-0.084453
H	0.146254	-0.138388	2.362150
H	-5.655239	0.073177	-1.210957
H	3.062126	-1.223323	-1.704943

H	2.414297	-2.144315	-0.333118
H	3.983343	-1.324763	-0.203069

**Vibrational frequencies**

	51.3747	59.2429	138.1404
	153.3776	156.102	191.2387
	234.501	295.7137	328.5009
	428.708	431.4504	516.9667
	555.0701	560.3407	601.4719
	668.6258	704.5308	771.8666
	780.8227	824.2915	973.984
	996.4475	1028.361	1102.425
	1197.892	1226.162	1252.847
	1403.207	1417.186	1450.244
	1477.203	1485.556	1495.842
	1518.822	2083.092	2200.623
	2386.589	3042.176	3044.569
	3105.908	3107.344	3150.081
	3152.095	3157.297	3486.136

**p46 + C<sub>2</sub>H<sub>6</sub>**

**Cartesian coordinates**

C	2.521446	0.000181	0.000008
C	-0.062167	-0.000256	0.000031
C	-1.415283	-0.000117	-0.000012
C	-2.625040	0.000148	-0.000021
C	1.171073	-0.000157	-0.000042
H	3.073889	0.932324	0.000042
H	3.074405	-0.931649	0.000042
H	-3.688466	0.000539	0.000136

**Vibrational frequencies**

	138.5862	147.7072	342.5825
	391.6841	502.5683	530.9046
	624.929	662.5262	733.3977
	737.137	1026.762	1312.018
	1474.326	2039.865	2149.387
	3158.906	3256.756	3477.589
	3158.5862	147.7072	342.5825
	391.6841	502.5683	530.9046
	624.929	662.5262	733.3977
	737.137	1026.762	1312.018
	1474.326	2039.865	2149.387
	3158.906	3256.756	3477.589

**p47 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C	1.977881	0.007894	0.127334
C	0.827533	-0.596323	-0.151654
C	-0.524127	0.003118	-0.033462
C	-0.701751	1.381351	-0.069006
C	-1.603503	-0.855261	0.100719
H	2.922653	-0.511293	0.016728
H	2.020929	1.031008	0.486787
H	0.847514	-1.634712	-0.474565
H	0.123179	2.060714	-0.241649
H	-1.689424	1.810721	0.049523
H	-2.611416	-0.470634	0.203388
H	-1.469639	-1.930470	0.116201

**Vibrational frequencies**

	53.0094	305.5123	408.3978
	438.3306	521.1501	547.2727
	557.8916	737.441	770.4004
	810.3416	828.2682	956.8675
	986.2355	1027.336	1044.008
	1076.708	1294.467	1348.404
	1378.32	1464.943	1494.782
	1539.441	1723.907	3155.004
	3159.606	3164.93	3169.651
	3247.711	3260.456	3267.144

**p48 + C<sub>2</sub>H<sub>6</sub>**

**Cartesian coordinates**

C	2.521446	0.000181	0.000008
C	-0.062167	-0.000256	0.000031
C	-1.415283	-0.000117	-0.000012
C	-2.625040	0.000148	-0.000021
C	1.171073	-0.000157	-0.000042
H	3.073889	0.932324	0.000042
H	3.074405	-0.931649	0.000042
H	-3.688466	0.000539	0.000136

**Vibrational frequencies**

	138.5862	147.7072	342.5825
	391.6841	502.5683	530.9046
	624.929	662.5262	733.3977
	737.137	1026.762	1312.018
	1474.326	2039.865	2149.387
	3158.906	3256.756	3477.589
	3158.5862	147.7072	342.5825
	391.6841	502.5683	530.9046
	624.929	662.5262	733.3977
	737.137	1026.762	1312.018
	1474.326	2039.865	2149.387

3158.906	3256.756	3477.589
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**p49 + H**

**Cartesian coordinates**

C	-3.539595	-0.878992	-0.000041
C	-2.904198	0.291438	-0.000038
C	-1.448548	0.489975	0.000020
C	-0.588890	-0.760673	0.000058
C	2.036759	-0.341179	0.000005
C	3.392608	-0.127109	-0.000020
C	4.580087	0.062627	-0.000039
C	0.846966	-0.527130	0.000027
C	-0.934843	1.719922	0.000027
H	-4.622111	-0.924040	-0.000096
H	-3.017247	-1.829784	0.000017
H	-3.491184	1.206708	-0.000092
H	-0.846035	-1.368956	0.875686
H	-0.846065	-1.369031	-0.875509
H	5.630114	0.229761	-0.000057
H	-1.584141	2.588657	0.000000
H	0.134594	1.893404	0.000063

**Vibrational frequencies**

	44.7814	71.6912	142.6197
	159.17	208.0271	241.532
	332.1893	392.4928	408.6296
	484.6113	527.7881	538.3277
	564.0647	633.7017	674.5343
	712.0638	770.5282	789.4442
	842.9196	939.9325	949.5283
	963.5273	971.3049	1038.727
	1065.038	1182.738	1182.738
	1282.831	1331.318	1391.549
	1439.134	1460.656	1480.116
	1694.595	1747.507	2203.628
	2407.726	3035.717	3068.849
	3160.302	3163.488	3172.081
	3252.082	3257.071	3483.105

**p50 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C	2.397209	-0.229417	-0.000001
C	1.352595	-1.065295	0.000000
C	-1.165072	-0.306840	0.000001
C	-2.478896	0.081802	0.000000
C	-3.632197	0.424823	-0.000001
C	-0.005142	-0.644297	0.000001
C	2.326713	1.261147	0.000000
H	3.389704	-0.672184	-0.000003
H	1.520972	-2.137787	-0.000001
H	-4.651891	0.725918	-0.000002
H	2.837011	1.667066	-0.879156
H	2.837022	1.667064	0.879150
H	1.295919	1.618387	0.000007

**Vibrational frequencies**

	77.012	108.2376	144.856
	206.4421	292.3581	374.8083
	479.0052	531.1382	560.6891
	583.6436	677.3186	687.3486
	743.681	771.9898	938.8297
	989.254	1070.004	1107.908
	1186.435	1279.45	1403.289
	1446.039	1483.654	1489.4
	1718.766	2199.471	2381.294
	3048.372	3107.996	3146.847
	3176.201	3196.246	3487.703







H 0.346013 -1.868386 -0.762732

**Vibrational frequencies**

61.4746 132.41 151.5626  
180.1868 256.0266 401.9295  
440.164 532.1963 545.3958  
579.7773 652.8958 663.0683  
693.2411 731.2909 748.5449  
801.3042 882.281 914.7623  
933.1947 967.165 978.2598  
1006.032 1034.077 1042.439  
1099.212 1111.229 1194.714  
1233.292 1276.433 1305.731  
1337.964 1396.325 1446.861  
1613.42 1685.687 1735.261  
2247.45 3001.234 3156.529  
3171.55 3230.494 3247.761  
3249.626 3254.797 3486.807

**p69 + C<sub>2</sub>H<sub>2</sub>**

**Cartesian coordinates**

C 1.699356 0.734507 -0.310511  
C 1.699097 -0.734442 -0.310921  
C -0.306763 -0.000083 0.606216  
C -1.650679 0.000080 0.030299  
C -2.755678 0.000197 -0.434214  
C 0.544207 -1.180444 0.196526  
C 0.544664 1.180257 0.196739  
H 2.514356 1.348362 -0.670945  
H 2.514632 -1.348442 -0.670145  
H -0.401741 -0.000460 1.702990  
H -3.731512 0.000297 -0.856184  
H 0.229298 -2.206173 0.324752  
H 0.229751 2.205989 0.324728

**Vibrational frequencies**

120.3521 160.6864 356.2029  
463.2666 528.5843 589.0102  
690.9542 703.8382 711.7942  
743.5076 815.4268 838.9255  
900.8862 977.3517 978.6567  
1006.039 1039.319 1050.314  
1108.327 1134.232 1213.841  
1277.681 1307.051 1404.032  
1603.54 1680.604 2252.745  
3022.041 3224.138 3235.043  
3258.396 3263.523 3485.867

**p70 + H**

**Cartesian coordinates**

C -3.638405 -0.591353 -0.164602  
C -2.380465 -0.265197 -0.094374  
C -1.117260 0.059941 -0.022327  
C -0.546640 1.396371 -0.235515  
C 1.234803 0.079979 0.592646  
C 2.494929 -0.359625 -0.004086  
C 3.525615 -0.722901 -0.497922  
C 0.748267 1.420289 0.073020  
C 0.041320 -0.873847 0.297829  
H -4.081948 -0.933573 -1.095369  
H -4.286810 -0.532811 0.705142  
H -1.132040 2.237613 -0.582632  
H 1.390368 0.160148 1.676238  
H 4.438069 -1.045136 -0.938421  
H 1.401573 2.281073 0.012519  
H 0.271535 -1.486709 -0.576729  
H -0.173728 -1.542544 1.131238

**Vibrational frequencies**

40.4582 114.3128 163.2029  
191.3017 249.6886 355.3056  
450.4935 480.9833 520.0337  
582.5546 601.9737 636.0264  
698.4771 710.1557 717.5924  
797.9687 855.9001 863.6407  
898.4588 975.5543 991.1414  
1020.242 1043.047 1062.469  
1121.344 1192.744 1207.894  
1257.898 1281.737 1302.871  
1348.437 1393.19 1481.836  
1493.233 1687.253 2088.458  
2251.124 3033.442 3083.593  
3131.291 3144.438 3209.551  
3221.345 3245.235 3487.244

**p71 + H**

**Cartesian coordinates**

C -1.451472 -0.475427 0.000505  
C -2.642910 -1.085676 0.000287  
C -0.019075 1.546765 0.000036  
C -1.229556 0.958600 0.000144  
C 2.274150 0.267194 0.000029  
C 3.475030 -0.390810 -0.000101  
C 4.530203 -0.969563 -0.000249  
C 1.212095 0.844400 0.000085

C -4.000453 -0.456877 -0.000552

H -0.557937 -1.093369 0.001024  
H -2.640408 -2.173235 0.000735  
H 0.049846 2.629943 -0.000161  
H -2.094497 1.613452 0.000018  
H 5.463506 -1.478838 -0.000393  
H -3.973865 0.632964 -0.001745  
H -4.567499 -0.780334 0.878193  
H -4.567220 -0.782220 -0.878770

**Vibrational frequencies**

22.8072 56.2529 82.9998  
133.119 179.1807 232.4621  
277.2283 355.1564 366.5652  
515.0628 520.5316 558.4816  
578.9632 657.3977 676.2723  
705.7704 747.7497 768.6264  
813.7587 941.386 998.5428  
1026.301 1034.061 1063.339  
1149.772 1189.346 1256.953  
1303.001 1378.055 1423.039  
1472.316 1479.418 1495.522  
1666.45 1740.7 2196.725  
2374.76 3045.076 3098.871  
3150.681 3165.68 3181.727  
3186.049 3204.288 3484.168

**p72 + H**

**Cartesian coordinates**

C -1.309902 -2.343472 0.119327  
C -2.131762 1.273476 -0.100930  
C -2.136729 -0.060697 -0.156304  
C -1.039760 -1.033060 0.005296  
C 1.505970 -0.342145 -0.016291  
C 2.830950 0.006269 -0.033266  
C 3.993674 0.314680 -0.047236  
C 0.333691 -0.628105 0.002602  
C -1.010384 2.228165 0.167959  
H -0.520368 -3.076140 0.226795  
H -2.334032 -2.699649 0.104917  
H -3.095310 1.749425 -0.271378  
H -3.094262 -0.540193 -0.342007  
H 5.022205 0.584026 -0.060315  
H -1.336713 2.981518 0.890677  
H -0.741000 2.763531 -0.748911  
H -0.115001 1.746821 0.553281

**Vibrational frequencies**

35.5111 66.2295 112.6553  
122.0304 220.5122 268.0216  
281.8086 330.542 378.341  
488.6348 541.8889 573.735  
608.0059 625.3985 683.9822  
695.1832 716.0301 721.8955  
805.2809 900.4318 947.372  
981.5078 1022.95 1076.32  
1078.896 1124.121 1304.322  
1375.271 1415.609 1429.036  
1471.211 1491.414 1506.869  
1665.168 1755.383 2200.962  
2386.821 3049.762 3104.002  
3146.183 3166.966 3175.305  
3193.45 3265.687 3487.305

**p73 + H**

**Cartesian coordinates**

C -2.790106 -0.573681 0.000018  
C -1.727133 0.503873 -0.000009  
C -0.708300 -0.375012 -0.000042  
C -1.610382 -1.597705 0.000018  
C 1.898361 -0.120104 -0.000027  
C 3.261678 0.007357 0.000001  
C 4.459879 0.120131 0.000028  
C 0.694218 -0.228222 -0.000037  
C -1.816494 1.983829 0.000008  
H -3.426360 -0.602355 -0.889479  
H -3.426354 -0.602336 0.889520  
H -1.544107 -2.225282 -0.891513  
H -1.544044 -2.225183 0.891610  
H 5.518294 0.220741 0.000059  
H -2.362133 2.337483 0.880808  
H -2.362482 2.337488 -0.880571  
H -0.823137 2.436650 -0.000183

**Vibrational frequencies**

66.4655 69.7995 110.1432  
177.3993 192.6564 232.3806  
305.7647 373.756 444.9594  
506.7268 520.093 572.6129  
591.6523 664.8657 696.9907  
705.2765 802.0041 911.0604  
940.2676 980.2407 987.9747  
1060.21 1100.746 1115.725  
1176.841 1221.676 1227.5  
1278.581 1352.247 1418.558

1460.142 1474.68 1481.93  
1488.92 1743.055 2197.368  
2374.229 3041.677 3055.214  
3074.202 3101.878 3102.824  
3130.344 3141.279 3484.432

**p74 + H**

**Cartesian coordinates**

C 2.415853 -0.504529 -0.676599  
C 1.776663 0.478343 -0.040427  
C 0.825032 -0.473163 0.686370  
C 1.567738 -1.615528 -0.099461  
C -1.759883 -0.132007 0.177011  
C -3.091684 0.054749 -0.094643  
C -4.259386 0.219048 -0.332154  
C -0.589900 -0.299321 0.416255  
C 1.855626 1.959093 0.014861  
H 3.249347 -0.514088 -1.369235  
H 0.992378 -0.523607 1.767522  
H 2.077280 -2.340084 0.541398  
H 0.928923 -2.145787 -0.808993  
H -5.291677 0.364974 -0.540165  
H 0.895150 2.401108 -0.268113  
H 2.625887 2.337677 -0.659844  
H 2.082354 2.299707 1.030154

**Vibrational frequencies**

63.6762 81.5629 149.1837  
182.6355 190.741 255.071  
315.4234 375.1657 456.3216  
512.9271 547.0201 596.8618  
666.9863 701.9236 708.9664  
712.5462 845.7795 913.2953  
920.1223 973.2689 994.8923  
1029.514 1059.096 1115.051  
1163.631 1205.139 1219.337  
1243.498 1301.285 1350.273  
1414.545 1479.777 1483.049  
1488.694 1748.477 2199.697  
2396.194 3044.571 3067.55  
3074.729 3108.107 3130.478  
3137.968 3215.708 3484.753

**p75 + H**

**Cartesian coordinates**

C 2.744102 -0.380195 -0.371669  
C 1.739673 0.653961 0.092380  
C 0.795938 -0.432620 0.607065  
C 1.619367 -1.443387 -0.254747  
C -1.804607 -0.157741 0.158767  
C -3.146868 -0.008655 -0.082947  
C -4.323790 0.122446 -0.293560  
C -0.624785 -0.288487 0.368332  
C 1.599425 1.958140 -0.052525  
H 3.539733 -0.540347 0.362181  
H 3.193284 -0.227644 -1.353735  
H 0.974613 -0.613946 1.672969  
H 1.864514 -2.392508 0.221122  
H 1.130664 -1.626738 -1.211867  
H -5.363953 0.240633 -0.478900  
H 2.368391 2.557189 -0.528104  
H 0.702022 2.462587 0.289755

**Vibrational frequencies**

69.2555 84.1869 132.1477  
191.051 239.6472 343.4483  
374.4439 439.538 500.7536  
537.7214 591.9207 613.9888  
681.5436 703.3123 708.6195  
773.1436 805.4811 901.2641  
914.8819 931.8358 954.4854  
982.7295 1053.871 1098.343  
1190.23 1206.308 1228.439  
1242.777 1261.542 1282.366  
1373.525 1435.428 1481.886  
1505.158 1787.761 2201.74  
2399.831 3058.693 3065.315  
3099.342 3126.546 3157.166  
3164.581 3247.155 3485.235

**p76 + H**

**Cartesian coordinates**

C 2.542481 -0.386984 -0.606032  
C 1.884243 0.548461 0.388514  
C 0.891234 -0.659814 0.662628  
C 1.694409 -1.392387 -0.404344  
C -1.687757 -0.251056 0.177568  
C -3.018860 -0.038630 -0.077715  
C -4.186091 0.147341 -0.301019  
C -0.517598 -0.437426 0.400465  
C 1.283886 1.832827 -0.156119  
H 3.407272 -0.261180 -1.247053  
H 2.499511 0.760489 1.269781  
H 1.011344 -1.078513 1.667475  
H 1.585293 -2.389670 -0.811660

H	-5.217927	0.311743	-0.497134
H	0.656635	1.631725	-1.028073
H	2.076317	2.524307	-0.455248
H	0.666235	2.327111	0.598242

**Vibrational frequencies**

70.1582	73.6588	167.9545
199.4911	232.548	265.8815
334.6013	412.2281	472.3075
496.7095	545.9401	598.3401
703.7792	714.2585	716.9515
783.7598	827.3173	879.6916
897.2677	959.9267	996.124
1041.55	1063.713	1100.806
1159.934	1181.786	1211.653
1235.241	1311.43	1349.845
1364.594	1417.396	1494.295
1498.556	1672.955	2200.053
2396.784	3050.79	3056.747
3066.157	3128.739	3133.565
3205.098	3237.884	3484.847

**p77 + H**

**Cartesian coordinates**

C	3.074648	-0.620740	-0.000019
C	1.653250	-0.277595	0.000028
C	0.727475	0.672297	0.000013
C	1.977425	-1.699033	-0.000001
C	-1.832451	0.048269	0.000007
C	-3.167094	-0.261960	-0.000002
C	-4.339506	-0.532893	-0.000011
C	-0.654129	0.313428	0.000013
C	1.062992	2.142624	-0.000007
H	3.642931	-0.479870	-0.914264
H	3.642988	-0.479895	0.914194
H	1.823122	-2.263463	-0.914153
H	1.823174	-2.263486	0.914146
H	-5.375738	-0.770531	-0.000019
H	0.641698	2.633120	0.881676
H	0.641683	2.633099	-0.881695
H	2.144482	2.284647	-0.000019

**Vibrational frequencies**

64.4001	85.0799	146.9406
173.6994	189.0012	206.8919
239.692	334.95	422.0989
463.4167	515.0121	546.469
594.3633	631.2403	670.6222
697.4495	757.3116	795.9914
872.1358	970.55	1028.143
1048.512	1068.51	1073.802
1096.398	1098.536	1167.378
1195.3	1314.483	1421.952
1446.269	1472.448	1480.632
1502.372	1865.128	2197.918
2381.234	3054.774	3122.277
3130.441	3134.06	3152.418
3210.733	3223.142	3486.641

**p78 + H**

**Cartesian coordinates**

C	2.378876	-0.801262	-0.000014
C	3.506900	-0.080665	-0.000008
C	-0.064356	-1.062136	0.000019
C	1.026026	-0.276227	-0.000021
C	-2.524485	-0.147783	0.000007
C	-3.808722	0.327352	0.000000
C	-4.936695	0.747007	-0.000007
C	-1.388216	-0.559873	0.000010
C	3.642736	1.409177	0.000021
H	2.465515	-1.885234	-0.000022
H	4.445847	-0.629205	-0.000041
H	0.046691	-2.143862	0.000075
H	0.882916	0.799606	-0.000086
H	-5.932808	1.118757	-0.000026
H	2.685551	1.930737	0.000483
H	4.206564	1.737887	-0.878793
H	4.207341	1.737776	0.878368

**Vibrational frequencies**

54.8534	55.897	87.9431
119.8503	166.2692	195.6057
281.7547	339.8001	366.229
464.3455	479.914	549.4704
572.2583	631.6737	670.2774
684.2684	744.4937	784.9582
881.912	941.6824	970.095
1022.188	1062.759	1066.634
1175.649	1218.237	1278.312
1324.165	1353.889	1423.21
1453.32	1482.003	1502.015
1685.293	1743.904	2197.085
2375.174	3045.809	3099.344
3150.863	3162.152	3167.496
3181.452	3204.027	3483.589

**p79 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	-2.125752	-0.303730	-0.000053
C	-1.182947	0.618447	-0.000066
C	1.401737	0.136957	0.000113
C	2.751049	-0.100636	0.000027
C	3.936054	-0.309458	-0.000122
C	0.211553	0.338826	0.000268
C	-3.588701	-0.378417	-0.000018
H	-1.466422	1.676047	-0.000446
H	4.983193	-0.493435	-0.000324
H	-3.952153	-0.908214	0.884943
H	-3.951945	-0.914188	-0.881465
H	-4.030630	0.627858	-0.003599

**Vibrational frequencies**

68.7101	78.6283	162.268
203.7665	209.1074	317.5549
396.628	455.0655	551.0526
554.8418	667.3877	708.5332
757.8705	786.9202	944.0024
1042.414	1065.658	1206.1
1293.294	1400.151	1450.7
1475.174	1751.678	2198.712
2381.472	3007.977	3060.959
3093.847	3119.624	3483.596

**p80 + H**

**Cartesian coordinates**

C	-1.432880	1.103760	-0.210407
C	-2.520789	-0.009992	-0.388506
C	-1.364900	-0.988464	-0.354165
C	-0.429774	-0.038503	-0.205832
C	2.180826	-0.030096	0.004153
C	3.545466	-0.015129	0.116816
C	4.744550	-0.002501	0.216001
C	0.976848	-0.051523	-0.094766
C	-3.560085	-0.128572	0.716102
H	-1.504655	1.655648	0.730279
H	-1.336540	1.808315	-1.039793
H	-3.010479	0.040671	-1.366950
H	-1.312584	-2.068742	-0.423734
H	5.803969	0.009279	0.305754
H	-4.146026	-1.045185	0.605776
H	-4.251487	0.718427	0.694439
H	-3.077771	-0.152288	1.697857

**Vibrational frequencies**

68.65	69.7515	148.996
207.642	245.2881	283.3738
333.6325	408.5679	479.1207
486.0167	507.2633	574.7934
589.7631	679.6212	697.4047
778.0584	873.7274	890.5114
911.8649	931.6554	1004.996
1072.484	1081.195	1100.961
1179.184	1211.096	1230.215
1270.028	1302.577	1370.262
1417.474	1482.418	1498.604
1501.973	1691.65	2199.824
2379.237	3044.35	3061.254
3073.73	3122.71	3123.455
3131.506	3216.758	3484.461

**p81 + H**

**Cartesian coordinates**

C	2.809699	-0.664595	-0.748557
C	1.497683	-0.660599	0.000934
C	0.624725	0.554722	0.000228
C	2.811116	-0.662887	0.747884
C	-1.962172	0.048532	0.000076
C	-3.304550	-0.226373	0.000020
C	-4.483117	-0.467963	-0.000018
C	-0.781646	0.301325	0.000124
C	1.073395	1.815437	-0.000455
H	3.088661	-1.574553	-1.265403
H	3.080539	0.250968	-1.261685
H	0.948680	-1.593908	0.002518
H	3.091014	-1.571699	1.266240
H	3.083038	0.253777	1.258465
H	-5.524980	-0.680176	-0.000034
H	0.387285	2.652066	-0.001093
H	2.134965	2.037943	-0.000420

**Vibrational frequencies**

31.9792	71.3629	113.8985
215.6318	265.4539	286.8793
338.4093	372.8869	497.1439
538.202	590.1844	654.7921
676.7259	682.2796	704.4695
737.4918	799.2076	838.5718
842.4166	929.9757	940.0669
961.3266	1060.794	1080.623
1081.461	1126.146	1132.711

1209.708	1230.228	1290.453
1436.719	1452.524	1476.609
1523.584	1697.371	2199.001
2383.881	3147.739	3152.354
3169.243	3198.773	3233.261
3247.871	3266.371	3484.343

**p82 + H**

**Cartesian coordinates**

C	-0.731440	2.552679	0.000050
C	-1.760959	-0.994834	0.000061
C	-1.797034	0.336331	-0.000120
C	-0.617335	1.216582	-0.000021
C	1.765074	0.083493	0.000020
C	2.999418	-0.512183	-0.000004
C	4.081793	-1.037113	-0.000038
C	0.680451	0.612332	0.000029
C	-2.967756	-1.876886	0.000007
H	-1.708818	3.022002	-0.000003
H	0.139631	3.195185	0.000152
H	-0.793108	-1.492163	0.000308
H	-2.755406	0.850966	-0.000343
H	5.038419	-1.501308	-0.000058
H	-2.970472	-2.529511	0.878968
H	-2.969931	-2.530203	-0.878435
H	-3.893581	-1.297381	-0.000495

**Vibrational frequencies**

62.0446	91.7114	111.4074
178.9556	189.4498	197.8876
255.1681	317.4126	378.1753
430.6105	537.0042	539.1074
625.4023	636.4123	659.1078
678.5646	715.5482	728.7091
849.7322	923.9915	944.5018
999.0282	1011.364	1073.657
1084.111	1135.08	1317.759
1350.54	1364.319	1419.058
1447.064	1484.332	1491.237
1679.663	1760.607	2201.97
2390.542	3037.465	3097.394
3127.239	3168.454	3170.387
3172.798	3267.207	3485.876

**p83 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	2.373337	-0.261508	0.000003
C	1.367434	-1.117446	0.000001
C	-1.139385	-0.307767	-0.000003
C	-2.439867	0.123416	-0.000001
C	-3.581143	0.504694	0.000002
C	0.007132	-0.688484	-0.000003
C	2.593591	1.187143	0.000000
H	1.552340	-2.189384	0.000003
H	-4.589981	0.840463	0.000005
H	3.159266	1.494734	-0.883826
H	3.159174	1.494753	0.883878
H	1.632599	1.719148	-0.000057

**Vibrational frequencies**

71.2897	75.1398	135.5964
180.264	304.3603	329.644
429.9255	516.441	549.5952
570.4799	672.5552	684.0669
747.9874	790.9418	928.8633
1039.606	1058.776	1197.823
1312.159	1397.15	1455.798
1466.631	1731.592	2196.295
2375.022	3013.516	3094.56
3116.232	3155.125	3485.013

**p84 + C<sub>2</sub>H<sub>4</sub>**

**Cartesian coordinates**

C	-2.181814	1.341987	0.000017
C	-1.591371	0.162080	0.000002
C	1.045421	0.038409	-0.000027
C	2.413541	-0.032342	-0.000005
C	3.614945	-0.095618	0.000024



2336.388      3483.639      3484.782

***C<sub>4</sub>H<sub>5</sub> (1,3-butadien-1-yl)***  
**Cartesian coordinates**  
 C -1.498603 -0.501629 0.034979  
 C -0.680114 0.543456 -0.056854  
 C 0.786817 0.486949 0.071322  
 C 1.543430 -0.574576 -0.081844  
 H -1.120056 -1.499362 0.232531  
 H -2.569506 -0.385350 -0.082292  
 H -1.098829 1.531712 -0.226999  
 H 1.282055 1.435349 0.304840  
 H 2.597154 -0.807554 -0.033701

**Vibrational frequencies**

107.8461	270.0826	511.2163
597.5106	721.9698	812.385
865.197	971.9167	981.8379
1044.622	1088.96	1280.779
1341.833	1449.481	1669.63
1715.556	3068.8	3156.728
3173.629	3252.292	3262.638

***C<sub>4</sub>H<sub>6</sub> (1,3-butadiene)***

**Cartesian coordinates**  
 C -1.838541 -0.110893 -0.000056  
 C -0.609535 0.401749 0.000067  
 C 0.609535 -0.401751 0.000062  
 C 1.838540 0.110895 -0.000053  
 H -2.718119 0.522073 -0.000067  
 H -2.002085 -1.184501 -0.000145  
 H -0.476726 1.481814 0.000151  
 H 0.476734 -1.481826 0.000156  
 H 2.002078 1.184507 -0.000150  
 H 2.718123 -0.522072 -0.000067

**Vibrational frequencies**

154.3644	304.6184	524.8894
531.3234	789.0897	903.08
946.9017	951.0523	1006.303
1009.948	1053.449	1235.38
1328.466	1329.704	1421.194
1475.546	1685.285	1752.834
3148.707	3151.175	3163.185
3168.233	3242.885	3243.183

***C<sub>4</sub>H<sub>6</sub> (1,2-butadiene)***  
**Cartesian coordinates**

C 1.739293 -0.366608 -0.000002  
 C 0.554259 0.561281 -0.000028  
 C -0.689767 0.175577 -0.000034  
 C -1.932191 -0.214933 0.000012  
 H 2.362973 -0.194819 0.882287  
 H 2.364306 -0.193238 -0.881039  
 H 1.422648 -1.410452 -0.001178  
 H 0.755915 1.630616 0.000147  
 H -2.467776 -0.381959 -0.929122  
 H -2.467628 -0.382051 0.929220

**Vibrational frequencies**

118.1403	209.7072	343.1082
545.3429	576.7384	885.7592
895.6724	897.6291	1028.268
1057.877	1097.03	1160.286
1369.603	1406.872	1476.431
1484.713	1508.697	2091.532
3046.126	3109.85	3138.721
3145.195	3158.171	3227.124