

Gas-Phase Formation of C₅H₆ isomers via the Crossed Molecular Beam Reaction of the Methylidyne Radical (CH; X²Π) with 1,2-butadiene (CH₃CHCCH₂; X¹A')

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Supporting Information

See supporting information for the discussion of the formation pathways of products **p12**, **p13**, **p17-p22** (figure S1-S2), products **p1-p3**, **p9**, **p15** (figure S3), products **p4**, **p6**, **p7**, **p11**, **p16**, **p33**, **p36**, **p37** (figure S4), and products **p22-p24**, **p31-p35** (figure S5); and rate constants (table S1); optimized Cartesian coordinates and calculated vibrational frequencies of the reactants, products, intermediates, and transition states.

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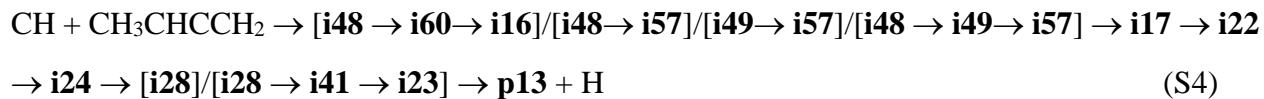
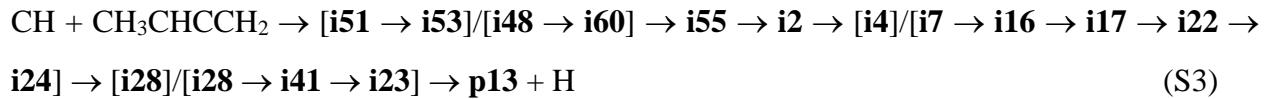
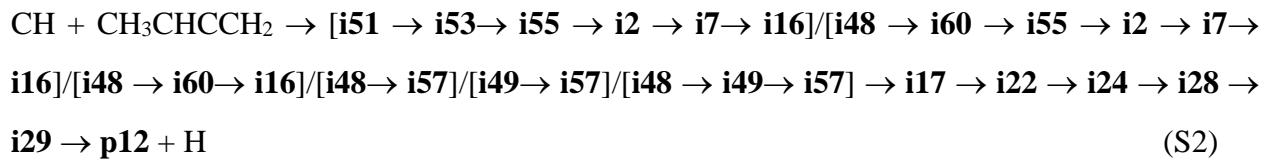
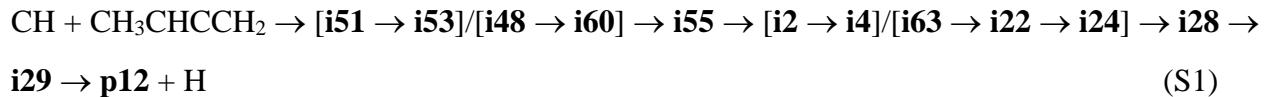
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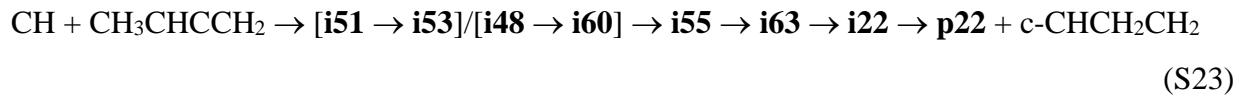
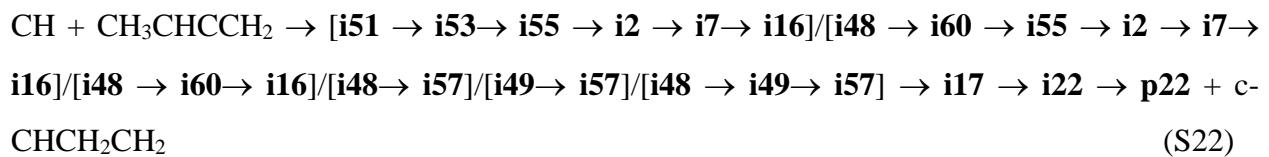
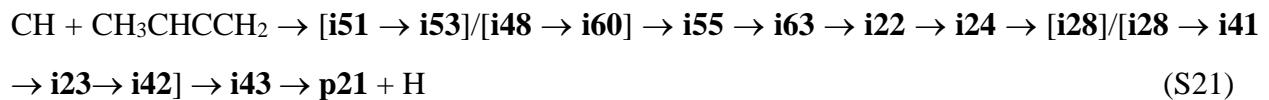
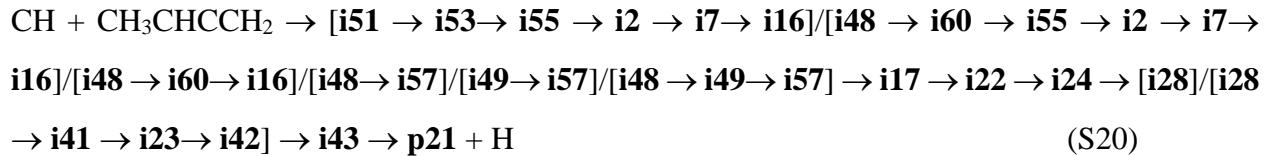
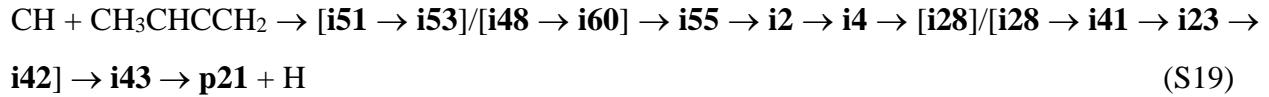
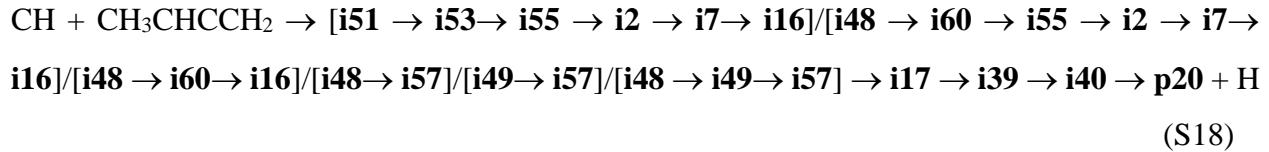
†These authors contributed equally to this work.

CH addition to the terminal and central carbon-carbon double bonds of 1,2-butadiene leading to products p12, p13, p17-p22 via intermediates i2, i4, i7, i9, i16, i17, i22-i29, i36, i39-i43, i48, i49, i51, i53, i55, i57, i60, i63, i64 (Figures S1-S2).

A 1,3-hydrogen migration from the CH₂ group of the c-CCH₂CH₂ moiety to the bare carbon atom in **i55** leads to **i2** which was considered earlier by us as an initial complex for CH addition to the double C=C bond in 1,3-butadiene.⁴⁰ The three-member ring opening in **i2** yields intermediate **i4**. The intermediates **i7**, **i16**, **i17**, and **i39** are rotational conformers connected via low barriers. The intermediates **i16**, **i17** and **i25** can also be formed via hydrogen migration from a CH₂ group of the c-CCH₂CH₂ moiety to the adjacent carbon atom in **i60** and from the CH₂ group to the adjacent bare carbon atom in **i57**. A hydrogen migration from the terminal CH₂ group to the CH moiety of the c-CHCHCH₂ group and from the CH₂ group to the terminal CH moiety of the c-CHCHCH₂ group in **i17** leads to **i22** and **i25**, respectively. A 1,2-H shift in **i55** forms **i63** and connects with its conformer **i22**. The product cyclopropene (**p18**) can be formed via vinyl group emission from **i17** and **i25** via loose exit transition state lying only 10 kJ mol⁻¹ above the separated products. The ring closure in **i39** yields a bicyclic intermediate **i40**. The rotational conformers **i22** and **i24** are connected via a low barrier of 1 kJ mol⁻¹. The product acetylene (**p22**) can be accessed via a C₃H₅ (cyclopropyl) group emission from **i22** via a tight exit transition state lying 26 kJ mol⁻¹ above the separated products. A hydrogen migration from one of the CH₂ moieties to the terminal CH group in **i24** leads to **i26**. A methylene walk in the three-member intermediate **i24** yields the four-member cyclic intermediate **i28**, which can also be formed via the ring closure of **i4**. The conformers **i26** and **i25** are connected via a low barrier of 6 kJ mol⁻¹ above **i26**. The C-C bond formation between two CH moieties in **i25** leads to **i40**. The product 2-methylenecyclo[1.1.0]butane (**p20**) can be formed via hydrogen atom emission from CH moiety of the CHCH₂ group in **i40** via a tight exit transition state lying 19 kJ mol⁻¹ above the separated products. 3-Methylene-cyclobutene (**p13**) can be accessed via atomic hydrogen loss from the CH moiety of the terminal CHCH₂ group in **i28** via a tight exit transition state lying 22 kJ mol⁻¹ above the separated products. A C-C bond formation between the terminal CH₂ group and non-adjacent CH group in **i28** leads to **i43**. The intermediate **i29** can be reached via a hydrogen migration from CH₂ group of c-CHCHCHCH₂ to the terminal CH₂ moiety in **i28**; the decomposition of **i29** accesses 1-methyl-1,3-cyclobutadiene (**p12**) via hydrogen emission from CH group of the CHCH₃ moiety in **i29**; cyclobutadiene (**p19**)

can be formed via CH₃ loss from **i29**. It should be noted that while an exit transition state **i29-p19** could be located at the DFT level, its refined CCSD(T)-F12 relative energy is slightly lower than that of the **p19** product thus indicating that the reverse CH₃ addition to cyclobutadiene may proceed without barrier. A hydrogen migration from CH moiety of the CHCH₂ group to the adjacent CH moiety in **i28** leads to **i41**; intermediate **i23** can be formed via a hydrogen migration from CH₂ moiety of cCCH₂CHCH₂ group to CH moiety in **i41**. A C-C bond formation between the terminal CH₂ group and nonadjacent CH moiety in **i23** accesses **i42**. The product 3-methylene-cyclobutene (**p13**) can be formed via hydrogen atom loss from CH₂ group in cCCHCH₂CH₂ moiety of **i23** via a loose exit transition state lying 10 kJ mol⁻¹ above the separated products. Bicyclo[2.1.0]pent-1(4)-ene (**p17**) can be accessed via hydrogen emission from CH group of **i42** via a loose exit transition state lying 2 kJ mol⁻¹ above the separated products. On the other hand, a hydrogen migration from the CH₂ group to the adjacent bare carbon atom in **i42** leads to **i43**. The product bicyclo[2.1.0]pent-2-ene (**p21**) can be formed via hydrogen emission from the CH₂ group in the cyclic moiety of **i43** via a loose exit transition state lying 12 kJ mol⁻¹ above the separated products. In brief, **p12**, **p13**, **p17**, **p20**, and **p21** are formed via pathways (S1)-(S2), (S3)-(S4), (S5)-(S6), (S14)-(S18), and (S19)-(S21), respectively, with hydrogen losses from 1,2-butadiene or possibly, from both reactants. The CHCH₂, CH₃, c-CHCH₂CH₂ group loss products **p18**, **p19**, and **p22** are accessed through pathways (S7)-(S10), (S11)-(S13), and (S22)-(S23), respectively. Considering the experimentally derived reaction energy of -190 ± 21 kJ mol⁻¹, the products 2-methylenebicyclo[1.1.0]butane (**p20**), and bicyclo[2.1.0]pent-2-ene (**p21**) with the reaction energies of -189, and -205 kJ mol⁻¹ could be among likely reaction products.

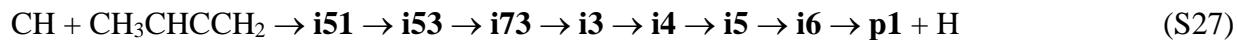
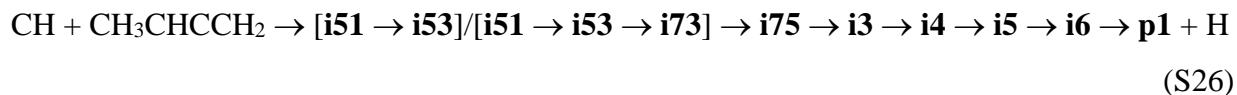
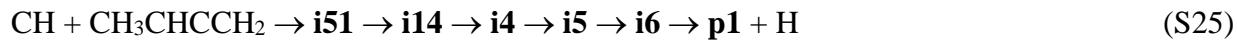
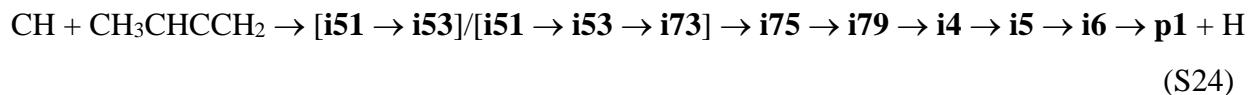


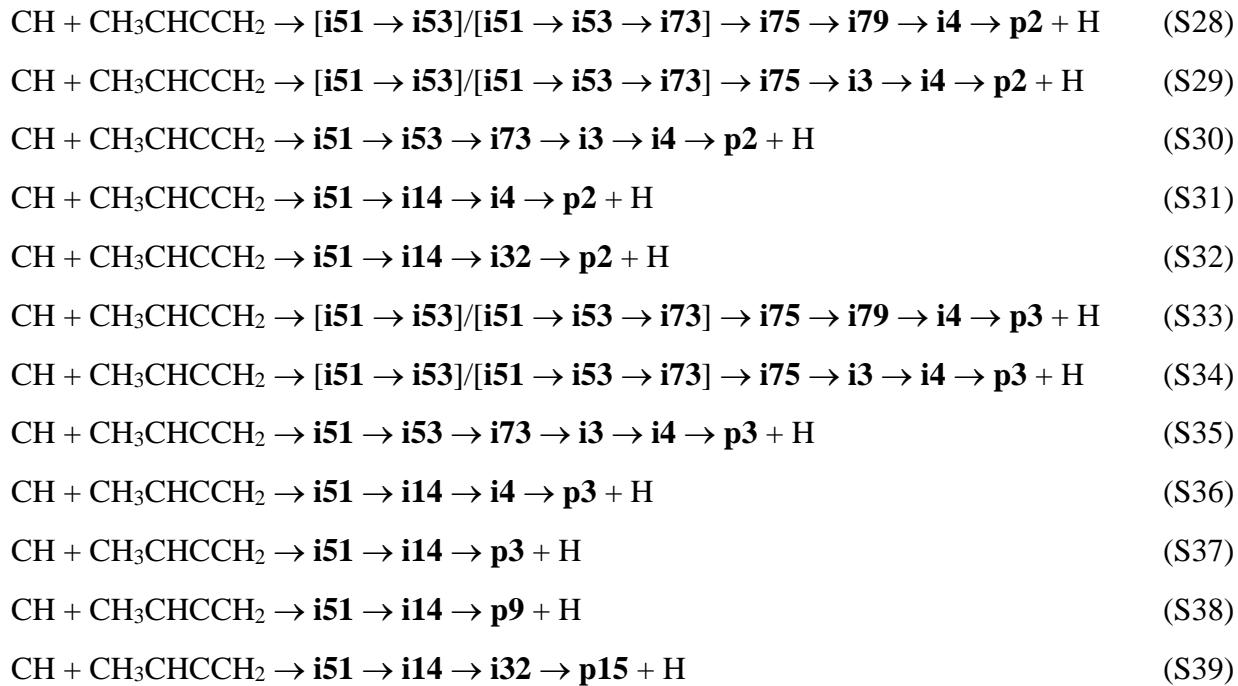


The methylidyne radical (CH) addition to the central carbon-carbon double bond of 1,2-butadiene leading to products p1-p3, p9, p15 via intermediates i3-i6, i14, i32, i51, i53, i73, i75, i79 (Figure S3).

The ring opening of the adduct **i51** leads to the acyclic intermediate **i14**. The product (Z)-3-penten-1-yne (**p9**) can be formed via hydrogen emission from the terminal CH₂ group of **i14** via a loose exit transition state lying 6 kJ mol⁻¹ above the separated products; the product cis-1,2,4-pentatriene (**p3**) can be accessed via atomic hydrogen loss from the terminal CH₃ group of **i14** via a loose exit transition state lying 8 kJ mol⁻¹ above the separated products. A rotation of CH₃CH group in **i14** leads to its conformer **i32** via a barrier of 54 kJ mol⁻¹ above **i14**; the decomposition of **i32** yields the products trans-1,2,4-pentatriene (**p2**) and (E)-3-penten-1-yne (**p15**) via hydrogen atom emission from the terminal CH₃ and CH₂ group of **i32**, respectively. The ring opening in **i53** leads to acyclic intermediates **i73** and **i75**; the intermediates **i73** and **i75** are also connected via a hydrogen migration from the CH moiety to the bare carbon moiety in **i73**. A hydrogen shift from

the central CH₂ group to the adjacent bare carbon moiety in **i73** and **i75** yields intermediate **i3**. The intermediate **i79** can be formed via a conformational change of **i75**. A 1,4-hydrogen migration from the terminal CH₃ group to the bare carbon moiety in **i14** or 1,2-H shift from the central CH₂ group to the adjacent bare C atom in **i79** both lead to **i4**. The conformers **i3** and **i4** are connected via a moderate barrier of 42 kJ mol⁻¹ above **i3**. The product trans-1,2,4-pentatriene (**p2**) and cis-1,2,4-pentatriene (**p3**) can be formed via hydrogen atom emission from the CH group in CH₂CH moiety of **i4** via loose exit transition states lying 13 and 11 kJ mol⁻¹ above the separated products, respectively. The rotation of the CHCH₂ group in **i4** leads to **i5** and eventually gives rise to a cyclic intermediate **i6**; the decomposition of **i6** yields the product cyclopentadiene (**p1**) via hydrogen atom emission from the CH₂ group of **i6**. In brief, **p1** can be formed via pathways (S24)-(S27) with the atomic hydrogen emission from the CH₂ and CH₃ groups of 1,2-butadiene. The product **p2** can be accessed via pathways (S28)-(S30) with the hydrogen loss from the CH₃ and CH groups of 1,2-butadiene or both from the methylidyne radical and the CH group of 1,2-butadiene; **p2** can also be formed via pathway (S31) with hydrogen emission from methylidyne and the CH₃ group of 1,2-butadiene and via pathway (S32) with the atomic hydrogen loss from the CH₃ group of 1,2-butadiene. The product **p3** can be formed through pathways (S33)-(S35) with the hydrogen atom emission from the CH₃ and CH groups of 1,2-butadiene or both from methylidyne radical and the CH group of 1,2-butadiene; **p3** can also be formed via pathway (S36) with the atomic hydrogen emission from the CH and CH₃ groups of 1,2-butadiene and via pathway (S37) with the hydrogen atom loss solely from the CH₃ group of 1,2-butadiene. The products **p9** and **p15** can be reached via pathways (S38) and (S39) with a hydrogen emission from the CH₂ group of 1,2-butadiene, respectively. Considering the experimentally derived reaction energy of -190 ± 21 kJ mol⁻¹, the fact that the products **p1-p3**, **p9** and **p15** have the reaction energies lower than -271 kJ mol⁻¹ suggests that pathways (S24)-(S39) are likely not open under our experiment conditions.

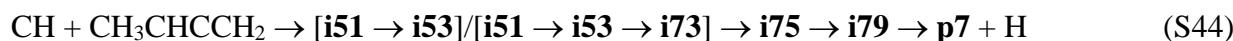
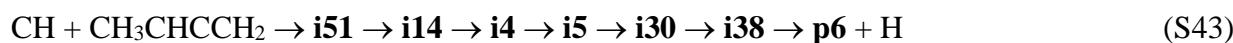
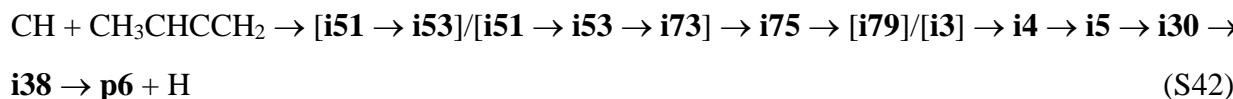
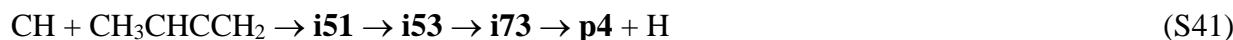
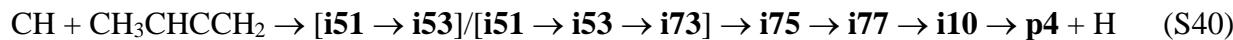


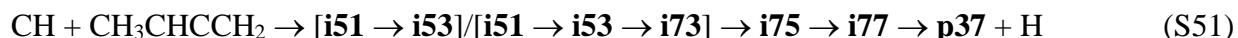
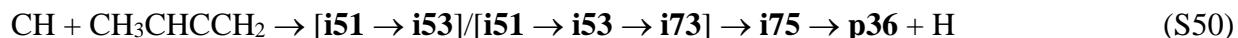
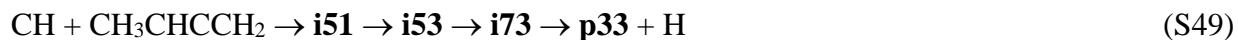
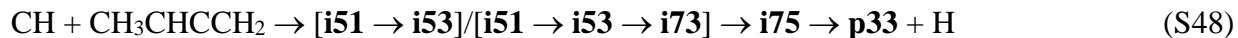
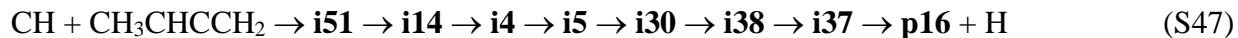
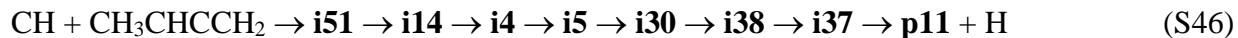
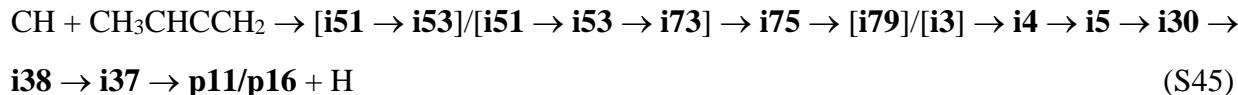


The methylidyne radical (CH) addition to the central carbon-carbon double bond of 1,2-butadiene leading to products p4, p6, p7, p11, p16, p33, p36, p37 via intermediates i3-i5, i10, i14, i30, i37, i38, i51, i53, i73, i75, i77, i79 (Figure S4).

The product allene (**p33**) can be formed via vinyl radical emission from **i73** and **i75** via a tight exit transition state lying 22 kJ mol⁻¹ above the separated products, respectively. The products **p4** and **p36** representing two different enantiomers/conformers of 4-penten-1-yne can be accessed with the atomic hydrogen emission from the terminal CCH₂ group of **i73** and **i75** via loose exit transition states lying close to 12 kJ mol⁻¹ above the separated products. A 1,4-hydrogen migration from the terminal CH₂ group to the non-adjacent bare carbon atom in **i75** leads to intermediate **i77**. Another conformer of 4-penten-1-yne, product **p7** can be formed via atomic hydrogen emission from the terminal CCH₂ group of **i79** via a loose exit transition state lying 13 kJ mol⁻¹ above the separated products. The decomposition of **i77** would lead to the product acetylene (**p37**) via allyl radical loss. The conformers **i77** and **i10** are connected via a low barrier of 16 kJ mol⁻¹ above **i77**. The product 4-penten-1-yne (**p4**) can be formed with the atomic hydrogen emission from the nonterminal CH moiety of the CHCH group in **i10** via a tight exit transition state lying 20 kJ mol⁻¹ above the separated products. The hydrogen migration between the terminal CH₂ groups of **i5** leads to

intermediate **i30** which can be subjected to a three-member ring closure ultimately forming cyclic intermediates **i38** and **i37**. The product cis-3-vinyl-cyclopropene (**p6**) can be produced via hydrogen atom emission from the terminal CH₃ group of **i38** via a tight exit transition state lying 34 kJ mol⁻¹ above the separated products. The product trans-3-vinyl-cyclopropene (**p11**) can be formed via atomic hydrogen loss from the terminal CH₃ group of **i37** via a loose exit transition state lying 10 kJ mol⁻¹ above the separated products. The product 3-ethylidene-cyclopropene (**p16**) can be accessed via hydrogen emission from the nonterminal CH group of the c-CHCHCH moiety of **i37**. In brief, **p4** can be formed via pathway (S40) with a hydrogen loss from the CH group of 1,2-butadiene and via pathway (S41) with hydrogen emission form the CH₂ group of 1,2-butadiene. The product **p6** can be accessed through pathways (S42)-(S43) with atomic hydrogen loss from the CH₂ and CH₃ groups of 1,2-butadiene. The products **p7** and **p36** can be formed via pathways (S44) and (S50), respectively, with hydrogen atom emission from the CH₂ or CH₃ group of 1,2-butadiene. **p11** can be reached via pathways (S45)-(S46), with hydrogen losses from the CH₂ and CH₃ groups of 1,2-butadiene. The product **p16** can be formed via pathway (S45) with atomic hydrogen emission from the methylidyne radical reactant. The products **p33** and **p37** can be formed via pathways (S48)-(S49) and (S51), respectively. Considering the experimentally derived reaction energy of -190 ± 21 kJ mol⁻¹, **p6**, **p11**, and 3-ethylidene-cyclopropene (**p16**) with reaction energies of -181, -185, and -170 kJ mol⁻¹ could be among likely reaction products. Due to high barriers of 186 kJ mol⁻¹, the isomerization processes from **i51** to **i53** are much less competitive than **i51** → **i14**; hence, we may rule out the pathways (S42) and (S45) leading to **p6**, and **p11**, **p16**. Further, from the CH plus 1,3-butadiene study,⁴⁰ we deduced that **i5** isomerizes to **i6** rather than to **i30**. The high barriers of over 200 kJ mol⁻¹ for these isomerization steps suggests that pathways (S43), (S46), (S47) can likely be eliminated, too. Therefore, **p6**, **p11**, and **p16** are unlikely to be formed via pathways (S42)-(S43), (S45)-(S46), and (S47), respectively.

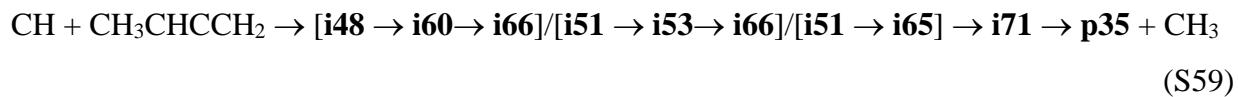
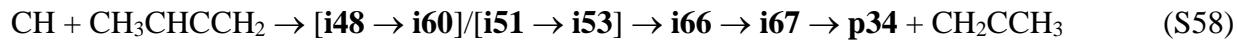
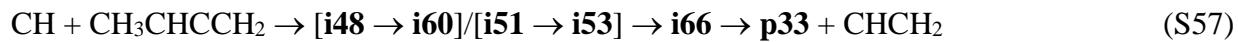
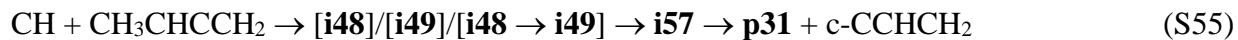
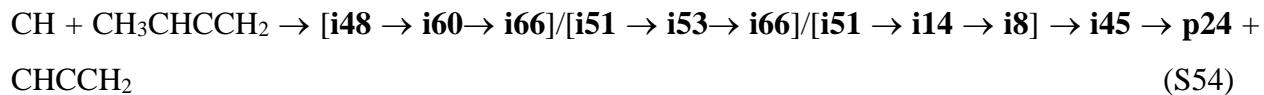
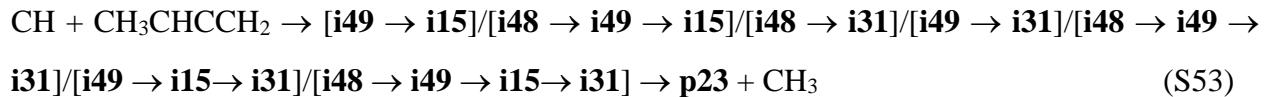
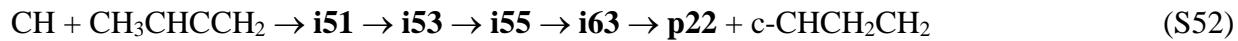




The methylidyne radical (CH) addition to the terminal and central carbon-carbon double bonds of 1,2-butadiene resulting in products p22-p24, p31-p35 via intermediates i8, i14, i15, i31, i45, i48, i49, i51, i53, i55, i57, i60, i63, i65-i67, i71 (Figure S5).

The product ethylene (**p31**) can be formed via c-CCHCH₂ group loss in **i57** via a tight exit transition state lying 18 kJ mol⁻¹ above the separated products. The methylenecyclopropene (**p32**) product can be accessed via CH₃ radical emission from **i51** via a tight exit transition state lying 20 kJ mol⁻¹ above the separated products. The ring opening in **i48** and **i49** can both lead to the linear intermediate **i31**. The intermediate **i15** can be formed via ring opening in **i49** accompanied with an H shift between terminal CH₃ and CH₂ via a barrier of 293 kJ mol⁻¹ above **i49**. The conformers **i15** and **i31** are connected via a low barrier of 34 kJ mol⁻¹ above **i15**; the decomposition of both intermediates leads to the product 1-buten-3-yne (**p23**) via CH₃ group loss. The product acetylene (**p34**) can be accessed via CH₂CCH₃ group emission in **i67** via a tight exit transition state lying 24 kJ mol⁻¹ above the separated products. An H migration from the terminal CH₃ group to the adjacent CH moiety in **i14** leads to intermediate **i8** and the ring opening in **i55** leads to the linear intermediate **i45**. The conformers **i8** and **i45** are connected via a low barrier of 10 kJ mol⁻¹ above **i8**. The product ethylene (**p24**) can be reached via a CHCCH₂ group loss in **i45** via a tight exit transition state lying 59 kJ mol⁻¹ above the separated products. The product acetylene (**p22**) may be formed via c-CHCH₂CH₂ (cyclopropyl) group emission in **i63** via a tight exit transition state lying 26 kJ mol⁻¹ above the separated products. The product allene (**p33**) can be accessed via a CHCH₂ (vinyl) group loss in **i66** via a tight exit transition state lying 27 kJ mol⁻¹ above the separated products. The product 1,2,3-butatriene (**p35**) can be reached via CH₃ group emission in **i71** via a tight exit transition state lying 45 kJ mol⁻¹ above the separated products. In brief, the

products **p22-p24**, **p31-p35** can be accessed via pathways (S52), (S53), (S54), (S55), (S56), (S57), (S58), (S59), respectively.



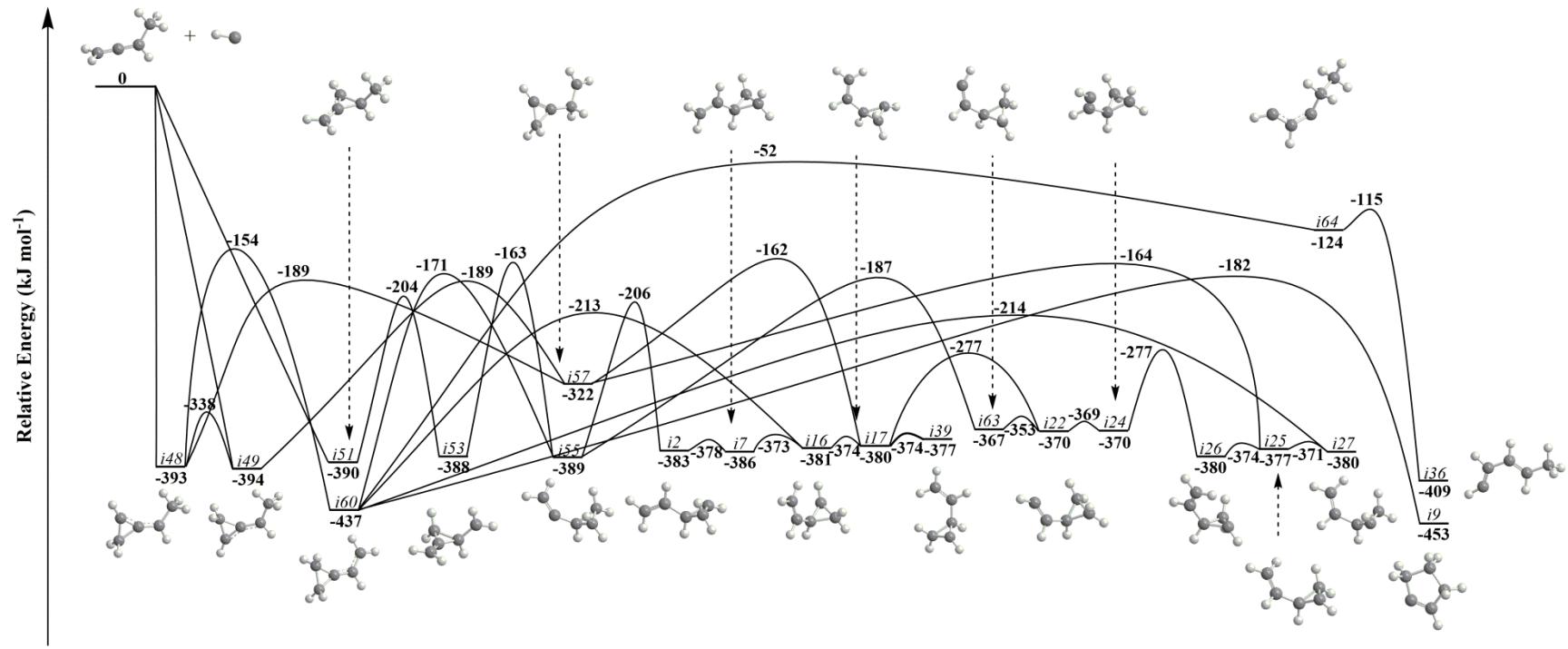


Figure S1. Portion of the C_5H_7 PES involving intermediates **i2**, **i7**, **i9**, **i16**, **i17**, **i22**, **i24-i27**, **i36**, **i39**, **i48**, **i49**, **i51**, **i53**, **i55**, **i57**, **i60**, **i63**, **i64**.

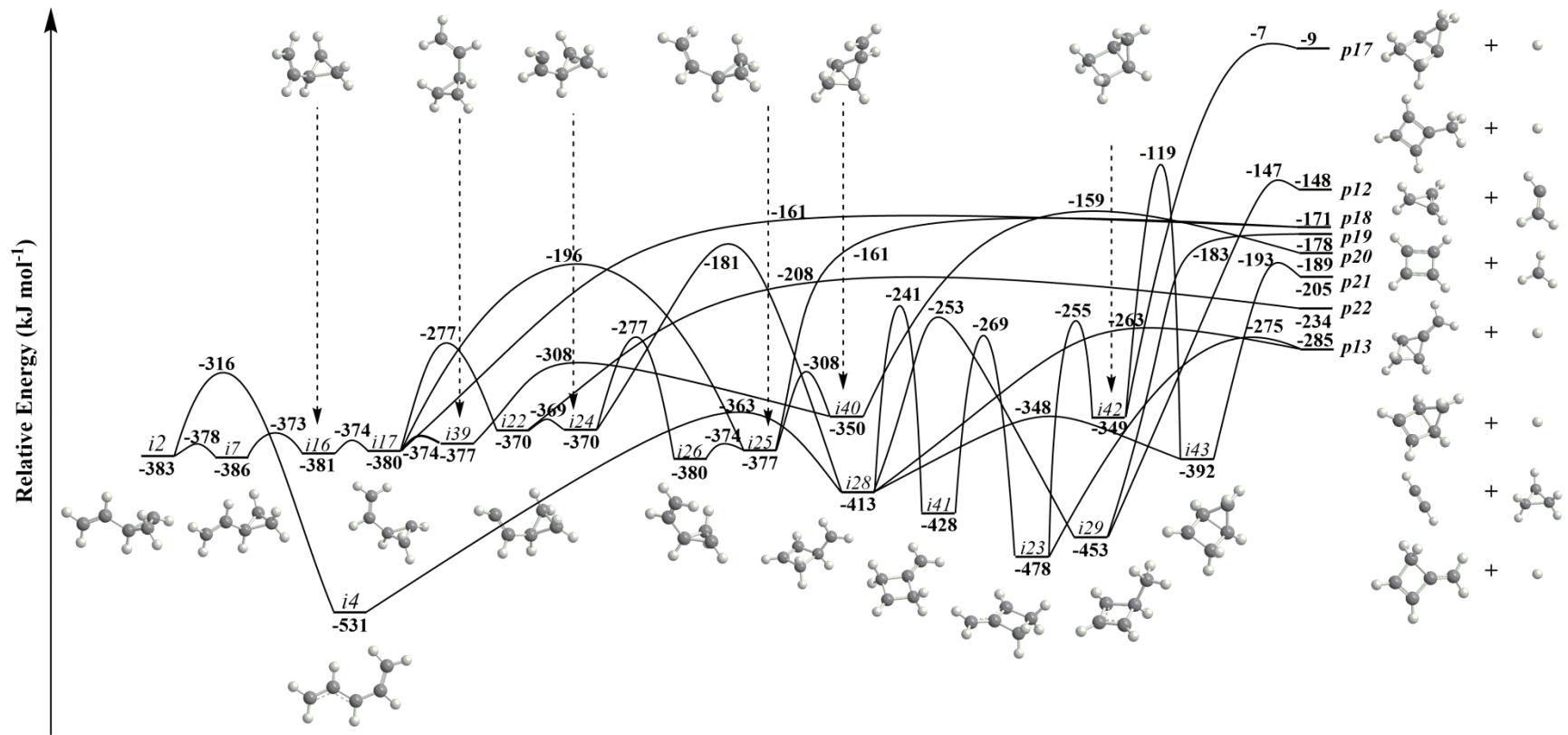


Figure S2. Portion of the C_5H_7 PES leading to \mathbf{p}_{12} , \mathbf{p}_{13} , \mathbf{p}_{17} - \mathbf{p}_{22} via intermediates \mathbf{i}_2 , \mathbf{i}_4 , \mathbf{i}_7 , \mathbf{i}_{16} , \mathbf{i}_{17} , \mathbf{i}_{22} - \mathbf{i}_{26} , \mathbf{i}_{28} , \mathbf{i}_{29} , \mathbf{i}_{39} - \mathbf{i}_{43} .

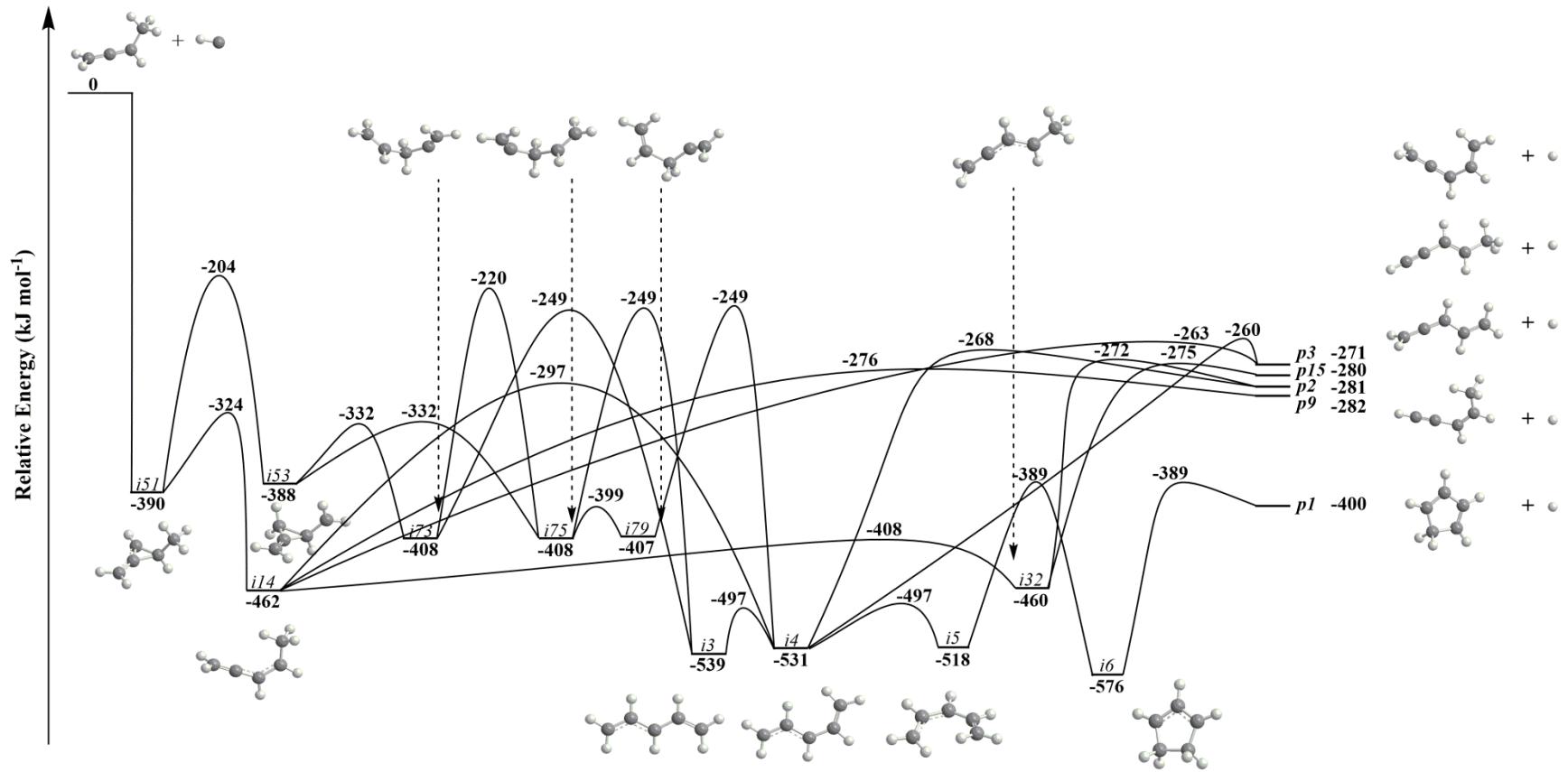


Figure S3. Portion of C_5H_7 PES leading to **p1-p3, p9, p15** via intermediates **i3-i6, i14, i32, i51, i53, i73, i75, i79**.

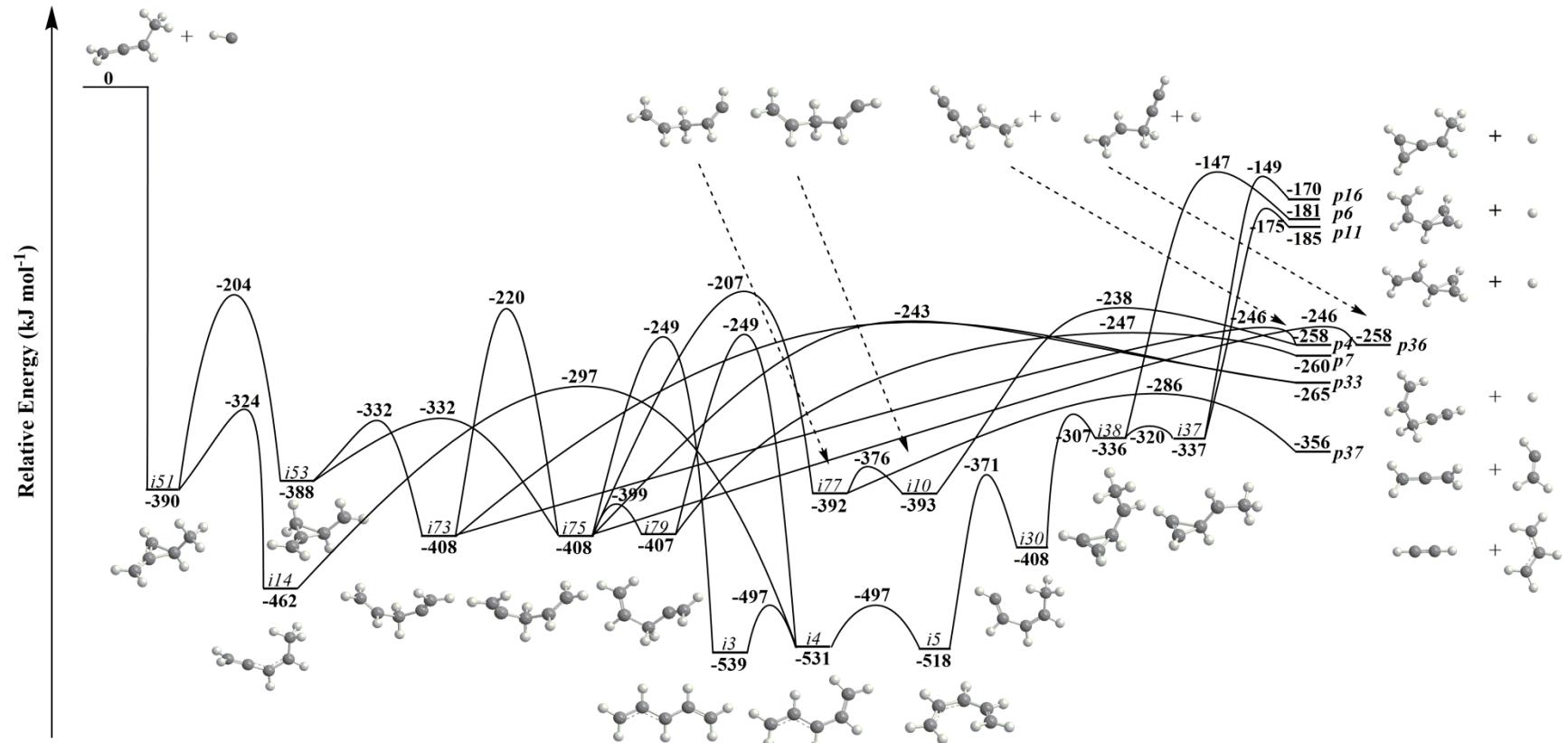


Figure S4. Portion of C_5H_7 PES leading to $\mathbf{p}4, \mathbf{p}6, \mathbf{p}7, \mathbf{p}11, \mathbf{p}16, \mathbf{p}33, \mathbf{p}36, \mathbf{p}37$ via intermediates $\mathbf{i}3-\mathbf{i}5, \mathbf{i}10, \mathbf{i}14, \mathbf{i}30, \mathbf{i}37, \mathbf{i}38, \mathbf{i}51, \mathbf{i}53, \mathbf{i}73, \mathbf{i}75, \mathbf{i}77, \mathbf{i}79$.

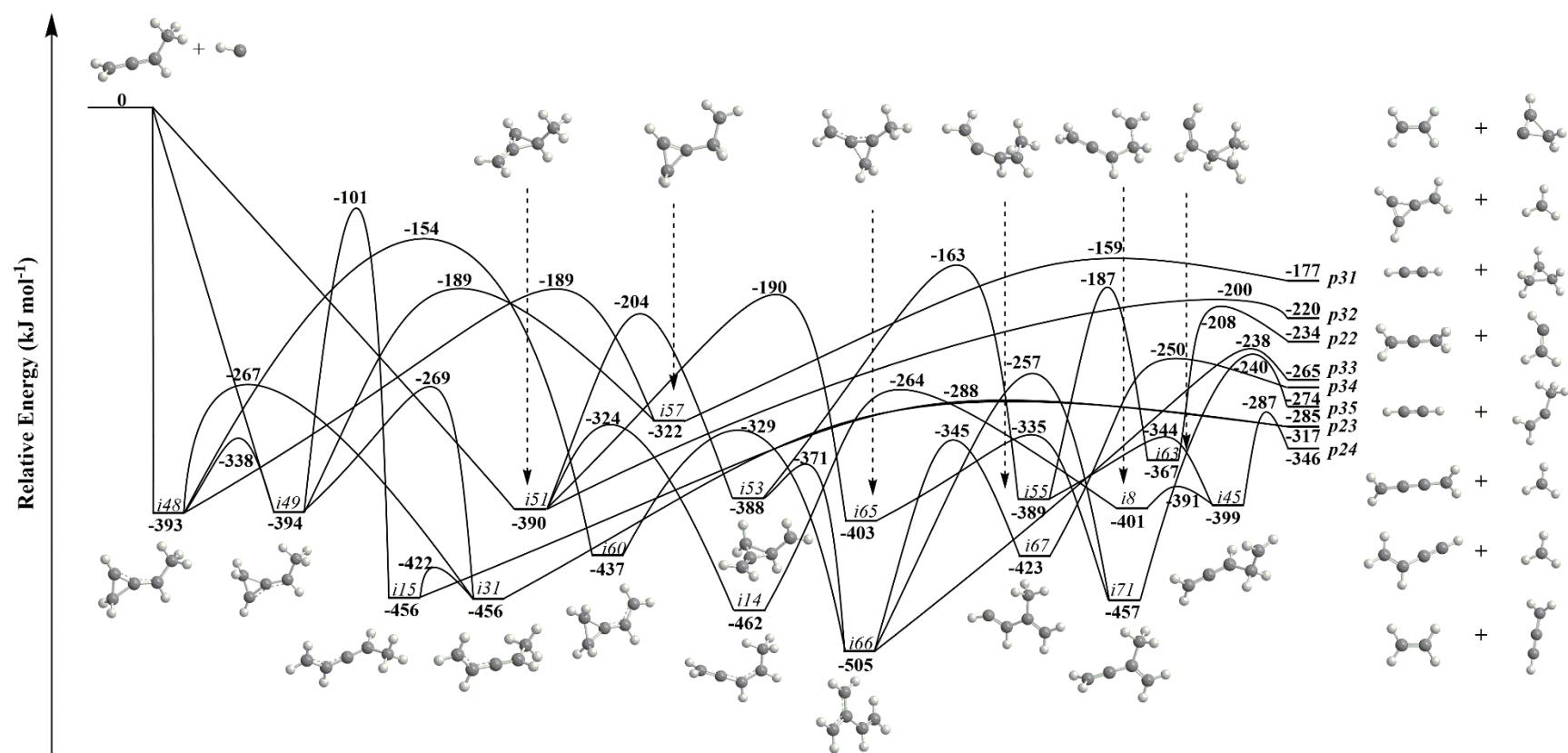


Figure S5. Portion of C₅H₇ potential energy surface (PES) leading to p22-p24, p31-p35 via intermediates **i8, i14, i15, i31, i45, i48, i49, i51, i53, i55, i57, i60, i63, i65-i67, i71**.

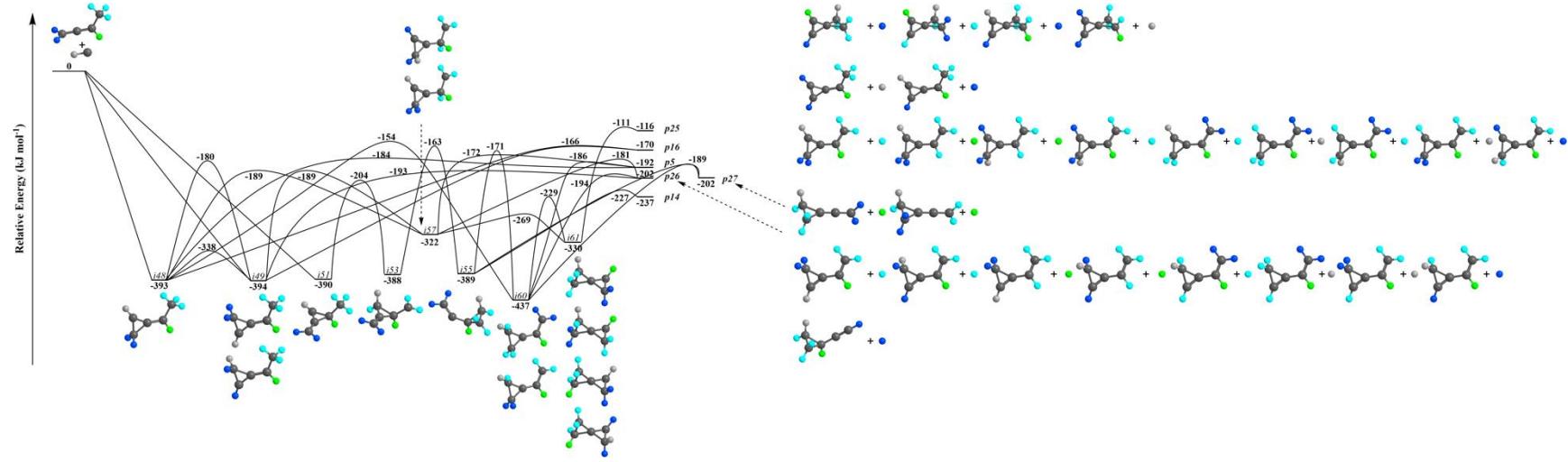


Figure S6. Portion of C₅H₆ potential energy surface (PES) leading to **p5**, **p14**, **p16**, **p25-p27** via intermediates **i48**, **i49**, **i51**, **i53**, **i55**, **i57**, **i60**, **i61**. H atoms from methylidyne radical, CH moiety, CH₂ moiety, and CH₃ moiety of 1,2-butadiene reactant are highlighted in grey, green, blue, and cyan, respectively.

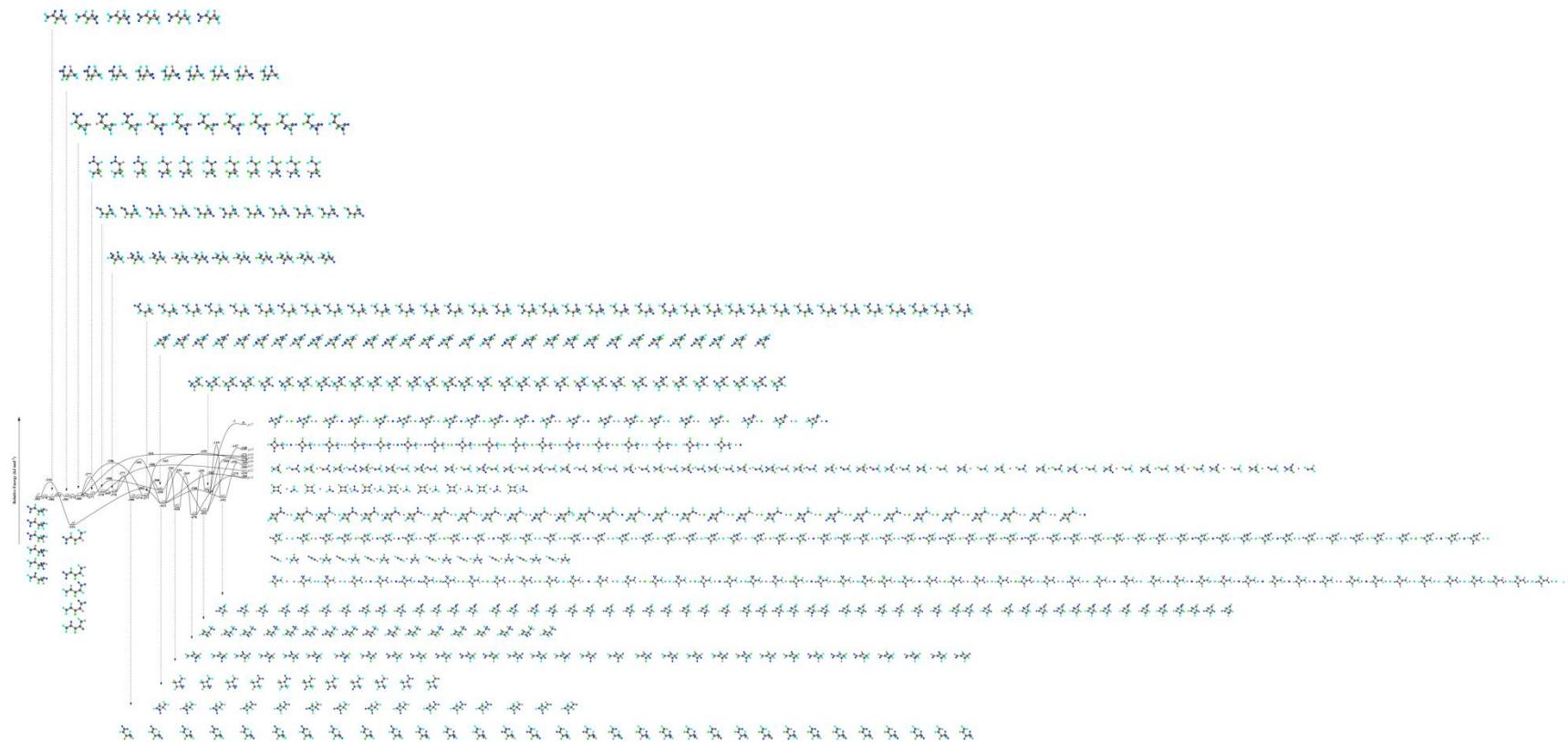


Figure S7. Portion of C₅H₆ PES leading to **p12, p13, p17-p22** via intermediates **i2, i4, i7, i16, i17, i22-i26, i28, i29, i39-i43**. H atoms from methylidyne radical, CH moiety, CH₂ moiety, and CH₃ moiety of 1,2-butadiene reactant are highlighted in grey, green, blue, and cyan, respectively.

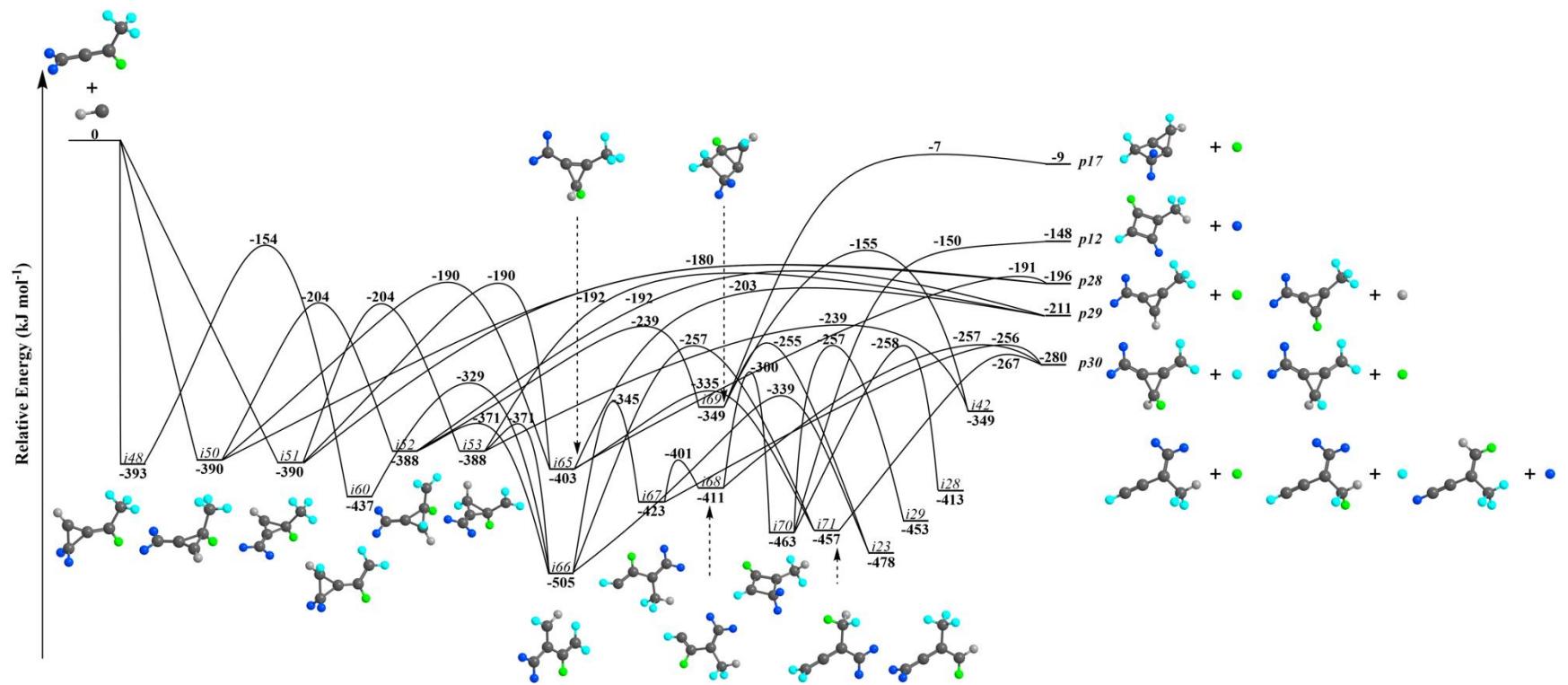


Figure S8. Portion of C_5H_6 PES leading to **p12**, **p17**, **p28-p30** via intermediates **i23**, **i28**, **i29**, **i42**, **i48**, **i50-i53**, **i60**, **i65-i71**. H atoms from methylidyne radical, CH moiety, CH_2 moiety, and CH_3 moiety of 1,2-butadiene reactant are highlighted in grey, green, blue, and cyan, respectively.

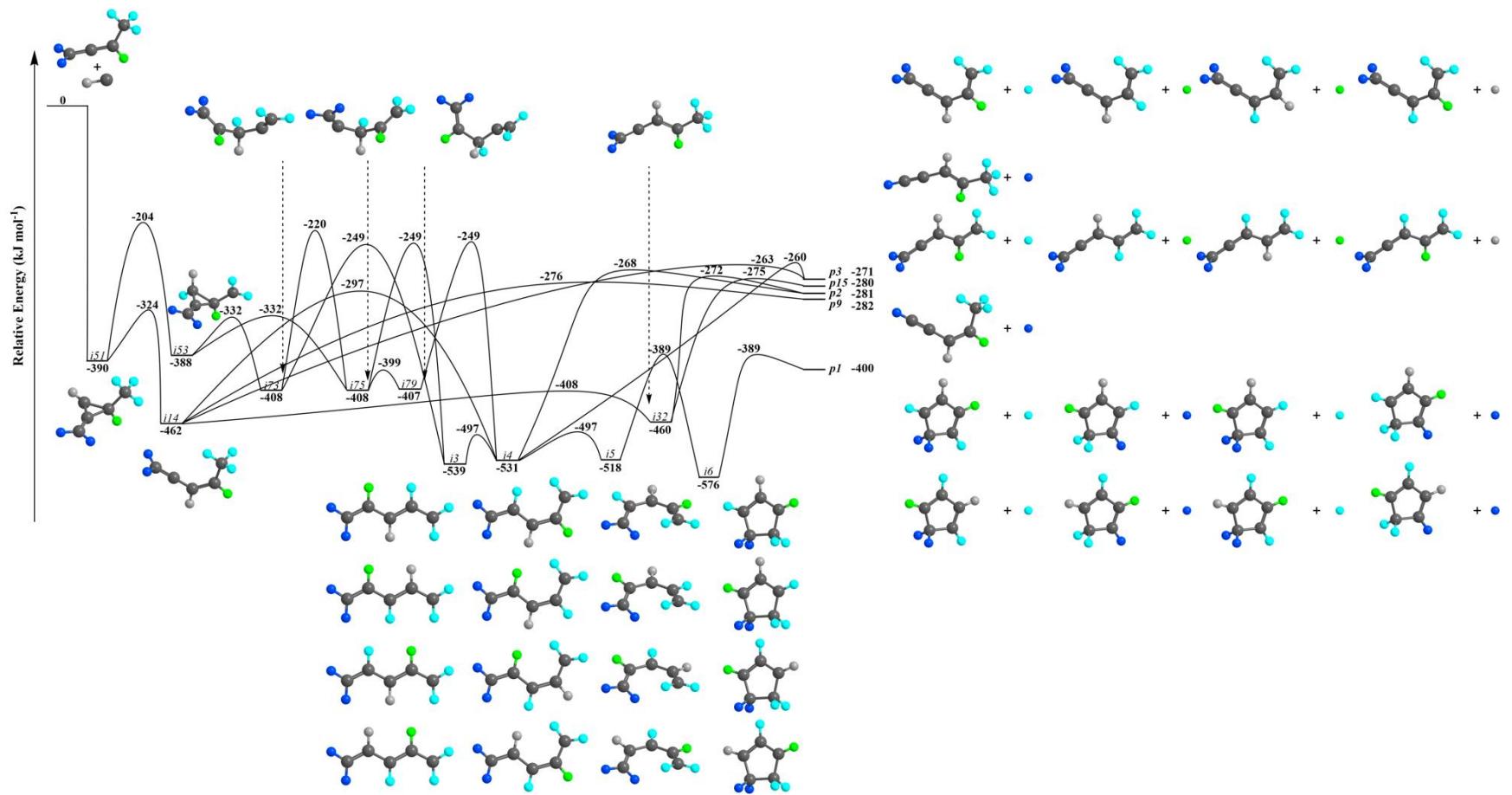


Figure S9. Portion of C₅H₆ PES leading to **p1-p3, p9, p15** via intermediates **i3-i6, i14, i32, i51, i53, i73, i75, i79**. H atoms from methylidyne radical, CH moiety, CH₂ moiety, and CH₃ moiety of 1,2-butadiene reactant are highlighted in grey, green, blue, and cyan, respectively.

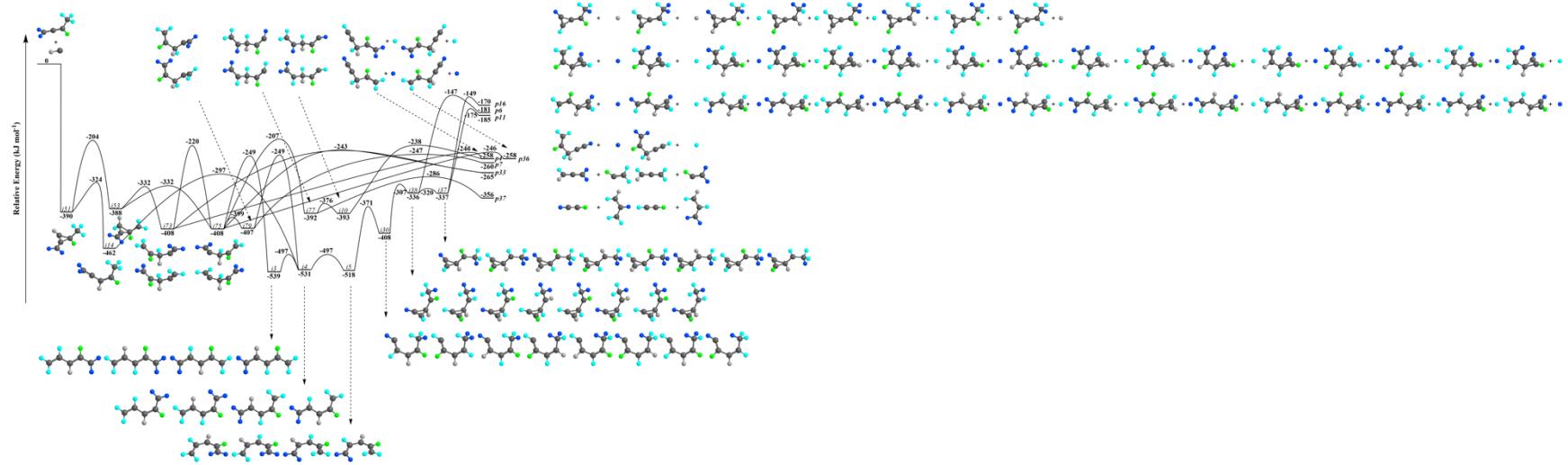


Figure S10. Portion of C_5H_6 PES leading to **p4, p6, p7, p11, p16, p33, p36, p37** via intermediates **i3-i5, i10, i14, i30, i37, i38, i51, i53, i73, i75, i77, i79**. H atoms from methylidyne radical, CH moiety, CH_2 moiety, and CH_3 moiety of 1,2-butadiene reactant are highlighted in grey, green, blue, and cyan, respectively.

Table S1. Rate constant (k , in s^{-1}) for all unimolecular reactions in the $\text{CH} + 1,2\text{-butadiene}$ system calculated using RRKM theory at $E_C = 20.6 \text{ kJ mol}^{-1}$.

Reaction	k								
i3-i4	6.42E+12	i16-i17	6.44E+12	i5-i16	1.40E+06	i63-i55	1.93E+09	i55-i53	2.14E+08
i4-i3	3.97E+12	i17-i16	1.21E+13	i16-i5	3.37E+08	i22-i63	1.02E+13	i50-p32	1.88E+10
i4-i5	2.77E+12	i4-i15	1.02E+08	i17-i39	2.62E+12	i63-i22	1.21E+13	i66-i67	8.05E+08
i5-i4	5.64E+12	i15-i4	1.36E+09	i39-i17	2.70E+12	i58-i59	1.56E+12	i67-i66	6.56E+11
i5-i6	3.86E+10	i15-p10	1.07E+09	i39-i40	1.32E+11	i59-i58	2.25E+12	i51-p32	1.88E+10
i6-i5	5.67E+10	i23-p13	1.58E+10	i40-i39	5.65E+11	i46-i66	5.86E+11	i42-i53	1.01E+11
i6-p1	2.10E+11	i1-i23	2.49E+10	i25-i40	1.32E+11	i66-i46	2.06E+04	i53-i42	2.75E+08
i1-i4	1.42E+13	i23-i1	1.64E+05	i40-i25	5.66E+11	i14-i50	2.21E+10	i75-p33	1.27E+11
i4-i1	1.95E+06	i4-i14	5.83E+09	i28-i41	8.78E+08	i50-i14	2.77E+12	i65-p29	2.08E+09
i4-p2	1.74E+09	i14-i4	3.45E+10	i41-i28	8.31E+08	i52-i54	7.88E+07	i67-p30	5.60E+10
i6-i13	1.97E+10	i3-i7	7.38E+08	i23-i41	2.14E+09	i54-i52	2.14E+08	i67-p34	2.94E+11
i13-i6	1.02E+11	i7-i3	6.90E+11	i41-i23	9.02E+09	i42-i69	2.80E+08	i71-p30	3.27E+09
i3-i10	2.45E+04	i24-p14	2.65E+10	i23-i42	1.52E+08	i69-i42	2.79E+08	i53-i74	6.95E+11
i10-i3	3.06E+06	i22-p14	2.65E+10	i42-i23	2.55E+11	i4-i78	5.18E+07	i74-i53	1.43E+11
i4-p3	1.98E+09	i10-p4	2.51E+10	i17-p18	3.49E+09	i78-i4	5.02E+09	i51-i65	2.16E+08
i10-i11	2.32E+12	i14-i15	9.18E+07	i25-p18	3.30E+09	i47-i50	6.86E+12	i65-i51	6.33E+07
i11-i10	2.59E+12	i15-i14	2.05E+08	i40-p20	8.63E+07	i50-i47	3.21E+09	i51-p28	3.38E+08
i11-i12	2.09E+12	i14-p10	5.16E+08	i42-p17	3.80E+02	i3-i72	4.91E+07	i14-i51	2.21E+10
i12-i11	2.44E+12	i8-i14	3.47E+09	i29-p19	4.58E+10	i72-i3	5.46E+09	i51-i14	2.76E+12
i12-i13	9.65E+10	i14-i8	1.27E+09	i28-i43	9.95E+10	i10-i77	9.69E+12	i53-p29	3.16E+08
i13-i12	1.15E+10	i14-p9	7.06E+10	i43-i28	1.26E+12	i77-i10	1.07E+13	i53-i66	4.48E+12
i13-p1	9.34E+11	i25-i27	1.20E+13	i42-i43	2.20E+07	i72-i78	2.12E+12	i66-i53	3.89E+09
i19-i21	9.87E+12	i27-i25	7.06E+12	i43-i42	3.68E+05	i78-i72	2.28E+12	i3-i74	4.91E+07
i21-i19	9.88E+12	i27-p6	6.40E+08	i43-p21	1.20E+09	i72-i77	3.29E+09	i74-i3	2.73E+09
i17-i22	1.63E+10	i12-p7	3.62E+10	i22-p22	8.21E+10	i77-i72	4.06E+09	i4-i79	5.22E+07
i22-i17	2.74E+10	i11-p4	3.94E+10	i14-p3	1.47E+10	i54-i55	3.54E+12	i79-i4	5.06E+09

i1-i8	1.89E+10	i21-p7	2.77E+10	i15-p23	4.67E+11	i55-i54	3.55E+12	i74-i79	2.11E+12
i8-i1	4.21E+04	i29-p12	1.20E+07	i31-p23	4.68E+11	i31-i48	1.97E+09	i79-i74	2.28E+12
i8-p3	1.11E+10	i20-p7	2.76E+10	i45-p24	7.22E+10	i48-i31	6.19E+10	i66-i71	3.05E+07
i6-i24	8.49E+05	i28-i29	9.98E+08	i31-i44	1.16E+08	i31-i49	1.84E+09	i71-i66	1.97E+08
i24-i6	4.36E+08	i29-i28	1.23E+09	i44-i31	1.29E+09	i49-i31	6.23E+10	i67-i68	3.91E+12
i10-i21	2.14E+12	i18-i20	1.00E+13	i30-i44	3.48E+12	i27-i60	1.36E+09	i68-i67	3.46E+12
i21-i10	3.07E+12	i20-i18	9.95E+12	i44-i30	3.93E+12	i60-i27	3.03E+08	i23-i66	5.75E+10
i12-i21	2.28E+12	i29-i30	4.72E+09	i30-i36	3.15E+09	i59-p26	3.47E+09	i66-i23	2.28E+08
i21-i12	2.52E+12	i30-i29	2.37E+09	i36-i30	1.34E+09	i48-p16	4.67E+08	i68-i70	2.22E+10
i15-p8	5.77E+10	i5-i30	2.07E+10	i34-i36	4.52E+12	i49-p16	5.86E+08	i70-i68	1.17E+10
i6-i9	2.76E+07	i30-i5	1.34E+12	i36-i34	2.00E+12	i48-p5	2.08E+09	i29-i70	2.48E+09
i9-i6	4.93E+09	i14-i30	9.58E+07	i8-i45	1.23E+12	i49-p26	2.19E+09	i70-i29	6.87E+08
i25-i26	2.69E+12	i30-i14	1.06E+09	i45-i8	1.20E+12	i16-i60	1.09E+09	i28-i70	4.28E+09
i26-i25	2.62E+12	i30-p9	2.27E+11	i30-i38	2.60E+11	i60-i16	2.75E+08	i70-i28	1.46E+09
i16-i18	7.80E+06	i31-i32	2.55E+08	i38-i30	1.57E+12	i60-p26	6.42E+08	i9-i60	1.89E+08
i18-i16	2.30E+06	i32-i31	1.51E+08	i14-i32	2.64E+12	i60-p5	6.50E+08	i60-i9	2.19E+07
i24-i28	1.25E+08	i32-p2	1.91E+10	i32-i14	3.51E+12	i61-i62	1.13E+13	i58-i62	5.15E+10
i28-i24	1.73E+07	i32-p15	1.03E+11	i48-i49 (H migration)	1.04E+08	i62-i61	1.13E+13	i62-i58	1.89E+12
i8-i9	5.66E+09	i32-i33	1.21E+09		i49-i48 (H migration)	1.13E+08	i60-i61	3.31E+08	i46-i50
i9-i8	3.73E+11	i33-i32	1.06E+10	i49-i59	3.57E+08	i61-i60	1.04E+11	i50-i46	2.95E+08
i18-i19	3.41E+12	i31-i33	9.40E+07	i59-i49	2.43E+09	i62-p25	1.77E+08	i2-i56	5.01E+08
i19-i18	3.41E+12	i33-i31	9.81E+08	i25-i59	8.43E+07	i46-i48	7.97E+13	i56-i2	2.80E+08
i17-i25	1.27E+09	i33-i34	1.05E+13	i59-i25	2.76E+08	i48-i46	6.15E+09	i60-i66	1.37E+11
i25-i17	1.31E+09	i34-i33	9.59E+12	i48-i49 (rotation)	1.57E+12	i69-p17	3.79E+02	i66-i60	4.21E+08
i24-i26	2.74E+10	i34-p15	6.07E+10		i49-i48 (rotation)	1.69E+12	i23-i69	2.23E+08	i57-i58
i26-i24	1.63E+10	i33-i35	4.48E+12	i50-i52	4.73E+08	i69-i23	3.74E+11	i58-i57	1.63E+12

i15-i16	6.89E+05	i35-i33	5.24E+12	i52-i50	1.39E+08	i52-i69	2.75E+08	i59-i62	7.45E+10
i16-i15	2.55E+07	i35-i36	1.96E+14	i57-p5	2.15E+09	i69-i52	1.01E+11	i62-i59	1.89E+12
i28-p13	7.77E+09	i36-i35	6.76E+13	i52-p29	3.17E+08	i71-p35	3.03E+09	i47-i49	2.86E+12
i17-p5	1.27E+09	i36-p15	5.48E+10	i48-i57	3.45E+08	i66-p33	3.47E+08	i49-i47	8.14E+08
i15-i31	5.77E+11	i11-i36	9.25E+03	i57-i48	1.97E+09	i47-i51	6.86E+12	i46-i51	2.14E+12
i31-i15	5.78E+11	i36-i11	2.30E+03	i15-i49	5.39E+03	i51-i47	3.21E+09	i51-i46	2.95E+08
i1-i7	6.03E+09	i36-i37	7.87E+10	i49-i15	1.83E+05	i70-p12	4.08E+07	i72-i73	2.79E+12
i7-i1	6.26E+05	i37-i36	7.30E+11	i17-i57	7.36E+07	i60-i64	2.62E+01	i73-i72	2.76E+12
i3-i15	1.05E+08	i37-p11	6.89E+08	i57-i17	1.91E+08	i64-i60	8.47E+08	i72-p4	2.43E+11
i15-i3	1.72E+09	i37-p16	1.50E+07	i48-i60	5.42E+06	i68-p30	4.42E+10	i74-i76	3.07E+12
i16-p6	5.30E+09	i37-i38	7.69E+11	i60-i48	1.61E+06	i50-i65	2.16E+08	i76-i74	2.86E+12
i22-i24	2.85E+12	i38-i37	1.18E+12	i36-i64	3.77E+04	i65-i50	6.33E+07	i76-p36	2.15E+11
i24-i22	2.85E+12	i38-p6	1.09E+08	i64-i36	2.71E+12	i52-i66	4.49E+12	i78-p7	1.64E+11
i7-i16	4.10E+12	i17-i38	4.31E+07	i60-p27	1.87E+08	i66-i52	3.89E+09	i79-p7	1.63E+11
i16-i7	2.66E+12	i38-i17	3.72E+07	i51-i53	4.72E+08	i55-i56	6.32E+12	i78-i79	2.83E+12
i2-i4	5.34E+11	i5-i17	2.74E+09	i53-i51	1.39E+08	i56-i55	4.55E+12	i79-i78	2.83E+12
i4-i2	7.01E+08	i17-i5	6.18E+11	i52-i72	6.96E+11	i56-p27	5.64E+08	i72-i74	1.41E+09
i26-p5	1.27E+09	i4-i28	4.93E+09	i72-i52	1.43E+11	i73-p33	1.30E+11	i74-i72	1.41E+09
i4-i11	7.39E+02	i28-i4	1.05E+12	i50-p28	3.50E+08	i65-i71	1.86E+12	i77-p37	1.62E+12
i11-i4	1.66E+05	i5-i25	2.93E+08	i55-i60	7.24E+07	i71-i65	1.05E+10	i57-p31	4.89E+09
i7-p11	3.69E+09	i25-i5	6.77E+10	i60-i55	7.54E+06	i74-i75	2.79E+12	i63-p22	9.73E+10
i2-i7	1.09E+13	i6-i25	2.32E+05	i55-p14	1.51E+11	i75-i74	2.71E+12	i45-i55	3.96E+10
i7-i2	1.08E+13	i25-i6	7.30E+07	i55-i63	1.26E+09	i53-i55	7.86E+07	i55-i45	2.98E+12
								i65-p28	2.23E+09

Optimized Cartesian coordinates and vibrational frequencies for all intermediates, transition states, reactants and products involved in the reactions of the methylidyne radical (CH) with 1,2-butadiene (C₄H₆).

REACTANTS

1,2-butadiene

C	0.553461	-0.559289	-0.000187
C	1.746400	0.364901	0.000062
C	-0.692711	-0.173928	0.000056
C	-1.937478	0.214056	0.000037
H	0.759435	-1.628862	0.000342
H	1.436517	1.410742	0.001404
H	2.371900	0.191112	-0.881717
H	2.373385	0.189233	0.880353
H	-2.479542	0.381768	-0.926279
H	-2.479733	0.381565	0.926088

Frequencies

168.4124	211.1632	339.7195
540.4038	572.4626	871.5966
879.2352	896.9325	1021.5979
1059.8893	1091.5140	1149.8380
1361.1250	1408.1836	1471.6498
1485.6411	1504.9465	2056.4778
3018.6767	3065.3246	3104.2583
3110.9812	3120.1311	3180.8861

Methylidyne

C 0.000000 0.000000 0.161146

H 0.000000 0.000000 -0.966877

Frequencies

2803.9026

INTERMEDIATE STATES

i39

C	1.179982	0.847460	0.116671
C	0.390457	-0.424033	0.444080
C	1.457357	-0.415539	-0.577767
H	0.654941	1.629035	-0.426529
H	1.892238	1.226777	0.846128
H	0.644253	-0.924056	1.380880
H	2.352841	-1.006648	-0.708226
C	-1.912893	0.407907	-0.145800
C	-1.046732	-0.577699	0.065623
H	-2.940053	0.204081	-0.426133
H	-1.631343	1.451057	-0.047789
H	-1.381907	-1.608817	-0.035171

Frequencies

95.8975	254.2380	299.2731
502.3137	608.5389	665.7189
752.5285	805.7032	896.7407
944.8324	982.2581	1019.4877
1039.3721	1057.6693	1068.3688
1096.5004	1119.1442	1231.4497
1323.3492	1375.5961	1446.0478
1464.3263	1702.3899	3061.9562
3080.6317	3118.5139	3135.4091
3150.4253	3205.0133	3214.0608

i40

C	1.206801	0.782909	-0.000257
C	0.633940	-0.387696	0.740746
C	0.634108	-0.388090	-0.740441
H	0.697177	1.744095	-0.000619
H	2.290581	0.864155	-0.000107
H	1.105614	-1.067068	1.434753
H	1.105604	-1.067994	-1.434062
C	-1.756627	0.449899	-0.000091
C	-0.687021	-0.547892	0.000000
H	-2.792317	0.136860	-0.000635
H	-1.546740	1.510904	0.000825
H	-1.047123	-1.575729	0.000106

Frequencies

125.0284	294.6140	319.6901
513.8423	529.8144	691.2239
712.5230	798.8728	838.3312
927.8164	952.9482	986.1515
1013.0707	1098.7550	1117.0617
1141.8644	1149.2032	1174.4729
1252.2916	1284.1596	1419.6512
1480.5546	1525.8283	3080.2548
3106.3641	3151.6577	3158.3175
3202.6863	3217.3536	3252.3575

i41

C -1.891194 -0.000072 -0.000127
C -0.567355 -0.000129 -0.000220
C 1.523876 0.000134 0.000933
C 0.497241 -1.103617 0.000052
C 0.496972 1.103683 0.000047
H -2.457636 0.925583 -0.000007
H -2.457880 -0.925580 -0.000111
H 0.489010 -1.757371 -0.884250
H 2.605165 0.000156 -0.003494
H 0.487957 -1.757755 0.884050
H 0.488653 1.757234 -0.884347
H 0.487496 1.757743 0.884047

Frequencies

105.5857	224.3357	355.8296
403.1250	638.4828	686.0456
832.4948	849.9176	890.1766
909.9089	946.2017	977.5514
1007.8631	1029.8322	1113.5764
1173.7088	1218.9164	1261.1558
1294.1048	1435.6085	1436.6540
1456.3345	1749.1496	2965.8889
2971.7263	2984.9484	2988.8714
3124.5170	3203.2702	3209.6390

i42

C	0.938085	0.772432	0.270657
C	-0.463640	0.778602	-0.349472
C	-1.372844	-0.227799	0.376640
C	-0.347744	-0.708654	-0.567421
C	1.061431	-0.774239	-0.004062
H	0.975039	1.054471	1.328302
H	1.666422	1.362177	-0.286855
H	-0.888288	1.566471	-0.959564
H	-1.284902	-0.386731	1.451414
H	-2.393086	-0.218658	0.006434
H	1.209013	-1.432688	0.856533
H	1.824078	-0.987100	-0.754315

Frequencies

265.5293	394.2286	617.4503
746.7308	771.3981	827.0902
886.8964	913.9602	944.2813
983.7896	1000.0348	1038.6418
1078.2583	1095.8115	1158.1438
1186.2962	1208.2433	1222.7951
1266.6367	1328.7857	1468.9899
1477.2398	1497.1656	3023.2544
3044.5275	3067.5347	3092.1079
3109.7072	3163.5035	3171.7391

i43

C	1.290412	-0.108182	0.501903
C	0.320261	-0.751577	-0.431927
C	-0.954499	0.846728	0.129336
C	0.426389	0.793981	-0.385206
C	-1.120342	-0.658139	0.119500
H	2.333795	-0.164161	0.207813
H	1.119697	-0.126424	1.574582
H	0.637775	-1.407471	-1.232447
H	-1.581506	1.659272	0.470877
H	0.897078	1.472401	-1.087716
H	-1.871812	-0.996613	-0.604538
H	-1.308352	-1.173870	1.069791

Frequencies

167.2692	322.5142	438.6453
704.2166	735.0590	789.1933
870.7669	912.1992	921.7510
974.4590	1004.2859	1009.1686
1034.7085	1054.6873	1068.8962
1109.5563	1198.5749	1234.1814
1237.4384	1317.0065	1333.6911
1470.9446	1488.8213	2993.2920
3022.7887	3094.4515	3155.2321
3174.9501	3186.7427	3201.6356

i44

C	-1.173532	0.626815	0.000029
C	-1.971961	-0.642509	-0.000006
C	0.161081	0.763386	-0.000017
H	-1.762721	1.540990	0.000064
H	-2.626408	-0.686194	-0.877958
H	-2.626193	-0.686452	0.878086
H	-1.353271	-1.540651	-0.000232
H	0.575289	1.767086	-0.000024
C	1.146500	-0.315311	0.000007
C	2.452851	-0.146502	-0.000034
H	0.767801	-1.342471	0.000033
H	3.335868	-0.767589	0.000160

Frequencies

115.8311	152.4098	222.9926
370.9634	391.4381	616.8109
637.6045	759.3961	787.7689
853.0161	930.6780	1009.7752
1030.6658	1058.7971	1153.9575
1251.4704	1286.0874	1407.3328
1431.0034	1481.6485	1489.3905
1630.9216	1697.4386	3015.0189
3038.0905	3053.1504	3108.9637
3132.2588	3159.9022	3240.9310

i45

C	1.177988	-0.337856	0.497418
C	-0.024825	-0.521285	-0.426250
C	-2.433029	0.319616	0.117577
C	-1.230876	-0.102243	-0.160940
C	2.211357	0.556164	-0.106480
H	0.818503	0.074376	1.446477
H	1.608128	-1.321645	0.713300
H	0.165629	-1.014936	-1.377034
H	-2.761302	1.318103	-0.156572
H	-3.152041	-0.313210	0.629701
H	2.005886	1.613107	-0.225986
H	3.111511	0.157829	-0.557838

Frequencies

50.2068	83.3549	200.1012
306.3574	342.7629	518.2573
556.4755	602.4890	772.3406
872.8351	893.9749	937.5026
1020.1180	1048.2980	1091.2853
1136.9295	1251.6670	1301.6761
1357.7071	1459.1989	1474.3797
1477.8971	2046.4780	3014.3861
3054.8307	3111.0965	3124.9587
3136.7117	3181.6867	3241.9355

i46

C	0.686089	-0.639700	0.035852
C	2.010246	0.040676	-0.012526
C	-0.562089	0.027980	0.035281
C	-1.782243	-0.687486	-0.008395
C	-0.638566	1.436168	-0.091057
H	0.674701	-1.722385	0.132266
H	2.681774	-0.460290	-0.718917
H	2.513721	0.009995	0.963950
H	1.903403	1.087824	-0.301713
H	-2.728982	-0.179507	0.123861
H	-1.806610	-1.737742	-0.281466
H	-1.518623	1.936274	0.327095

Frequencies

119.4985	172.6819	236.9924
264.5968	453.8842	468.0614
546.4032	594.1722	700.1991
751.8040	804.6867	862.5714
977.9895	1013.2208	1053.9071
1128.4585	1240.6114	1366.6076
1402.6683	1434.2472	1476.0679
1478.9518	1499.3888	2987.8491
3034.7950	3069.1646	3101.0085
3126.7467	3144.0879	3231.7565

i47

C	0.643128	-0.591968	-0.232744
C	1.927032	0.065134	0.150311
C	-0.651499	-0.023832	-0.089189
C	-0.908594	1.359106	-0.051668
C	-1.663749	-0.954925	0.239600
H	0.695604	-1.632728	-0.538177
H	1.777723	1.067691	0.553116
H	2.595838	0.139287	-0.717417
H	2.465629	-0.527397	0.900138
H	-0.151739	2.088537	-0.312911
H	-1.903321	1.710805	0.187359
H	-1.557647	-1.967283	-0.169968

Frequencies

66.6071	94.6810	270.8704
375.6570	459.3346	476.6104
547.8187	646.1667	704.5462
748.6819	836.0030	861.9693
977.6924	1004.5152	1061.7908
1113.6603	1270.5890	1353.1348
1401.0573	1428.3401	1472.4103
1485.9185	1496.0722	2997.3659
3032.3701	3047.9224	3109.4939
3147.4646	3156.1702	3250.6316

i48

C	0.902980	-0.611895	0.000036
C	2.132910	0.241494	0.000027
C	-0.367021	-0.111945	-0.000117
C	-1.839931	-0.442237	0.000092
C	-1.230558	0.921330	-0.000235
H	1.034573	-1.689926	0.000058
H	1.883375	1.304170	-0.000752
H	2.758003	0.036955	-0.877977
H	2.757298	0.038021	0.878772
H	-2.301412	-0.825051	-0.912444
H	-2.301419	-0.824899	0.912660
H	-1.420700	1.980240	0.000865

Frequencies

125.4532	189.9981	204.1736
315.5127	475.1913	491.8469
711.1210	739.9821	913.2839
983.4396	986.1096	1023.5133
1040.9411	1050.4838	1092.1311
1129.1974	1159.6868	1392.9224
1412.4646	1477.1107	1480.9633
1504.6890	1603.3423	3000.1326
3025.7890	3035.8815	3085.4485
3100.6802	3151.8831	3267.7185

i49

C	-0.924853	0.639232	0.000096
C	-2.065086	-0.327784	-0.000101
C	0.390794	0.276808	0.000237
C	1.362323	-0.882260	0.000047
C	1.703060	0.571594	-0.000191
H	-1.161315	1.700611	0.000229
H	-1.711367	-1.360461	-0.000259
H	-2.708030	-0.185619	-0.877864
H	-2.708130	-0.185928	0.877641
H	1.497777	-1.466832	-0.912258
H	1.498241	-1.466666	0.912390
H	2.495402	1.299358	-0.000407

Frequencies

134.1725	195.4356	200.0122
329.1288	459.9308	523.7834
685.8353	734.6475	921.2228
938.1827	985.6219	1020.2772
1040.4566	1058.1125	1095.3389
1130.8498	1215.7486	1372.5767
1408.7360	1477.3122	1480.9319
1499.2948	1609.9129	2997.0274
3025.0477	3030.6718	3084.2853
3100.4599	3135.5917	3268.5353

i50

C	0.665339	0.158336	0.492576
C	1.760088	-0.596349	-0.249581
C	-0.776979	0.111693	0.045680
C	-1.903543	-0.644716	-0.061781
C	-0.103755	1.265813	-0.147261
H	0.844902	0.234479	1.569265
H	1.871523	-1.611415	0.144884
H	2.725518	-0.090703	-0.145738
H	1.527865	-0.670215	-1.315087
H	-2.807663	-0.238330	-0.501306
H	-1.927158	-1.669359	0.288239
H	-0.081894	2.276879	-0.518057

Frequencies

182.1636	187.7330	317.3992
379.0315	400.5632	528.9903
581.2013	719.3468	792.0466
816.0606	958.1602	997.5567
1048.8587	1079.0977	1111.4310
1156.7369	1203.5508	1355.3787
1404.9851	1467.9706	1490.7634
1497.5579	1595.2310	3015.4040
3026.1280	3072.4773	3093.2724
3133.1724	3225.3569	3253.5088

i51

C	0.665429	0.158361	-0.492720
C	1.759896	-0.596496	0.249625
C	-0.777073	0.111813	-0.045894
C	-1.903489	-0.644702	0.061842
C	-0.103560	1.265832	0.147332
H	0.844992	0.234981	-1.569335
H	1.526767	-0.671461	1.314852
H	2.725230	-0.090370	0.147146
H	1.872155	-1.611141	-0.145670
H	-2.807542	-0.238223	0.501423
H	-1.927251	-1.669323	-0.288281
H	-0.081575	2.276685	0.518757

Frequencies

181.8802	187.7067	317.4245
379.0715	400.6032	529.0410
581.2982	719.2135	792.1409
816.0583	958.1957	997.4847
1048.8440	1079.1125	1111.3611
1156.7089	1203.3132	1355.2651
1405.0104	1467.9250	1490.7405
1497.5613	1595.0727	3015.4307
3026.4996	3072.4458	3093.3005
3133.1008	3225.2571	3253.3164

i52

C	0.713652	0.058759	0.479343
C	1.715913	-0.705524	-0.247084
C	-0.713553	0.045101	0.074856
C	-1.807744	-0.681070	-0.042202
C	-0.013535	1.293125	-0.189351
H	0.904500	0.201540	1.539993
H	1.558953	-0.969659	-1.285423
H	2.642154	-0.999089	0.227950
H	0.264015	1.536202	-1.210756
H	-2.712253	-0.272584	-0.482206
H	-1.840393	-1.709356	0.302387
H	-0.185373	2.150601	0.454680

Frequencies

171.9146	194.9493	326.2350
344.0312	444.4479	514.2539
649.5269	681.9806	817.4299
857.5561	920.8470	943.0554
990.3189	1028.8663	1074.4155
1107.9358	1132.6461	1170.4250
1346.1227	1435.1621	1465.0997
1468.3953	1821.6869	3095.1028
3119.6337	3121.4094	3146.2135
3179.3880	3201.3954	3251.1779

i53

C -1.716025 -0.705353 -0.247157
C -0.713731 0.058789 0.479328
C 0.013764 1.293131 -0.189471
C 0.713516 0.045016 0.075119
C 1.807701 -0.681159 -0.042196
H -1.558746 -0.970084 -1.285289
H -2.642146 -0.999056 0.228015
H -0.904772 0.201944 1.539890
H -0.263547 1.535947 -1.210993
H 0.185347 2.150623 0.454588
H 2.712080 -0.272451 -0.482249
H 1.840428 -1.709466 0.302301

Frequencies

171.9063	194.9655	326.2674
344.0172	444.4286	514.1629
649.3213	681.9411	817.4317
857.4923	920.7803	943.0019
990.2663	1028.7491	1074.3726
1107.8829	1132.7023	1170.4294
1346.1173	1435.1141	1465.0665
1468.3460	1821.6002	3095.1741
3119.6672	3121.4437	3146.2520
3179.5360	3201.4917	3251.2514

i54

C -1.048076 -0.498135 0.181413
C -2.102325 0.189957 -0.180077
H -2.090042 1.283871 -0.221529
H -3.043057 -0.284707 -0.446584
C 0.338159 -0.334243 0.547203
C 1.146006 0.876056 0.056535
C 1.433088 -0.487010 -0.496410
H 0.595188 -0.690954 1.540295
H 0.632944 1.585551 -0.579757
H 1.846901 1.314522 0.756947
H 2.342589 -0.990465 -0.191440
H 1.114363 -0.697571 -1.509921

Frequencies

115.6645	189.8277	325.8702
476.2905	575.3041	759.9330
796.9484	814.2913	855.0799
889.8412	945.7624	1023.6321
1043.4004	1073.3036	1099.0255
1121.9745	1197.8595	1200.5496
1358.3959	1422.5023	1465.2351
1496.5523	1747.4297	3026.9044
3125.3881	3128.0021	3132.7416
3143.0980	3207.5955	3222.8491

i55

C	1.048216	-0.498363	0.181593
C	2.102216	0.190050	-0.180189
C	-0.338099	-0.334025	0.547269
C	-1.433003	-0.487045	-0.496454
C	-1.145998	0.875979	0.056508
H	-0.595384	-0.691082	1.540184
H	2.089631	1.283976	-0.220937
H	3.042963	-0.284267	-0.447185
H	-1.114289	-0.697761	-1.509932
H	-2.342473	-0.990551	-0.191444
H	-1.847028	1.314401	0.756855
H	-0.633407	1.585712	-0.579907

Frequencies

115.8671	189.9013	325.9104
476.3480	575.3417	759.9773
797.1253	814.3122	855.1882
889.7826	945.6810	1023.7792
1043.5441	1073.2881	1099.1161
1121.9869	1197.9015	1200.6047
1358.4713	1422.4316	1465.2872
1496.6087	1747.1115	3027.0414
3125.3435	3127.8720	3132.6340
3143.3237	3207.4963	3222.7082

i56

C -1.018180 -0.000502 -0.251369
C -2.309377 0.000092 -0.030573
C 0.249140 -0.000252 0.442059
C 1.441549 0.749523 -0.134783
C 1.442064 -0.749140 -0.134690
H -2.717284 0.000992 0.984903
H -3.038019 -0.000178 -0.836547
H 0.174487 -0.000246 1.530872
H 1.290023 1.259324 -1.077887
H 2.083877 1.268326 0.566217
H 2.084792 -1.267468 0.566343
H 1.290944 -1.259076 -1.077767

Frequencies

91.7579	214.5081	274.7060
419.0381	551.3942	757.7890
806.7649	819.1788	858.6833
890.3583	955.2121	973.7409
1055.6238	1073.6595	1101.1819
1154.1221	1198.5159	1210.7488
1335.2854	1423.1223	1464.7165
1499.8603	1743.1676	3031.9095
3060.1942	3127.8567	3132.0855
3146.9144	3209.4063	3223.7220

i57

C	1.011735	-0.648985	0.002235
C	2.105707	0.363684	0.003481
C	-0.355644	-0.079090	-0.011195
C	-1.822532	-0.428458	0.022150
C	-1.162834	0.929593	-0.041460
H	1.117022	-1.334297	-0.851941
H	1.925526	1.370753	0.355850
H	3.119578	0.074345	-0.241958
H	1.090722	-1.314492	0.881765
H	-2.300479	-0.840949	-0.869217
H	-2.278492	-0.767352	0.955285
H	-1.332481	1.991529	-0.081047

Frequencies

81.2747	112.5139	197.6030
282.0916	431.3278	458.9284
693.5495	727.4240	859.4734
920.4461	1001.0294	1005.9430
1030.8801	1064.9432	1090.3531
1104.7221	1153.5542	1201.3417
1354.9364	1441.4259	1455.6597
1523.4014	1854.4448	2911.7594
2984.0071	3016.6625	3075.4857
3145.0264	3251.9554	3270.0440

i58

C -1.062246 0.526359 -0.352093
C -1.999133 -0.433448 0.309258
H -1.226714 0.507368 -1.438572
H -1.282625 1.560964 -0.039164
H -1.728532 -0.922289 1.235947
H -3.006965 -0.557408 -0.065905
C 0.369115 0.243256 -0.081379
C 1.453389 -0.799179 -0.216078
C 1.526763 0.589486 0.376177
H 1.453486 -1.669902 0.442423
H 1.896992 -0.994768 -1.194856
H 2.167032 1.317194 0.844817

Frequencies

59.2028	114.1807	180.1127
305.4530	446.9905	491.6648
655.3038	753.7187	832.2912
925.0221	996.2803	1005.7182
1048.2916	1065.8247	1078.9588
1112.2907	1142.7976	1240.2175
1333.7327	1449.9297	1456.8385
1522.7580	1853.3492	2936.9458
2998.0933	3020.3278	3080.5506
3143.7911	3251.8686	3264.7231

i59

C	1.062113	-0.563673	0.302422
C	1.992717	0.453552	-0.272979
C	-0.369881	-0.260180	0.060109
C	-1.419716	0.820752	0.171594
C	-1.554975	-0.600444	-0.323748
H	1.297538	-1.565568	-0.076867
H	1.666874	1.473763	-0.427485
H	3.039594	0.215755	-0.411134
H	1.211111	-0.625647	1.397297
H	-1.425819	1.645326	-0.544180
H	-1.815458	1.093572	1.152601
H	-2.235381	-1.337241	-0.714618

Frequencies

79.9547	127.9614	185.3943
302.9427	446.5634	494.9456
646.4385	739.2521	867.1518
914.9012	960.4035	1009.1899
1057.1250	1069.2658	1090.7030
1103.5120	1157.4949	1218.6214
1339.6662	1447.8758	1453.9706
1522.5090	1857.0553	2898.3933
3018.3202	3020.1388	3078.3303
3145.5158	3253.5841	3266.6149

i60

C 1.068399 -0.568744 0.000338
C 2.143056 0.301087 -0.000226
C -0.250769 -0.186721 0.000018
C -1.657257 -0.571176 -0.000273
C -1.217119 0.908524 0.000187
H 1.272382 -1.637949 0.000730
H -1.369850 1.482541 0.911731
H 1.993822 1.374384 -0.000471
H 3.161176 -0.066275 -0.000427
H -2.102359 -0.966674 -0.911220
H -2.102680 -0.966540 0.910565
H -1.370352 1.482696 -0.911173

Frequencies

137.2889	203.5768	260.2405
512.1901	550.0246	696.2496
747.1474	784.7103	844.3501
957.4475	982.2640	994.9040
1033.6815	1063.4700	1075.6079
1118.6947	1150.9098	1221.9391
1384.3951	1451.1838	1464.8221
1508.1168	1609.8028	3070.1708
3074.3255	3123.7737	3134.5508
3143.5860	3147.9901	3238.9239

i61

C -1.249601 -0.533702 -0.628252
C -1.372173 0.493980 0.442572
C -0.042218 -0.026364 -0.046122
C 1.227304 -0.548009 0.544088
C 1.258113 0.570482 -0.484362
H -1.669564 -1.523242 -0.744863
H -1.733320 0.194924 1.425671
H -1.650896 1.507495 0.159247
H 1.449592 -0.290330 1.574486
H 1.566639 -1.531839 0.238731
H 1.610267 0.335164 -1.482742
H 1.498734 1.569504 -0.138074

Frequencies

273.7830	299.9723	313.5329
585.7983	624.2718	790.1789
826.7779	848.6797	881.5220
913.7916	982.5570	1017.9582
1049.7217	1061.9311	1064.1807
1082.2605	1121.1682	1169.6581
1179.8398	1432.4002	1459.1345
1477.9839	1531.5352	3062.5771
3106.8579	3112.7332	3132.8206
3186.4073	3198.9537	3202.3461

i62

C 1.249668 -0.533706 -0.628128
C 1.372236 0.493946 0.442506
C 0.042219 -0.026320 -0.046185
C -1.258233 0.570621 -0.484138
C -1.227247 -0.548217 0.543920
H 1.669372 -1.523366 -0.744922
H 1.650697 1.507442 0.158704
H 1.733404 0.195558 1.425808
H -1.498547 1.569494 -0.137108
H -1.610699 0.336104 -1.482586
H -1.566268 -1.531947 0.237821
H -1.449816 -0.291228 1.574425

Frequencies

273.7905	299.9842	313.5729
585.7946	624.2727	790.2388
826.7344	848.7475	881.5243
913.8759	982.6053	1018.0819
1049.8122	1061.9336	1064.2290
1082.2811	1121.4305	1169.6529
1179.8577	1432.4297	1459.1298
1478.0196	1531.5218	3062.3796
3106.7751	3112.6482	3132.5628
3186.3090	3198.6978	3202.2436

i63

C -1.158326 -0.552441 -0.103179
C -1.990218 0.400582 0.234842
C 0.277275 -0.385738 -0.502913
C 1.367155 -0.405110 0.552298
C 1.057990 0.864523 -0.200536
H -2.000822 1.475801 0.334518
H -1.514369 -1.585133 -0.098719
H 0.527023 -0.893089 -1.430816
H 1.051508 -0.463370 1.587090
H 2.286296 -0.933310 0.327082
H 1.768518 1.209022 -0.942154
H 0.558597 1.659185 0.339930

Frequencies

90.6405	250.2982	323.7491
490.6226	684.3539	753.5642
802.2475	825.7475	856.2591
872.3567	926.7037	992.7332
1048.6685	1077.7003	1109.9893
1124.7244	1195.4113	1220.0817
1268.8159	1379.5490	1465.2896
1503.1679	1659.2937	3073.1176
3120.0814	3122.9962	3129.5717
3200.5268	3214.8687	3237.2235

i64

C -1.528373 -0.502054 -0.011584
C -2.103094 0.725416 -0.094985
C -0.154256 -0.718578 -0.096649
C 0.894495 0.153360 0.467794
C 2.224664 0.148470 -0.296227
H -2.185487 -1.379748 -0.037991
H 2.090173 0.533238 -1.309959
H -3.064615 1.126978 -0.384557
H 0.509191 1.180111 0.592293
H 1.061396 -0.206908 1.496581
H 2.621565 -0.866069 -0.374709
H 2.967161 0.772714 0.208250

Frequencies

66.1690	159.2100	202.6966
260.3673	374.6472	417.9094
566.2599	720.5175	771.4589
806.4349	875.7179	991.0598
1006.9830	1074.8635	1228.5590
1256.4503	1281.6030	1323.3269
1362.5769	1411.8850	1412.9578
1495.5027	1504.4218	2930.3998
2971.0341	3018.0739	3031.9366
3096.2333	3103.9057	3217.1410

i65

C	-0.592743	0.051614	-0.001480
C	-1.924742	-0.580030	0.000431
C	0.753100	-0.027895	-0.000317
C	1.915994	-0.736704	0.000277
C	0.137111	1.353325	0.000216
H	0.173135	1.954253	-0.912118
H	-1.853544	-1.669915	0.002107
H	-2.504818	-0.272042	-0.878259
H	-2.503367	-0.269105	0.879041
H	2.876616	-0.237184	0.001803
H	1.908159	-1.820810	-0.000815
H	0.171499	1.952950	0.913479

Frequencies

96.1142	169.0119	216.5755
390.4111	407.4729	534.9058
682.8243	769.8005	786.2115
943.5381	947.0349	1014.2724
1038.3387	1046.1080	1102.2853
1176.1518	1320.5801	1402.3756
1468.5602	1470.6685	1478.5541
1497.4671	1678.9253	2998.1039
3013.6217	3036.1946	3070.8769
3094.9080	3135.3879	3227.3765

i66

C	1.996652	0.006215	-0.048993
C	0.821302	-0.613694	0.058022
C	-1.620804	-0.845805	-0.039685
C	-0.525790	0.004723	0.012661
C	-0.695841	1.390345	0.027478
H	2.083378	1.077772	-0.190251
H	2.925057	-0.550585	-0.004255
H	0.818709	-1.694005	0.181851
H	-2.630765	-0.456425	-0.079762
H	-1.499284	-1.921960	-0.044889
H	-1.688468	1.820034	-0.022673
H	0.138255	2.074466	0.103084

Frequencies

9.0586	298.5053	421.6241
432.3502	498.5458	530.9952
555.8227	726.3443	755.3731
807.7095	815.4688	937.9183
980.7809	1024.2338	1030.0119
1072.3589	1299.0119	1349.1209
1363.8221	1456.1845	1490.6096
1527.0091	1690.7963	3133.4019
3142.3230	3143.3694	3154.6335
3220.4134	3236.9171	3247.1541

i67

C	-0.909119	-0.619354	0.000307
C	-2.012550	0.096628	-0.000249
C	0.466453	-0.096591	0.000171
C	0.643132	1.399589	0.000111
C	1.504977	-0.942856	-0.000196
H	-0.998751	-1.712026	0.001112
H	0.165923	1.844767	-0.878399
H	-3.078129	-0.074014	-0.000874
H	1.699143	1.674016	-0.000281
H	0.166175	1.845255	0.878469
H	2.527972	-0.584715	-0.000499
H	1.360311	-2.017782	-0.000397

Frequencies

148.8837	191.0557	255.9820
423.7149	440.5414	536.0724
638.3165	742.2827	753.2568
857.3275	868.2724	921.9137
986.4685	1042.8941	1069.1773
1251.5343	1315.8675	1411.0835
1440.4498	1478.0684	1495.1117
1633.5283	1685.2857	3020.2033
3026.5229	3074.7763	3110.8768
3135.1036	3217.9748	3248.0611

i68

C -0.405689 0.118291 -0.036563
C -1.576969 -0.824358 0.089520
C -0.552354 1.447033 -0.041990
H -1.475508 -1.461543 0.974694
H -1.635332 -1.492296 -0.777440
H -2.519713 -0.280469 0.164744
H 0.298286 2.107325 -0.162379
H -1.528464 1.905596 0.069396
C 2.084469 -0.029264 0.182335
C 0.922497 -0.528612 -0.169392
H 3.120039 -0.333668 0.175188
H 0.908975 -1.543489 -0.587657

Frequencies

86.5814	183.6875	261.9897
387.9703	421.6076	534.2414
638.4565	727.0633	745.7327
847.5440	905.5469	926.1493
982.1316	1028.6683	1069.7789
1234.6409	1302.2352	1410.7243
1437.2248	1481.2728	1495.3768
1642.6822	1694.5403	3003.5502
3015.0076	3059.1414	3109.8237
3137.0929	3222.6032	3243.0089

i69

C -1.060672 -0.774850 -0.004099
C 0.348555 -0.707839 -0.568216
C 1.373047 -0.227516 0.376597
C 0.462846 0.779219 -0.348692
C -0.939023 0.771844 0.270498
H -1.206094 -1.433194 0.857012
H -1.823663 -0.989720 -0.753349
H 0.888123 1.567841 -0.957333
H 1.284858 -0.388271 1.451108
H 2.393453 -0.216899 0.006526
H -0.978056 1.054446 1.327894
H -1.667133 1.360646 -0.288389

Frequencies

265.4215	394.3174	617.3811
746.5942	771.4194	827.1699
887.1263	913.5621	944.4514
983.9252	1000.2483	1038.5869
1078.0304	1095.7809	1158.1577
1186.1263	1208.3927	1222.9149
1266.6705	1328.7968	1469.0669
1477.2429	1497.1900	3023.4015
3044.3064	3067.1437	3092.1242
3109.6048	3163.1664	3171.3506

i70

C	-0.440876	0.046853	0.000375
C	-1.922974	0.002557	-0.000165
C	1.602398	0.137665	-0.000104
C	0.539189	1.043671	0.000057
C	0.636047	-1.051078	0.000083
H	-2.349897	1.008681	0.000103
H	-2.311759	-0.529490	0.878274
H	-2.311109	-0.528747	-0.879334
H	2.679490	0.220681	-0.001015
H	0.485958	2.126910	0.000300
H	0.662533	-1.687991	0.891419
H	0.662084	-1.688048	-0.891227

Frequencies

116.2623	205.8022	315.0394
406.4199	509.0801	648.3295
872.5659	878.1197	929.1981
936.5931	979.2948	1024.2874
1052.0792	1087.0630	1163.3354
1201.0054	1261.7328	1362.8006
1404.7678	1452.6359	1468.5903
1477.4229	1526.8660	2986.4884
3016.1658	3017.6500	3053.0713
3086.2731	3174.7525	3225.6724

i71

C -0.899155 0.012524 -0.000032
C -2.195573 -0.076836 -0.000018
C 0.447969 0.099872 -0.000176
C 1.106714 1.334708 0.000085
C 1.266307 -1.185824 0.000004
H 0.624474 -2.066615 -0.007848
H -2.771430 -0.114162 -0.924563
H -2.771327 -0.115194 0.924548
H 2.188710 1.381541 -0.000259
H 0.554118 2.264618 0.000615
H 1.903005 -1.232096 0.887761
H 1.914878 -1.224756 -0.879427

Frequencies

12.7285	179.2822	184.4376
370.5201	469.0290	496.3083
520.3292	598.3282	714.8033
771.7372	882.5971	960.2037
984.0276	1000.9527	1050.5734
1273.3095	1283.2833	1403.6567
1447.5073	1480.9413	1490.3401
1498.3342	1909.5470	3032.1142
3065.3658	3087.8317	3122.6590
3123.0276	3146.5371	3246.8768

i72

C	-1.226587	0.273891	-0.360654
C	-2.206382	-0.535107	0.025129
C	1.265227	0.281157	-0.229490
C	2.331406	-0.462888	-0.090053
C	-0.000583	0.591658	0.464367
H	-1.276917	0.760101	-1.331858
H	-2.183002	-1.043354	0.984487
H	-3.069031	-0.720043	-0.604759
H	2.458019	-1.125806	0.772064
H	3.140533	-0.464430	-0.815620
H	-0.039108	0.040981	1.418184
H	-0.008976	1.660288	0.721710

Frequencies

80.7962	122.4452	246.2096
352.9428	422.6350	515.6415
638.5466	866.0162	885.5077
922.8542	949.7220	951.6886
1013.2872	1033.7850	1134.5028
1226.9993	1298.9671	1324.5637
1412.8639	1442.7777	1453.1916
1708.6934	1741.6453	2953.2330
3001.2813	3027.5324	3126.1681
3141.2778	3145.4177	3211.2546

i73

C 1.026521 -0.035543 0.463444
C 2.030546 -0.498737 -0.273518
H 0.877515 -0.411542 1.472976
H 2.200369 -0.152675 -1.288666
H 2.723234 -1.238221 0.112688
C -1.352976 0.430107 -0.109597
C -1.985230 -0.714366 -0.060771
C 0.015133 0.987507 -0.006644
H -3.063887 -0.781788 -0.177315
H -1.457692 -1.660377 0.090671
H 0.316720 1.394911 -0.978336
H -0.000226 1.835882 0.690496

Frequencies

75.5130	155.7144	202.0040
404.4071	433.5156	474.8439
659.2508	886.8853	890.8017
910.9392	929.3940	949.1514
1016.1076	1030.9095	1116.0611
1237.4975	1302.1301	1323.1444
1409.7826	1445.7365	1461.7327
1698.4543	1736.6489	3000.0899
3038.4101	3040.6318	3124.7854
3139.2680	3143.2712	3209.2360

i74

C	-1.265260	0.281467	-0.229765
C	-2.330336	-0.463966	-0.089348
C	1.226426	0.273505	-0.361039
C	2.205366	-0.535901	0.026030
C	0.000608	0.593655	0.463302
H	-2.455750	-1.126319	0.773366
H	-3.139874	-0.467130	-0.814441
H	1.277292	0.758060	-1.333040
H	2.181455	-1.042629	0.986181
H	3.067788	-0.722868	-0.603571
H	0.009195	1.662928	0.717937
H	0.039066	0.045397	1.418490

Frequencies

80.7957	122.2231	246.3628
352.7414	422.6096	515.6904
638.6895	865.9913	885.5320
922.8588	949.7262	951.6451
1013.2228	1033.7651	1134.4941
1227.0235	1298.9741	1324.5581
1412.8728	1442.7783	1453.2244
1708.7265	1741.6163	2953.3944
3001.3423	3027.6418	3126.1617
3141.2749	3145.4789	3211.2210

i75

C 1.352990 0.430169 -0.110158
C 1.985968 -0.713850 -0.060758
H 1.458610 -1.659833 0.091176
H 3.064458 -0.781367 -0.178667
C -1.026594 -0.036289 0.463383
C -2.031056 -0.498232 -0.273759
C -0.015291 0.987100 -0.005954
H -0.877390 -0.413599 1.472401
H -2.201055 -0.150708 -1.288373
H -2.724018 -1.237931 0.111555
H 0.000528 1.834376 0.692359
H -0.317243 1.395673 -0.976973

Frequencies

75.2258	154.9614	201.7202
404.3059	433.5460	474.5569
659.1867	886.7313	890.7018
910.9191	929.4361	949.2024
1016.0360	1030.8898	1116.0752
1237.5323	1302.0077	1323.1379
1409.7453	1445.7566	1461.6079
1698.4984	1736.7282	3000.8535
3038.8260	3041.1856	3124.8048
3139.2300	3143.4260	3209.2092

i76

C	1.210606	0.048238	-0.388507
C	2.437566	-0.264317	-0.057960
C	-1.157718	-0.339331	0.299338
C	-2.355381	-0.135365	-0.236797
C	-0.003105	0.632581	0.218456
H	3.133716	-0.714811	-0.760350
H	2.824174	-0.078631	0.949740
H	-0.956735	-1.260622	0.841204
H	-2.585243	0.769147	-0.792111
H	-3.151183	-0.865158	-0.140689
H	0.254233	0.976751	1.236896
H	-0.310770	1.522483	-0.341870

Frequencies

82.9890	103.1011	280.4523
330.9545	414.0816	534.5517
649.8026	869.7767	890.8581
896.7228	949.8353	959.2507
1024.3637	1037.3101	1129.2611
1233.9298	1298.6986	1325.9577
1413.8000	1441.7085	1453.9799
1706.8551	1736.0331	2918.1709
3024.9996	3037.7215	3125.5199
3139.0819	3146.7823	3211.1283

i77

C 1.176182 -0.405295 -0.151876
C 2.139731 0.510141 -0.161995
C -1.340491 -0.372308 -0.214854
C -2.262154 0.551763 -0.272721
C -0.089089 -0.315870 0.659065
H 1.281154 -1.294801 -0.770921
H 2.071844 1.414381 0.435347
H 3.031783 0.389313 -0.766013
H -2.467465 1.516053 0.169701
H -1.439802 -1.269017 -0.829309
H -0.091233 0.597357 1.258888
H -0.131353 -1.163872 1.356595

Frequencies

83.6894	114.7030	280.6781
387.7436	425.3328	624.8616
679.8102	818.0388	845.6225
936.3406	941.6009	951.2902
993.2894	1031.4618	1123.4000
1223.6715	1267.2353	1310.8075
1327.7416	1450.0672	1473.7610
1665.7044	1706.4227	2994.1131
3072.5093	3086.2543	3121.0947
3129.6457	3210.7012	3229.6555

i78

C	1.051517	0.004448	-0.359498
C	-0.026746	0.959519	-0.055530
C	-1.722286	-0.920592	0.015435
C	-1.411722	0.368532	0.086378
C	2.175153	-0.436123	0.143624
H	-0.055823	1.733077	-0.835759
H	0.226454	1.501137	0.874331
H	-2.745785	-1.258057	0.131157
H	-0.966596	-1.678653	-0.160215
H	-2.196822	1.100374	0.263460
H	2.553119	-0.076053	1.106321
H	2.789953	-1.176527	-0.361747

Frequencies

83.5468	143.0108	231.4525
325.5212	453.4620	558.0482
620.9191	849.9584	891.9107
909.6014	948.7139	955.1399
1024.3535	1035.2861	1097.6705
1217.6557	1320.7675	1338.3575
1414.9687	1437.4011	1447.1163
1709.2338	1744.6046	2919.0922
2999.4486	3024.8645	3128.3357
3139.2893	3143.2306	3218.7102

i79

C -1.051223 0.002753 -0.358682
C -2.176220 -0.435487 0.143397
C 0.026521 0.958804 -0.055892
H -2.555989 -0.072192 1.104171
H -2.790344 -1.177197 -0.360865
H 0.054716 1.731646 -0.836860
H -0.226843 1.501014 0.873584
C 1.411938 0.368986 0.086162
C 1.723407 -0.919957 0.015837
H 2.196544 1.101446 0.262799
H 0.968239 -1.678637 -0.159381
H 2.747140 -1.256679 0.131623

Frequencies

83.5930	142.9246	231.1823
325.6139	453.4957	557.9898
620.7092	849.9029	891.8820
909.7013	948.7244	955.1620
1024.3047	1035.2129	1097.7048
1217.6850	1320.7648	1338.3319
1414.9698	1437.3506	1447.0764
1709.2364	1744.6587	2919.0565
2999.4731	3024.8487	3128.4086
3139.3383	3143.2736	3218.7164

TRANSITION STATES

i17 — i39

C	1.252174	-0.663370	-0.441174
C	0.402213	0.609261	-0.272420
C	1.293385	0.106671	0.798851
H	0.713281	-1.607936	-0.461024
H	2.100120	-0.631616	-1.122783
H	0.755754	1.487204	-0.810432
H	2.087792	0.566865	1.369390
C	-1.824099	-0.504395	0.184498
C	-1.086048	0.551018	-0.150888
H	-2.902593	-0.429977	0.256468
H	-1.390381	-1.473654	0.406993
H	-1.589729	1.494000	-0.351809

Frequencies

-96.9714	252.2925	284.5075
528.6948	576.7976	682.8183
737.1914	801.4338	890.8974
923.7334	975.8745	1019.7221
1026.0512	1048.7362	1060.7619
1097.6972	1112.4280	1239.6364
1335.3145	1389.0485	1443.9521
1469.8609	1698.5882	3073.2161
3094.5425	3129.4524	3139.0662
3144.1386	3203.8917	3215.6960

i39 — i40

C	-1.214991	-0.792982	0.033648
C	-0.542796	0.400674	0.679417
C	-0.855044	0.409117	-0.748653
H	-0.691427	-1.736120	-0.094812
H	-2.270131	-0.907938	0.273430
H	-0.967441	1.003535	1.473432
H	-1.352718	1.104026	-1.407832
C	1.766278	-0.450223	-0.068541
C	0.824347	0.544961	0.130126
H	2.723171	-0.215299	-0.516997
H	1.548966	-1.492949	0.124558
H	1.142816	1.575466	-0.007760

Frequencies

-613.2894	257.7864	297.9033
480.2741	535.7022	627.9620
744.8888	796.2655	841.9028
896.5139	958.5163	985.6811
1004.7306	1047.5915	1071.3307
1088.8728	1115.3629	1233.5883
1274.4138	1331.9507	1421.9531
1505.1650	1516.1094	3085.3038
3132.6655	3147.1036	3153.6727
3158.8244	3219.3027	3238.5399

i25 — i40

C	-1.215170	0.792831	0.033745
C	-0.854729	-0.408982	-0.748845
C	-0.542722	-0.400610	0.679506
C	1.766237	0.450289	-0.068476
C	0.824334	-0.544949	0.130044
H	-0.691795	1.736092	-0.094528
H	-2.270395	0.907537	0.273246
H	-1.352845	-1.104035	-1.407551
H	-0.967590	-1.004089	1.472916
H	2.723237	0.215430	-0.516731
H	1.548757	1.493014	0.124429
H	1.142928	-1.575428	-0.007633

Frequencies

-613.4227	257.8178	297.8198
480.0813	535.7161	628.2751
744.7668	796.2526	841.8467
896.4090	958.4866	985.7451
1004.5590	1047.6082	1071.3865
1088.9530	1115.3540	1233.5231
1274.3852	1331.9115	1421.9415
1505.1438	1516.1188	3085.3623
3132.8006	3147.1398	3153.7455
3158.9549	3219.2042	3238.5647

i28 — i41

C	1.921680	-0.003654	-0.093315
C	0.560962	-0.027084	0.086544
C	-1.542996	-0.069173	-0.134888
C	-0.550147	-1.040943	-0.018652
C	-0.537899	1.061577	0.026247
H	2.461779	0.932507	-0.035567
H	2.496611	-0.916023	-0.194044
H	0.117547	-0.711205	1.156792
H	-2.620186	-0.102843	-0.064448
H	-0.509382	-2.119537	-0.116272
H	-0.642578	1.695910	0.912450
H	-0.413388	1.696853	-0.854530

Frequencies

-1731.9350	279.9674	342.2449
451.5669	544.4280	591.8894
680.3495	712.8253	862.8520
884.6271	907.2834	949.4404
980.3332	1056.7504	1057.8143
1143.2836	1152.6086	1197.2884
1251.9811	1401.7849	1429.6182
1450.7745	1554.4844	1588.9928
3035.9770	3084.8565	3143.7382
3183.0782	3222.7200	3233.8532

i23 — i41

C	-1.923695	-0.016138	0.004714
C	-0.585663	-0.031419	-0.008016
C	1.551410	-0.023814	-0.002045
C	0.448209	-1.066166	0.024548
C	0.487803	1.072004	0.001878
H	-2.475274	0.916611	-0.009489
H	-2.498075	-0.934729	0.044959
H	1.129326	-0.825721	-1.004896
H	2.559815	-0.067115	0.385644
H	0.451674	-2.106907	0.322797
H	0.482281	1.795252	-0.817923
H	0.481863	1.615801	0.952426

Frequencies

-1872.9783	217.3373	352.6217
454.7218	577.4477	629.2305
710.6359	767.2832	833.7272
874.1138	894.6348	929.2656
967.3294	1012.2551	1083.8437
1149.9207	1183.9127	1228.3522
1256.7734	1279.0487	1436.1724
1459.2341	1679.1736	2176.8167
3031.0530	3075.0720	3135.2202
3186.5469	3203.7378	3218.1996

i23 — i42

C	-1.282918	-0.470536	0.304080
C	0.034912	-0.957359	-0.257142
C	1.690463	0.172399	0.279338
C	0.508376	0.322159	-0.584860
C	-0.788752	0.972681	-0.073559
H	-1.414792	-0.626022	1.378907
H	-2.174544	-0.847683	-0.208033
H	0.468449	-1.944648	-0.365084
H	1.634822	0.426709	1.333601
H	2.564211	-0.365014	-0.067288
H	-0.667760	1.658845	0.768236
H	-1.382875	1.461751	-0.847482

Frequencies

-856.8590	229.0143	344.3163
511.6344	573.6973	698.8608
765.3602	838.2891	855.6402
889.8924	945.0463	956.4267
1036.0788	1066.7135	1158.8120
1173.6723	1201.2453	1237.3424
1276.0562	1353.6171	1440.3273
1454.5159	1482.9617	3023.9285
3049.8521	3067.8885	3100.5685
3110.0767	3182.2670	3223.2542

i28 — i43

C	1.443640	-0.128154	0.480204
C	0.455857	-0.497697	-0.547564
C	-1.138853	0.641624	0.251010
C	0.078134	0.957147	-0.343826
C	-0.937200	-0.854012	0.061808
H	2.424033	0.221315	0.183016
H	1.255971	-0.309372	1.529506
H	0.782255	-0.923022	-1.494648
H	-1.882550	1.221202	0.781736
H	0.540284	1.869782	-0.693029
H	-1.616855	-1.303907	-0.669671
H	-0.912607	-1.489451	0.953302

Frequencies

-621.4759	338.0369	398.3169
580.1880	608.5684	683.9703
804.0687	822.1623	840.9397
906.8458	933.5047	1000.8683
1026.3081	1068.2070	1088.5246
1119.5446	1195.5277	1217.8539
1263.4252	1316.4654	1379.1500
1453.1331	1477.8835	3017.0494
3055.9071	3104.4108	3143.5371
3191.1408	3216.4331	3253.7609

i42 — i43

C	1.082603	0.712280	0.205333
C	-0.356616	0.763379	-0.350842
C	-1.422469	-0.055898	0.397357
C	-0.388882	-0.743969	-0.445732
C	0.995209	-0.805797	0.080492
H	1.217561	1.068446	1.235746
H	1.823268	1.215398	-0.422390
H	-0.698102	1.462048	-1.107104
H	-1.380162	-0.189491	1.476413
H	-2.421782	0.061272	-0.007663
H	1.435319	-1.609729	0.663346
H	0.564826	-1.227914	-1.157996

Frequencies

-2142.1985	319.0566	369.5164
615.0428	711.9104	754.9429
819.5627	856.8403	885.9102
909.4898	972.7902	1003.3277
1029.8287	1040.0783	1065.0198
1131.2631	1168.1848	1177.1901
1229.2236	1253.1335	1316.9427
1455.1617	1469.2259	2036.4404
2989.5705	3058.9712	3086.1008
3144.0360	3146.5555	3186.2949

i43 — p21

C	1.253446	-0.200588	0.536846
C	0.362885	-0.619002	-0.613412
C	-1.014149	0.753684	0.160676
C	0.453829	0.853339	-0.207938
C	-1.096526	-0.551766	-0.181437
H	2.321697	-0.205556	0.335259
H	0.967864	-0.472653	1.548415
H	0.750418	-1.061195	-1.521142
H	-1.687314	1.443339	0.654567
H	0.928660	1.646960	-0.769233
H	-1.893251	-1.282701	-0.193753
H	-1.144989	-1.482194	1.777476

Frequencies

-420.8632	255.0915	321.8913
431.0184	485.1051	742.9114
782.8992	786.8689	826.7528
850.6699	888.8905	930.8833
960.5090	1022.5478	1027.6942
1042.9807	1087.0638	1099.7397
1198.6317	1218.6186	1287.5048
1306.4389	1469.1328	1537.9363
3091.3994	3180.0758	3181.7944
3191.1116	3198.9520	3217.4851

i22 — p22

C	1.509785	-0.471683	0.547469
C	0.603095	-0.333421	-0.608902
C	1.255397	0.886517	-0.109732
H	1.078608	-0.625457	1.533052
H	2.474589	-0.953568	0.409595
H	0.685298	-0.783845	-1.588849
H	0.655996	1.597122	0.453177
H	2.046211	1.344029	-0.698048
C	-2.216234	0.450954	0.165481
C	-1.632359	-0.594916	-0.042238
H	-2.568189	1.445274	0.300384
H	-1.490615	-1.648257	-0.121781

Frequencies

-392.4140	39.8703	133.1437
145.8694	268.9354	542.2898
645.1910	692.2486	738.0851
764.0989	788.1542	809.9602
854.4784	945.0313	1028.9713
1065.6493	1086.2173	1113.2220
1163.9798	1253.2206	1455.0739
1483.8232	1933.6123	3083.6190
3087.5732	3150.7119	3162.6479
3191.4317	3389.0631	3479.9453

i17 — p18

C	1.645287	-0.515283	0.508119
C	1.349170	0.873375	0.023042
C	0.887619	-0.087644	-0.729713
C	-2.253292	0.390136	0.196966
C	-1.467485	-0.605868	-0.119785
H	1.085671	-0.933327	1.345132
H	2.662195	-0.902539	0.421174
H	1.500855	1.924736	0.194485
H	0.567282	-0.395379	-1.708732
H	-3.303304	0.238853	0.458975
H	-1.898336	1.418100	0.217916
H	-1.582157	-1.678742	-0.200722

Frequencies

-266.2992	36.4741	105.0020
140.1618	200.5570	263.3912
590.8511	747.1768	772.8483
809.4848	853.3992	918.0390
930.7435	1010.7625	1036.0044
1061.8401	1069.5869	1094.2299
1152.2093	1389.4445	1502.9003
1626.1996	1653.0756	3032.0966
3050.5191	3096.6887	3140.9300
3210.6534	3252.4066	3291.1297

i25 — p18

C	-1.334773	0.901906	-0.105101
C	-0.889817	-0.338862	0.636565
C	2.232883	0.416796	-0.042242
C	1.471934	-0.647258	-0.064229
C	-1.689435	-0.529449	-0.378465
H	-2.086679	1.560593	0.333714
H	-0.614828	1.418505	-0.739933
H	-0.515537	-0.701424	1.576782
H	3.261636	0.400399	-0.412188
H	1.882996	1.371650	0.344423
H	1.600030	-1.668391	-0.396785
H	-2.272376	-1.200131	-0.985182

Frequencies

-273.5319	40.6033	111.0926
141.3255	187.3677	242.2074
591.8032	743.4177	774.5697
811.2944	858.3864	916.6010
929.3527	1008.1530	1033.0354
1063.1987	1069.2268	1092.3427
1152.9263	1390.2976	1499.8339
1621.7341	1647.9107	3032.3705
3042.4782	3097.3729	3136.5596
3216.4178	3252.6514	3291.0414

i40 — p20

C	-1.474727	-0.592670	-0.000532
C	-0.581367	0.334890	0.766016
C	-0.581353	0.336266	-0.765426
C	1.892266	-0.376272	-0.000321
C	0.640352	0.110796	0.000068
H	-1.265126	-1.660348	-0.001304
H	-2.531562	-0.337538	-0.000378
H	-0.841662	1.126350	1.450098
H	-0.841679	1.128931	-1.448081
H	2.425926	-0.512635	-0.932549
H	2.425750	-0.514796	0.931682
H	1.257326	1.891976	0.001697

Frequencies

-900.5658	267.0766	278.8209
375.5842	582.1413	621.7903
649.3662	736.4130	747.1154
809.9595	865.8252	884.4661
983.9757	997.7501	1029.9579
1043.8418	1104.2594	1143.5768
1215.3851	1223.8465	1288.8720
1460.1768	1522.1195	1740.9256
3101.4438	3168.8392	3189.2341
3262.6321	3270.5022	3271.4675

i42 — p17

C	0.999288	0.721072	0.420459
C	-0.469780	0.636619	-0.040895
C	-1.476376	-0.415513	0.323433
C	-0.310245	-0.578833	-0.603371
C	1.180867	-0.669606	-0.223305
H	1.096060	0.744600	1.508224
H	1.555150	1.553987	-0.008359
H	-1.493108	2.969671	-1.329333
H	-1.497180	-0.878619	1.313253
H	-2.446935	-0.321619	-0.147133
H	1.385333	-1.481476	0.478275
H	1.858160	-0.748968	-1.072854

Frequencies

-253.5010	55.8359	61.1233
214.5383	302.7154	315.3455
727.2459	729.1536	853.0097
864.6207	946.1013	1005.0460
1022.2977	1080.5934	1131.9884
1178.8914	1205.7544	1206.6290
1230.6354	1243.7836	1454.5373
1469.6845	1482.3982	1555.0073
3077.1077	3083.9361	3089.5107
3146.6906	3160.7760	3204.7529

i29 — p19

C	0.228989	-0.487389	0.763327
C	-2.736266	0.102727	-0.319805
C	1.528392	0.419101	-0.556866
C	0.749540	0.947081	0.394391
C	1.012393	-1.012708	-0.188909
H	-0.452329	-0.882356	1.502194
H	-3.265260	0.443975	0.558821
H	-2.902330	-0.896507	-0.694785
H	-2.076906	0.773929	-0.849908
H	2.228401	0.814050	-1.280019
H	0.557842	1.945005	0.763143
H	1.212291	-2.010961	-0.552272

Frequencies

-60.0322	46.4893	54.7739
66.0369	139.8869	168.8989
505.8165	535.3834	573.3196
590.1883	710.7637	720.3803
852.4525	861.3749	867.8741
1050.3777	1086.3784	1186.2822
1259.7032	1375.1979	1401.7554
1405.2119	1592.2824	3104.9446
3195.1353	3211.6763	3230.2156
3243.3617	3281.3365	3288.1569

i14 — p3

C	-1.326333	0.489347	-0.040674
C	-1.678578	-0.785214	-0.245888
C	1.125315	0.246802	0.023855
C	2.182143	-0.506599	-0.033675
C	0.048355	0.990405	0.078025
H	-2.103999	1.240197	0.063181
H	-2.719698	-1.064844	-0.348355
H	-0.935187	-1.562871	-0.389021
H	-1.805302	-1.619629	1.875168
H	2.604173	-0.952188	0.862092
H	2.676129	-0.708081	-0.979578
H	0.178469	2.058966	0.226654

Frequencies

-416.9732	68.2368	148.3526
184.3261	247.5923	338.2893
409.8052	535.8455	662.5199
739.3805	902.5620	927.5679
931.5399	953.7209	1017.5915
1026.8992	1060.2235	1161.1524
1344.0241	1385.6491	1449.5526
1486.5950	1671.3562	2061.9386
3139.6636	3156.5814	3166.7550
3182.9931	3221.2591	3256.8638

i15 — p23

C	-2.565025	0.780458	-0.084908
C	0.200261	-0.637496	-0.046485
C	2.297476	0.557626	0.325056
C	1.442519	-0.115455	-0.463769
C	-0.926655	-0.991239	0.255424
H	-2.955405	0.813509	0.923826
H	-3.150850	0.284447	-0.847448
H	-1.885269	1.562000	-0.392577
H	3.238672	0.925628	-0.064072
H	2.074822	0.750895	1.367533
H	1.706166	-0.291567	-1.504404
H	-1.719596	-1.608279	0.605235

Frequencies

-380.9707	52.7295	64.0092
116.4313	227.5121	340.5424
408.0382	435.0846	562.8394
651.2047	664.0684	691.3335
759.9685	901.0282	925.2271
996.7550	1111.7786	1311.8672
1409.2684	1416.6130	1438.9702
1627.8235	2077.4646	3096.1795
3130.2748	3146.6615	3237.5050
3260.2288	3271.4080	3437.1607

i31 — p23

C	-2.565068	0.780434	0.084834
C	0.200259	-0.637451	0.046532
C	2.297547	0.557519	-0.325100
C	1.442494	-0.115345	0.463805
C	-0.926650	-0.991237	-0.255356
H	-3.151288	0.284218	0.846936
H	-2.954958	0.813824	-0.924078
H	-1.885424	1.561846	0.393080
H	3.238713	0.925593	0.064033
H	2.075005	0.750538	-1.367647
H	1.706033	-0.291212	1.504509
H	-1.719573	-1.608327	-0.605120

Frequencies

-380.9810	52.6906	64.0087
116.4337	227.5114	340.5416
408.0477	435.0874	562.8387
651.2094	664.0653	691.3355
759.9779	901.0283	925.2279
996.7557	1111.7790	1311.8678
1409.2668	1416.6140	1438.9713
1627.8241	2077.4600	3096.1814
3130.2761	3146.6625	3237.5055
3260.2331	3271.4062	3437.1584

i45 — p24

C	-1.431148	-0.256844	0.609454
C	0.275456	0.903997	-0.083305
C	2.471718	-0.466284	-0.060343
C	1.373393	0.287108	-0.092909
C	-2.350503	-0.306123	-0.398537
H	-0.803514	-1.114598	0.815290
H	-1.568413	0.428873	1.438285
H	-0.142020	1.864740	-0.309628
H	2.794643	-1.025430	-0.931742
H	3.092124	-0.517979	0.827681
H	-2.320829	-1.085921	-1.150555
H	-3.085489	0.479189	-0.535487

Frequencies

-536.6371	46.3484	133.6019
224.6544	320.5437	375.6158
420.8875	488.6077	723.3846
743.2971	784.5356	818.1863
859.9466	981.4755	1014.1680
1028.2465	1152.9821	1237.2176
1279.9298	1462.3892	1466.7905
1561.3030	1928.9790	3125.9595
3131.2375	3137.5711	3206.1596
3207.7850	3233.7097	3327.8002

i31 — i44

C -1.086305 0.665548 -0.000005
C -2.135848 -0.413881 0.000002
C 1.195090 -0.642580 -0.000001
C 2.289343 0.117032 0.000005
C 0.214874 0.430527 -0.000005
H -1.433681 1.694745 0.000009
H -2.779393 -0.329993 -0.881421
H -2.779087 -0.330272 0.881678
H -1.688957 -1.410145 -0.000237
H 1.066467 -1.719247 -0.000009
H 3.364216 -0.038982 0.000005
H 1.387515 1.194013 -0.000002

Frequencies

-2273.0946	85.3579	129.7726
183.8948	351.6544	490.2647
668.8390	687.0573	786.6970
886.4128	919.9918	979.4140
1013.6678	1041.1486	1068.0261
1117.3492	1215.9741	1352.0406
1406.0151	1480.6620	1492.3080
1610.6956	1765.9075	1934.2523
3040.5396	3101.6867	3134.1363
3176.0307	3182.3476	3219.7007

i30 — i44

C	1.180196	0.563913	-0.148253
C	1.721069	-0.823557	0.030446
C	-0.088157	0.946602	-0.000981
H	1.905493	1.324436	-0.430304
H	2.496037	-0.842966	0.805027
H	2.193151	-1.176835	-0.893026
H	0.940151	-1.534646	0.303433
H	-0.343194	1.991540	-0.162590
C	-1.220565	0.061883	0.402630
C	-2.074530	-0.504018	-0.411806
H	-1.354600	-0.090995	1.482915
H	-2.945116	-1.139473	-0.337670

Frequencies

-142.0267	154.6594	218.0063
280.8609	481.1736	518.8266
690.5035	710.0151	795.9826
853.0795	923.9991	990.1307
1005.0565	1067.4243	1113.4367
1242.8544	1263.2076	1394.6735
1422.9678	1484.5574	1490.3920
1661.4087	1716.5918	2981.8377
3015.3112	3056.0714	3106.8281
3121.1227	3141.8799	3231.5850

i30 — i36

C	-1.005400	0.351305	0.504811
C	-1.908134	-0.541473	-0.285968
H	-1.171723	0.447014	1.575936
H	-2.115040	-0.130884	-1.281092
H	-2.859792	-0.707399	0.224594
H	-1.444769	-1.527501	-0.449147
C	1.431749	0.301856	-0.194073
C	1.734415	-0.951301	0.227704
C	0.196120	0.956143	-0.065528
H	2.241387	0.878343	-0.658898
H	2.523419	-1.630487	-0.073414
H	0.134013	1.971732	-0.459650

Frequencies

-746.2991	87.9199	127.7117
239.9593	264.5242	334.4937
416.4157	555.4742	657.1212
766.8098	873.5584	916.0154
979.9605	1051.9568	1087.7924
1170.8324	1196.1614	1321.9529
1384.2518	1396.6545	1448.6241
1472.5084	1483.5306	2957.5085
3011.6887	3026.0026	3082.7408
3086.9616	3118.8556	3192.9223

i34 — i36

C 0.949956 -0.347698 -0.187127
C 2.376364 -0.036661 0.158259
C -1.489537 0.160937 -0.363417
C -2.409828 -0.260046 0.466258
C -0.077116 0.478447 -0.001563
H 0.758660 -1.330715 -0.614312
H 2.477707 0.965270 0.581873
H 3.019498 -0.100538 -0.726598
H 2.770261 -0.755771 0.884961
H -1.769525 0.320652 -1.413838
H -3.454249 -0.533356 0.426757
H 0.098618 1.464586 0.426697

Frequencies

-188.3460	172.4862	197.9251
250.4142	405.5378	479.4331
650.4958	767.4444	804.4527
858.3838	931.8892	988.7742
1060.6087	1070.1909	1119.6842
1243.2187	1299.3080	1329.2140
1413.2419	1480.1648	1491.6197
1662.9191	1724.9861	2987.3540
3012.7100	3056.2428	3092.4026
3111.1990	3127.1963	3232.1198

i8 — i45

C	1.358673	-0.436895	0.306340
C	1.747857	0.942047	-0.112284
H	1.349021	-0.514364	1.398515
H	2.099230	-1.159343	-0.052130
H	1.501699	1.799472	0.501184
H	2.087899	1.125247	-1.124558
C	-0.011358	-0.883356	-0.232113
C	-2.231854	0.448693	0.077365
C	-1.124569	-0.221585	-0.077716
H	-0.042068	-1.822952	-0.779906
H	-2.550850	1.191035	-0.648590
H	-2.877419	0.287485	0.935935

Frequencies

-107.3130	87.7839	164.7449
298.5825	332.0289	525.2546
546.2175	670.4208	773.5608
865.6920	872.5868	884.7788
1019.9158	1057.6236	1086.4283
1147.4948	1272.5785	1286.3878
1354.9918	1459.6504	1473.1345
1486.7141	2045.1783	3019.5552
3054.9755	3110.9462	3122.9998
3136.6225	3181.6490	3240.9081

i30 — i38

C	-0.989870	0.654012	-0.115840
C	-1.758911	-0.621577	0.004636
C	1.287327	-0.266386	0.632322
C	1.594619	-0.379632	-0.613104
C	0.380293	0.801809	0.113648
H	-1.527913	1.525421	-0.478468
H	-2.114491	-0.971700	-0.974346
H	-2.652491	-0.488143	0.625943
H	-1.158800	-1.422450	0.440917
H	1.489200	-0.698120	1.607385
H	2.101867	-0.883646	-1.419376
H	0.781878	1.809282	0.067975

Frequencies

-633.2210	73.7318	169.4576
246.5614	351.5738	505.3217
635.1879	660.2172	704.4669
844.3157	877.2293	930.4571
993.0536	1021.4621	1094.5928
1144.0393	1245.7626	1378.9800
1410.2759	1437.2818	1477.9170
1505.7210	1713.9642	2987.9411
3028.3784	3097.2917	3133.4145
3138.0012	3153.5088	3258.5167

i14 — i32

C	1.147678	-0.419439	0.416767
C	2.124282	0.588800	-0.089210
H	1.401492	-1.033600	1.274859
H	2.952960	0.733521	0.607301
H	2.552857	0.291580	-1.059311
H	1.642360	1.560356	-0.257926
C	-1.243397	-0.136702	-0.104928
C	-2.386859	0.446870	0.118951
C	-0.095998	-0.724291	-0.322806
H	-3.096031	0.045633	0.836979
H	-2.671534	1.355235	-0.403705
H	-0.056334	-1.484151	-1.110842

Frequencies

-249.6919	61.6528	144.6709
283.3177	313.9106	346.1478
563.4945	629.1905	864.4266
867.0749	881.6745	979.9308
1017.1676	1060.1945	1101.1122
1161.2560	1313.1344	1360.5136
1404.3654	1467.0437	1471.1849
1485.1271	2044.2995	2959.8448
3012.2119	3028.6906	3092.0054
3113.0824	3153.4384	3184.1294

i48 – i49 (hydrogen migration)

C	0.899111	-0.618394	0.011768
C	2.091600	0.295066	-0.025587
C	-0.356502	-0.206461	0.110871
C	-1.268479	0.912034	0.038217
C	-1.753404	-0.542922	-0.007894
H	1.082572	-1.687757	-0.049794
H	1.798800	1.334026	0.141469
H	2.610743	0.243233	-0.990010
H	2.823743	0.019491	0.741593
H	-1.449826	1.721689	-0.657294
H	-2.170633	0.378321	0.793051
H	-2.369353	-1.044934	-0.743271

Frequencies

-1866.6142	165.0440	206.2647
240.5917	403.3171	513.2156
613.9431	725.4988	740.6593
810.6821	869.6339	918.5498
1020.2719	1046.6989	1057.0352
1096.6054	1127.0210	1204.7754
1367.9064	1414.9047	1483.2645
1498.0759	1846.9614	2242.1729
3006.7353	3046.6327	3094.0225
3141.3833	3172.0378	3185.3007

i49 – i59

C	0.980701	-0.611516	0.037123
C	2.075481	0.393348	-0.093833
C	-0.396458	-0.276876	-0.006388
C	-1.370928	0.877379	0.030007
C	-1.666172	-0.593919	-0.058468
H	1.261024	-1.653335	-0.080663
H	1.830056	1.442285	-0.169013
H	3.089065	0.051122	-0.234496
H	1.547167	-0.154069	1.050753
H	-1.486341	1.514225	-0.850260
H	-1.538413	1.407184	0.971561
H	-2.438303	-1.337909	-0.138527

Frequencies

-1818.3076	160.1412	190.2605
267.6073	455.7781	506.0768
615.3319	627.7490	663.5285
837.5135	921.9549	957.2825
1003.3777	1062.3738	1082.6815
1088.7741	1133.1048	1218.1369
1233.0493	1366.4158	1425.6260
1515.2569	1762.3909	2196.7927
3010.0274	3067.1128	3153.5210
3166.7197	3275.4703	3290.6768

i25 – i59

C	1.066148	-0.559054	0.007827
C	2.080585	0.381034	-0.087682
C	-0.359477	-0.265402	0.037142
C	-1.348523	0.872072	0.028859
C	-1.648919	-0.586060	-0.121865
H	1.310054	-1.616210	-0.063962
H	0.343305	-0.531917	1.182968
H	1.864742	1.441584	-0.100483
H	3.114827	0.067095	-0.074938
H	-1.385135	1.526922	-0.845096
H	-1.575675	1.388861	0.965131
H	-2.410997	-1.331869	-0.249309

Frequencies

-1718.2856	193.1252	228.3604
257.4184	428.7886	523.5915
608.7476	668.6021	700.6218
825.2970	936.8627	958.7437
992.7644	1059.0915	1069.9713
1086.5573	1126.5078	1180.7525
1255.1971	1395.3486	1493.9926
1504.6941	1568.6296	1702.0692
3011.4339	3069.1219	3138.3372
3154.1288	3251.6692	3289.8848

i48 – i49 (CHCH₃ moiety rotation)

C	0.979993	0.259390	0.563352
C	2.085938	-0.171229	-0.347812
H	1.188726	0.374583	1.623073
H	1.921638	0.180046	-1.370831
H	2.170843	-1.268215	-0.398522
H	3.050335	0.208408	-0.001397
C	-0.390710	0.211097	0.161345
C	-1.607375	-0.750839	0.030915
C	-1.496237	0.702148	-0.299848
H	-2.126204	-1.067029	0.937016
H	-1.607425	-1.495156	-0.766586
H	-2.027572	1.563963	-0.670467

Frequencies

-186.3506	96.3871	179.0362
262.6764	458.5976	475.0872
643.1924	752.0942	852.9073
948.8942	964.5770	995.6293
1031.8967	1074.8975	1099.9307
1110.2463	1134.8552	1343.8639
1401.8823	1476.6565	1484.7550
1517.2778	1838.5117	2958.4429
3030.1760	3045.2793	3092.2163
3099.2899	3146.1508	3242.4055

i50 – i52

C	0.594280	-0.143759	0.652569
C	1.667103	-0.563489	-0.321498
C	-0.721260	0.051840	0.013673
C	-1.961683	-0.396370	-0.125349
C	0.208504	1.126404	-0.142523
H	0.690294	-0.222900	1.730013
H	1.540464	-1.474406	-0.906124
H	2.689865	-0.326106	-0.035410
H	1.152614	0.563733	-1.013535
H	-2.714835	0.185593	-0.645114
H	-2.262545	-1.351500	0.290321
H	0.182477	2.177831	0.118614

Frequencies

-2148.8279	193.4619	331.7129
435.3648	549.7158	582.0816
694.7766	716.6536	768.9972
882.8734	885.1363	921.3569
959.3559	1011.6421	1040.0034
1061.2424	1088.6956	1167.0602
1247.7973	1275.9182	1436.1311
1459.1416	1749.3561	1782.6101
3068.8929	3129.5032	3154.5636
3173.0201	3173.3062	3213.4615

i57 – p5

C 1.028440 -0.498260 -0.148182
C 2.090587 0.323747 -0.015597
C -0.341908 -0.036243 -0.061704
C -1.780765 -0.473444 -0.038761
C -1.208289 0.917564 0.055229
H 1.173296 -1.511451 -0.509843
H 0.910395 -1.422717 1.589765
H 1.962997 1.360952 0.273329
H 3.100423 -0.041137 -0.157815
H -2.261168 -0.797384 -0.963238
H -2.178525 -0.951679 0.858302
H -1.435807 1.963233 0.163597

Frequencies

-819.1920	69.6751	209.1977
253.2440	373.2774	407.7378
474.0048	628.3250	721.5687
785.6506	924.4877	940.6761
1019.1634	1025.3989	1036.3206
1067.9501	1103.6505	1118.7236
1172.9054	1308.8547	1436.9650
1526.6040	1616.1450	1853.8313
3057.4120	3126.4603	3165.9965
3188.7672	3265.3964	3303.3960

i52 – p29

C	0.688968	-0.006754	0.077572
C	1.839197	-0.655627	-0.153022
C	-0.731150	-0.006313	-0.014790
C	-1.884996	-0.652849	-0.041851
C	-0.021566	1.309116	-0.080183
H	0.793497	-0.002336	2.063636
H	1.874785	-1.739191	-0.177325
H	2.775855	-0.118494	-0.251191
H	-2.822888	-0.125889	-0.178634
H	-1.928583	-1.730000	0.078096
H	0.063075	1.817971	-1.038483
H	-0.098462	1.972503	0.777547

Frequencies

-701.9868	208.2616	260.5144
310.2680	373.2809	431.8225
449.6281	591.1157	729.7768
745.5558	816.4596	891.9593
918.2360	954.6399	996.0296
1026.5538	1048.0789	1105.1874
1160.7044	1428.8275	1435.4296
1472.7318	1646.5412	1839.7114
3079.6480	3129.1399	3130.0723
3156.3598	3212.7401	3218.6768

i48 – i57

C	0.955713	-0.579572	-0.012440
C	2.164773	0.287232	-0.046229
C	-0.371854	-0.073755	-0.036005
C	-1.828006	-0.465197	0.005286
C	-1.231271	0.915583	-0.015760
H	1.105376	-1.631268	-0.229614
H	2.054718	1.360117	0.012169
H	3.128596	-0.153580	-0.252199
H	1.572847	-0.324939	1.039401
H	-2.296568	-0.869180	-0.894597
H	-2.258841	-0.856175	0.930808
H	-1.442257	1.969283	0.024921

Frequencies

-1832.3500	137.4077	197.9302
283.7524	453.3996	468.4165
625.4481	630.8996	713.2714
829.4010	921.0189	1001.5187
1012.0246	1047.7881	1085.4538
1094.9671	1139.6514	1166.4992
1236.1975	1390.6749	1432.7866
1518.8239	1751.0027	2202.1922
3012.8631	3071.6774	3162.7781
3167.1936	3273.7985	3284.7843

i15 – i49

C	-1.039412	-0.766183	0.044399
C	-1.746340	0.472523	-0.041342
C	0.334171	-0.666825	-0.067639
C	1.027963	0.942650	0.107521
C	1.612646	-0.480746	-0.069241
H	-1.480899	-1.695843	0.382532
H	-0.336848	1.087131	0.283113
H	-2.754868	0.501175	0.366709
H	-1.664776	1.051337	-0.964718
H	1.356451	1.396036	1.046113
H	1.156433	1.568086	-0.773682
H	2.590341	-0.916436	-0.182256

Frequencies

-1817.7139	157.7246	215.9457
348.7161	481.4783	486.8656
600.0665	624.6124	687.5140
784.8780	824.3943	899.9943
937.6426	972.6048	1046.7514
1058.1009	1127.3730	1167.1218
1344.8346	1356.3904	1447.2765
1473.3725	1498.0362	1827.3160
3025.1329	3042.1699	3134.9415
3136.4581	3186.0255	3249.7090

i17 – i57

C	1.043250	-0.526923	0.009006
C	2.172183	0.273607	-0.095594
C	-0.336236	-0.057448	0.071583
C	-1.769527	-0.484103	-0.111403
C	-1.255310	0.914071	0.042870
H	1.142608	-1.604864	-0.076444
H	0.351510	-0.438024	1.189327
H	2.100374	1.353531	-0.103756
H	3.156530	-0.173734	-0.102474
H	-2.089852	-0.842895	-1.093236
H	-2.293128	-0.967952	0.716316
H	-1.494200	1.958712	-0.028509

Frequencies

-1734.7265	182.1433	208.7905
321.2107	413.0605	477.6843
610.2897	694.8679	717.2364
806.1612	934.2030	989.3713
1019.0229	1052.3255	1064.8296
1087.2199	1121.1189	1147.7772
1246.3084	1410.4866	1496.2046
1517.9637	1622.7255	1691.8232
3012.5402	3069.5878	3152.2067
3155.5906	3250.0162	3289.9131

i48 – i60

C	-0.884426	-0.829036	0.174466
C	-1.731964	0.366315	-0.170164
C	0.374753	-0.439213	0.385835
C	1.690257	-0.242387	-0.251533
C	0.711214	0.921171	0.041898
H	-1.229468	-1.847604	0.029027
H	-0.566972	1.144157	-0.496043
H	-2.231581	0.924520	0.623043
H	-2.359796	0.258446	-1.056575
H	2.604724	-0.213561	0.340002
H	1.832064	-0.637783	-1.254362
H	0.992027	1.710725	0.731893

Frequencies

-2344.7676	235.6399	261.4764
383.4953	560.2281	620.3542
734.6016	785.3194	833.6957
889.8832	919.4359	990.0505
1009.3038	1021.3208	1058.5384
1084.1824	1102.5939	1117.5626
1286.7120	1357.4924	1437.8923
1456.2137	1548.6113	1712.4287
3057.8651	3067.1447	3130.2286
3142.4626	3149.5599	3159.3720

i36 – i64

C	1.509160	0.445667	0.072540
C	2.141004	-0.698631	-0.124272
C	0.112652	0.683068	-0.292794
C	-0.834304	-0.170663	0.284955
C	-2.285842	-0.191257	-0.132502
H	2.096883	1.323611	0.367626
H	3.158855	-1.055437	-0.180775
H	-0.519069	-1.000936	0.937345
H	-0.653849	0.972989	0.788678
H	-2.441913	-1.055885	-0.785497
H	-2.536587	0.708760	-0.695899
H	-2.960343	-0.302206	0.720964

Frequencies

-907.0551	157.6465	197.2650
256.1056	298.0995	444.5152
493.6355	631.1957	773.1569
841.0793	857.9777	947.5636
1044.9690	1091.3541	1120.0767
1195.5801	1244.8892	1301.3031
1406.7653	1455.9110	1484.0023
1504.8586	1563.0882	2188.9076
2960.6496	3011.4618	3028.3902
3084.1594	3120.3397	3233.2969

i60 – p27

C	1.036371	-0.000004	-0.022620
C	2.336065	0.000047	0.137154
C	-0.257167	0.000026	0.101303
C	-1.517193	-0.762966	0.025242
C	-1.517195	0.762986	0.024961
H	0.930707	-0.000697	-2.059094
H	2.763069	0.000257	1.135692
H	3.020749	-0.000121	-0.701916
H	-1.740413	-1.276603	-0.905171
H	-1.859492	-1.273867	0.920178
H	-1.859493	1.274215	0.919710
H	-1.740415	1.276284	-0.905639

Frequencies

-564.4924	113.9092	172.6515
198.0396	420.7900	472.7019
550.3846	602.4167	657.4878
767.2192	869.4893	910.6783
946.5211	1002.0097	1016.6640
1046.0136	1070.8371	1076.7386
1169.1445	1363.8244	1449.5005
1462.5665	1528.4893	2035.9993
3098.4136	3098.9514	3124.8774
3173.1772	3186.2786	3208.1075

i51 – i53

C	-1.667114	-0.563473	-0.321508
C	-0.594278	-0.143773	0.652571
C	-0.208508	1.126389	-0.142509
C	0.721265	0.051829	0.013676
C	1.961693	-0.396358	-0.125355
H	-1.540502	-1.474396	-0.906132
H	-2.689866	-0.326074	-0.035400
H	-0.690300	-0.222919	1.730014
H	-1.152601	0.563740	-1.013526
H	-0.182489	2.177821	0.118608
H	2.714826	0.185621	-0.645129
H	2.262583	-1.351480	0.290315

Frequencies

-2148.8085	193.4619	331.7103
435.3609	549.7195	582.0871
694.7802	716.6599	768.9973
882.8742	885.1361	921.3575
959.3562	1011.6460	1039.9923
1061.2509	1088.6917	1167.0568
1247.7974	1275.9158	1436.1269
1459.1413	1749.3855	1782.6154
3068.8894	3129.5028	3154.5581
3173.0188	3173.3074	3213.4605

i52 – i72

C	0.964065	0.124394	0.459343
C	1.818069	-0.682845	-0.256969
C	-0.888746	0.069187	0.071830
C	-1.998468	-0.611980	-0.038076
C	0.032886	1.152066	-0.155345
H	1.014294	0.132904	1.542111
H	1.843028	-0.656366	-1.340403
H	2.431208	-1.423814	0.239564
H	-2.884984	-0.190805	-0.520897
H	-2.100587	-1.623592	0.347766
H	0.245562	1.404702	-1.197144
H	-0.115359	2.052038	0.444310

Frequencies

-570.8508	130.7543	206.8098
373.1573	387.8011	502.0007
526.2023	742.5581	855.9296
876.2615	899.1055	933.2541
964.5891	1020.3409	1066.0585
1175.3361	1191.7891	1267.2713
1406.5646	1432.0024	1455.6320
1516.0748	1798.8479	3032.8400
3036.5972	3096.7781	3132.9541
3138.9956	3170.2709	3232.0379

i50 – p28

C	0.603082	0.140950	0.049832
C	1.880707	-0.589726	-0.125734
C	-0.843367	0.053698	-0.008520
C	-1.982190	-0.635440	0.002485
C	-0.094863	1.264223	-0.124844
H	1.012574	0.481746	2.082816
H	1.974862	-1.400702	0.597962
H	2.740676	0.075460	-0.033452
H	1.887632	-1.039492	-1.125618
H	-2.937900	-0.135125	-0.091904
H	-1.981290	-1.713051	0.107169
H	-0.076763	2.328937	-0.296285

Frequencies

-555.1200	169.1407	200.1299
243.9273	332.1956	423.7000
443.6346	514.8370	693.9460
707.8857	774.1597	783.0910
849.5996	989.2110	1033.3097
1052.0069	1095.4777	1183.4211
1403.4244	1449.7350	1472.4543
1486.6723	1616.1363	1843.7335
3022.1256	3088.8848	3121.8277
3140.6499	3224.2846	3246.4693

i55 – i60

C	1.094633	-0.384493	0.111038
C	2.270481	0.177385	-0.150503
C	-0.277007	-0.151649	0.267022
C	-1.557475	-0.614512	-0.301951
C	-1.365632	0.854175	0.102368
H	0.436327	-0.838384	1.158722
H	2.339736	1.054272	-0.795418
H	3.202895	-0.237659	0.213848
H	-1.589139	-0.858552	-1.360273
H	-2.231392	-1.204099	0.312840
H	-1.895820	1.199792	0.983031
H	-1.252611	1.599194	-0.680592

Frequencies

-1991.3430	149.2316	181.1084
349.6639	440.8848	593.9037
668.3599	768.7621	823.5696
846.0306	934.3505	958.3374
982.1365	1026.4971	1053.4866
1070.5880	1089.9276	1163.2395
1322.1841	1452.0314	1454.7029
1494.6540	1712.5878	2143.4309
3070.6522	3090.3470	3098.2073
3166.3504	3184.3800	3186.4028

i55 – p14

C	1.032505	-0.200377	0.185111
C	2.194079	-0.157571	-0.149082
C	-0.344611	-0.151040	0.575786
C	-1.427357	-0.634594	-0.380137
C	-1.291925	0.830804	-0.103990
H	2.603121	1.927378	-0.319760
H	3.203977	-0.313654	-0.440056
H	-0.524723	-0.332528	1.630078
H	-1.099541	-1.004896	-1.342903
H	-2.260415	-1.171728	0.056385
H	-2.029734	1.312033	0.526083
H	-0.868829	1.460066	-0.875950

Frequencies

-381.0079	48.9971	171.6990
206.0823	297.8740	507.8507
531.9394	673.0667	716.5168
758.8904	815.1295	819.7298
885.0926	963.0674	1056.9373
1078.5631	1111.3437	1138.0040
1201.2391	1212.8914	1380.5067
1469.0102	1502.2858	2173.6427
3131.5637	3135.7461	3144.8335
3215.0592	3230.0538	3467.6677

i55 – i63

C	1.088937	-0.380194	0.288919
C	2.086155	0.290401	-0.201871
C	-0.356758	-0.430251	0.518794
C	-1.304429	-0.383976	-0.669592
C	-1.192206	0.809280	0.230171
H	2.338920	1.222582	-0.715424
H	2.134908	-1.000786	-0.134918
H	-0.678497	-1.045045	1.351663
H	-0.855852	-0.322804	-1.653587
H	-2.198309	-0.993772	-0.614069
H	-2.006927	1.029058	0.909546
H	-0.664443	1.679211	-0.141737

Frequencies

-1990.6271	109.0528	184.8977
246.6016	376.0747	538.6035
651.4547	754.5116	806.1063
827.1578	852.6196	891.3988
939.1575	1048.7199	1074.8756
1114.8431	1123.2619	1199.1252
1210.4427	1362.0756	1466.7710
1497.6117	1827.7061	2327.3986
3017.4505	3123.7654	3127.1655
3149.3211	3203.5192	3218.3661

i22 – i63

C	1.148286	-0.539344	0.135977
C	1.928220	0.441104	-0.210767
C	-0.315248	-0.465334	0.458864
C	-1.327193	-0.294098	-0.662748
C	-1.088378	0.817681	0.323859
H	1.558886	-1.557151	0.191257
H	2.567324	1.243773	-0.493305
H	-0.618095	-1.135899	1.257287
H	-0.930721	-0.173740	-1.663749
H	-2.253929	-0.852936	-0.603180
H	-1.855481	1.027497	1.059570
H	-0.542103	1.688411	-0.018994

Frequencies

-687.3554	80.2421	246.6429
328.2672	558.7835	632.4403
762.0381	773.1061	812.4896
830.7314	920.0079	972.7063
1048.2402	1076.1370	1105.1937
1123.0096	1197.3836	1216.6538
1269.0159	1383.3908	1464.4850
1500.9466	1659.4585	2977.6303
3119.7704	3123.6328	3134.4862
3199.2452	3213.8556	3437.5653

i58 – i59

C	1.055095	-0.657647	0.000002
C	2.002630	0.492183	0.000001
H	1.243760	-1.311894	-0.867433
H	1.243757	-1.311889	0.867442
H	1.639909	1.510962	0.000053
H	3.070581	0.315859	-0.000051
C	-0.382725	-0.275699	0.000001
C	-1.340408	0.892996	-0.000005
C	-1.636374	-0.588698	0.000002
H	-1.485739	1.474533	-0.913015
H	-1.485741	1.474541	0.912999
H	-2.415844	-1.330926	0.000001

Frequencies

-81.2647	115.3367	203.4994
295.6133	444.8026	494.3115
640.5989	709.4451	873.2634
904.1768	961.1464	1009.6067
1061.6118	1064.1943	1097.7701
1107.5757	1175.5802	1181.3714
1336.1274	1436.7461	1454.7160
1525.0090	1849.7309	2944.6116
2945.2024	3017.7873	3077.0481
3148.8130	3257.8137	3267.7983

i46 – i66

C	-0.607591	-0.821645	-0.098317
C	-1.831014	-0.072409	0.103248
C	0.545689	0.009761	-0.036273
C	1.869423	-0.459899	0.087201
C	0.206589	1.383169	-0.177774
H	-0.566287	-1.878426	-0.339340
H	-1.345301	1.027534	-0.260837
H	-2.053440	0.212409	1.135180
H	-2.732197	-0.439671	-0.391020
H	2.080516	-1.520178	0.158768
H	2.708729	0.223056	0.094327
H	0.809403	2.141409	0.334419

Frequencies

-1594.8049	223.4466	318.2100
377.0164	390.1539	551.1930
563.3923	628.9720	689.7584
710.5872	782.4442	895.0968
940.7417	976.4189	1027.9506
1040.8743	1199.6437	1258.6798
1335.9267	1354.4686	1429.4609
1485.2072	1496.8017	1772.9763
3041.7237	3062.7213	3100.6720
3141.7039	3172.1776	3239.9971

i14 – i50

C	0.780663	0.192624	0.513538
C	1.841708	-0.602876	-0.191184
C	-0.949969	0.221824	-0.086838
C	-2.003193	-0.630766	-0.033196
C	-0.069595	1.172219	-0.173224
H	0.792627	0.185309	1.600764
H	1.940012	-1.610265	0.226905
H	2.824976	-0.120024	-0.095527
H	1.625182	-0.691838	-1.258873
H	-2.883967	-0.383533	0.548176
H	-1.954452	-1.608812	-0.495887
H	0.057929	2.111015	-0.700139

Frequencies

-644.3830	119.6069	136.5212
249.2352	311.6215	396.1651
417.3275	634.1398	722.5510
792.0145	884.2439	960.0357
1006.9575	1031.4238	1084.6297
1142.6522	1225.9825	1371.2494
1404.8033	1438.9349	1480.1939
1488.7839	1875.2781	2982.3876
3040.5903	3086.8229	3118.5783
3133.4363	3156.1134	3219.8279

i52 – i54

C	0.836765	-0.462115	-0.258133
C	2.052838	-0.189263	0.144529
H	2.379142	0.762253	0.562374
H	2.826434	-0.952867	0.064648
C	-0.572231	-0.038931	-0.448722
C	-0.594928	1.314186	0.142185
C	-1.609773	-0.855797	0.252178
H	-0.785657	0.000423	-1.522196
H	-0.443034	1.415234	1.208626
H	-0.612711	2.209215	-0.469189
H	-2.641569	-0.761446	-0.062043
H	-1.398639	-1.281288	1.225558

Frequencies

-409.0133	138.9874	210.3382
259.4117	312.2617	407.7623
457.9478	556.3992	574.8189
634.8524	768.4012	902.9263
910.8509	978.4010	1023.5135
1113.2669	1134.5271	1274.0312
1303.8003	1426.8317	1443.3145
1457.2989	1742.5886	3031.5454
3064.7563	3119.2187	3133.1216
3139.7429	3249.0718	3253.0165

i42 – i69

C	1.015757	0.766513	0.133300
C	-0.436380	0.837609	-0.409955
C	-1.412336	-0.000045	0.352194
C	-0.436332	-0.837565	-0.409968
C	1.015806	-0.766504	0.133268
H	1.089562	1.250198	1.111568
H	1.741270	1.237698	-0.529938
H	-0.385766	0.000014	-1.396883
H	-1.316135	-0.000054	1.435348
H	-2.438994	-0.000058	0.005392
H	1.089646	-1.250243	1.111504
H	1.741325	-1.237607	-0.530021

Frequencies

-1303.8987	230.0640	377.1766
415.6965	633.6685	735.7594
745.5228	868.1121	904.1991
973.9426	1000.1710	1065.1226
1074.4068	1128.3665	1170.3553
1215.5792	1230.5630	1254.6575
1255.9059	1324.8866	1466.1964
1476.8889	1494.3221	2203.8007
3038.6146	3046.1748	3095.5276
3108.0934	3111.1163	3186.3576

i4 – i78

C	-1.056290	-0.045858	0.252493
C	0.033485	0.842743	-0.022923
C	1.863330	-0.839289	-0.037204
C	1.433061	0.431797	-0.057883
C	-2.276338	-0.377554	-0.133511
H	-0.432285	0.682263	1.189253
H	-0.210323	1.830856	-0.416665
H	2.920957	-1.073262	-0.026879
H	1.167587	-1.670897	-0.025094
H	2.155930	1.242162	-0.091478
H	-2.589743	-0.246332	-1.171937
H	-2.995608	-0.835822	0.536970

Frequencies

-1910.4716	131.5237	223.9092
254.3979	319.2566	537.7467
596.5167	678.1261	850.3283
867.3238	893.9475	910.0534
1002.1327	1014.3581	1029.9191
1086.7409	1148.5107	1317.9972
1329.9723	1438.6224	1443.9912
1637.0649	1700.8491	2107.5468
3051.6270	3079.0598	3137.6391
3149.5032	3170.3823	3227.2500

i47 – i50

C	-0.667483	-0.483122	0.358065
C	-1.890249	0.155949	-0.212264
H	-0.794920	-1.441370	0.851138
H	-1.676130	1.128482	-0.657876
H	-2.651859	0.286052	0.566363
H	-2.346980	-0.477347	-0.984364
C	0.666811	-0.032381	0.132913
C	1.078392	1.303721	0.047986
C	1.435642	-1.117398	-0.316674
H	0.430324	2.116996	0.351612
H	2.081847	1.535601	-0.284688
H	1.219037	-2.109027	0.097663

Frequencies

-91.8999	92.4608	261.2330
373.5944	436.0775	492.5040
556.4647	643.7994	728.1136
756.7622	831.5413	875.9922
985.6476	1009.0111	1056.5731
1112.3157	1270.2336	1365.5234
1398.5212	1421.7517	1472.1392
1483.2859	1494.9099	2995.9566
3034.9255	3060.1296	3108.1441
3144.4247	3164.6970	3247.6770

i3 – i72

C 1.244896 -0.408971 -0.048780
C 2.453422 0.162794 -0.146695
C -1.282353 -0.261710 0.112274
C -2.519899 0.071588 -0.227925
C 0.019252 0.311032 0.269354
H 1.136075 -1.475965 -0.228310
H 2.595286 1.227268 0.009182
H 3.331786 -0.418986 -0.396516
H -2.705364 0.874854 -0.944406
H -3.388120 -0.470874 0.130061
H 0.101886 1.386248 0.450501
H -0.563455 -0.370940 1.230122

Frequencies

-1861.5061	134.9403	179.9150
257.5103	378.6433	468.3024
581.8199	686.4474	845.1498
867.6243	897.9569	910.9718
1000.0660	1012.8424	1077.8644
1117.9487	1185.3595	1267.8542
1315.1788	1431.7012	1460.7424
1652.9565	1669.4671	2095.8594
3051.6456	3057.8660	3134.5607
3141.8800	3174.0744	3224.2916

i10 – i77

C	1.187874	-0.373355	-0.204204
C	2.155264	0.533975	-0.116751
C	-1.330730	-0.336938	-0.221420
C	-2.255869	0.568420	-0.161950
C	-0.062335	-0.384329	0.633540
H	1.278522	-1.177372	-0.933113
H	2.102442	1.355152	0.591719
H	3.035565	0.488946	-0.748024
H	-1.417321	-1.167088	-0.935851
H	-3.011661	1.315917	-0.109213
H	-0.059036	0.450107	1.337615
H	-0.093739	-1.312304	1.221577

Frequencies

-693.4680	78.9160	117.2852
284.7739	417.5198	435.2875
630.0448	657.2603	753.0552
923.8296	935.8206	947.9466
977.7535	1031.1755	1106.3105
1221.3445	1267.9921	1309.7135
1327.2838	1450.5190	1472.9590
1667.8926	1707.4129	2979.5363
2992.6925	3083.2308	3118.7688
3129.0536	3209.5494	3438.0097

i72 – i78

C	1.128985	0.206615	-0.361059
C	-0.015760	0.900550	0.260039
C	-1.803918	-0.869013	0.064068
C	-1.375884	0.365889	-0.169716
C	2.169078	-0.506620	-0.011473
H	0.043135	1.969626	0.030690
H	0.080984	0.820578	1.356557
H	-2.784891	-1.197624	-0.259358
H	-1.187276	-1.600044	0.578363
H	-2.019522	1.062442	-0.699778
H	2.377209	-0.737026	1.038588
H	2.875361	-0.902483	-0.736213

Frequencies

-132.3355	101.6481	253.4774
322.6678	418.3018	536.8049
658.3617	865.5746	883.5025
890.5589	941.9656	954.6482
1019.7488	1040.3766	1108.5871
1218.0807	1318.6778	1333.4129
1412.8270	1442.8152	1455.2751
1704.1687	1734.7783	2935.0911
3025.8450	3043.2184	3127.9833
3146.6097	3146.9707	3213.2475

i72 – i77

C 1.216017 -0.307256 -0.315619
C 2.236755 0.496726 -0.040982
C -1.285276 -0.193753 -0.152347
C -2.401058 0.458037 -0.156134
C 0.001008 -0.481070 0.560068
H 1.223167 -0.897193 -1.229319
H 2.257530 1.106988 0.856862
H 3.090336 0.574908 -0.704673
H -3.026983 1.168443 0.386701
H -2.177715 -0.445568 -1.047290
H 0.068191 0.171430 1.441723
H -0.039201 -1.515112 0.926083

Frequencies

-2104.4208	69.4566	123.0677
179.5453	290.2638	397.9880
419.3193	609.6745	636.0357
826.6905	892.7463	915.9859
948.9339	955.3099	1030.6987
1119.1497	1221.8712	1287.6507
1323.6738	1445.4776	1457.1408
1709.8645	1844.4594	2350.9335
2983.1789	3025.4946	3052.7533
3125.5190	3137.2847	3210.9770

i54 – i55

C	1.069765	-0.553208	-0.001401
C	2.042163	0.325003	0.000860
H	1.858344	1.404558	0.003211
H	3.087687	0.027509	0.000525
C	-0.372848	-0.690360	-0.001979
C	-1.245644	0.311877	-0.748851
C	-1.245726	0.307520	0.750616
H	-0.738847	-1.712807	-0.005026
H	-0.732784	1.119066	-1.257476
H	-2.113830	-0.073865	-1.270040
H	-2.114005	-0.081176	1.269444
H	-0.732828	1.111722	1.263891

Frequencies

-152.8472	179.0943	269.0194
476.1079	558.5900	756.0531
808.5797	817.5817	854.0793
870.9345	933.5683	1001.1433
1049.2996	1071.4948	1107.3696
1112.0441	1200.4950	1208.0265
1362.0312	1419.4300	1469.8595
1500.2859	1739.7216	3021.5497
3122.5153	3123.7689	3127.6901
3137.1250	3203.3329	3219.2291

i31 – i48

C	0.988141	-0.549655	-0.034532
C	2.304920	0.198744	-0.019631
C	-0.195531	0.034308	0.072293
C	-2.158707	-0.378627	-0.025274
C	-1.351891	0.760342	0.098665
H	1.054411	-1.633340	-0.128530
H	2.153801	1.275344	0.074183
H	2.866572	0.011455	-0.942976
H	2.935475	-0.130774	0.813459
H	-2.907458	-0.485564	-0.813106
H	-2.068742	-1.205800	0.667380
H	-1.555654	1.778005	-0.219535

Frequencies

-839.5182	67.3925	134.7159
197.1665	360.2935	443.2361
630.4440	678.3597	748.1272
831.8938	857.4731	973.0471
1027.7476	1056.2368	1078.1141
1225.8756	1311.6710	1365.8032
1397.4297	1479.7925	1480.9130
1491.3623	1722.2543	3001.9588
3048.3093	3060.1787	3083.7505
3107.3517	3131.1278	3192.9800

i31 – i49

C 1.073084 -0.619359 -0.006934
C 2.088427 0.494167 -0.042340
C -0.241447 -0.488795 0.090208
C -1.756962 0.824847 0.002570
C -1.602470 -0.568614 0.047699
H 1.474354 -1.637810 -0.036793
H 1.600127 1.468924 -0.086096
H 2.745767 0.396473 -0.913026
H 2.731667 0.472875 0.846445
H -2.333125 1.325841 -0.778445
H -1.324636 1.461844 0.762906
H -2.257947 -1.341628 -0.342215

Frequencies

-856.7142	73.5312	135.5030
249.7515	326.0981	455.1641
631.7991	672.7543	742.0084
830.6467	853.9613	971.7837
1030.1694	1056.9526	1101.6864
1214.7830	1313.5707	1355.4328
1399.3073	1479.2243	1480.8838
1491.2389	1722.4823	2999.6820
3029.2143	3046.8980	3060.5115
3107.3888	3127.9990	3198.8386

i27 – i60

C 1.072579 -0.543905 0.018910
C 2.083801 0.340310 -0.068465
C -0.293853 -0.200666 0.279196
C -1.655912 -0.574285 -0.128477
C -1.279208 0.875379 -0.025664
H 1.286539 -1.605435 -0.092897
H 1.916242 1.405118 0.047973
H 3.097132 0.014299 -0.268199
H -2.001011 -1.212442 -0.933100
H -1.049686 -0.870907 1.031048
H -1.702057 1.518051 0.741616
H -1.111600 1.370319 -0.979444

Frequencies

-1851.5845	142.1301	204.8737
274.9821	514.0423	648.2639
694.4718	716.4374	866.5836
884.7071	901.5404	983.9884
993.0312	1012.4377	1053.5998
1089.2616	1121.1257	1206.0778
1309.9416	1404.5390	1472.3448
1545.8534	1623.4906	2252.7033
3087.2424	3121.8296	3140.0116
3158.6133	3165.1965	3227.6567

i59 – p26

C 1.052791 -0.528954 -0.063928
C 1.990323 0.448560 -0.104019
C -0.360587 -0.242976 -0.038178
C -1.382521 0.857788 0.099175
C -1.599586 -0.615865 -0.131651
H 1.337136 -1.557654 -0.266182
H 1.152046 -1.112379 1.800383
H 1.713590 1.489780 0.012137
H 3.042337 0.214724 -0.208306
H -1.531876 1.562077 -0.721581
H -1.582692 1.283395 1.084436
H -2.333063 -1.391262 -0.269282

Frequencies

-724.5765	131.4007	198.8390
244.1756	380.6821	414.7743
534.4918	647.1778	667.2626
753.2995	915.2045	937.3810
974.7193	1007.3756	1028.0831
1062.8521	1094.0276	1099.1822
1212.9882	1293.4379	1422.8797
1516.3293	1585.9681	1831.5483
3024.4113	3086.5615	3143.8433
3149.0451	3240.1220	3270.0690

i48 – p16

C	0.938482	-0.616436	-0.057569
C	2.143603	0.271141	0.096509
C	-0.314749	-0.175101	-0.090279
C	-1.744831	-0.363295	-0.192812
C	-1.299793	0.874708	-0.059500
H	1.107767	-1.685526	-0.146942
H	1.854675	1.321792	0.182635
H	2.824956	0.183614	-0.758407
H	2.725101	0.013125	0.989847
H	-2.578717	-1.014884	-0.391261
H	-2.730039	-0.687883	1.943756
H	-1.540009	1.923653	0.002278

Frequencies

-247.6923	138.3090	156.6803
180.2050	206.8053	292.4389
440.8300	510.0241	678.1108
780.5491	782.8747	876.4578
896.9116	950.2098	1053.1398
1069.3989	1089.4874	1115.9811
1357.5804	1415.3001	1482.1280
1499.9504	1572.4869	1833.0742
2999.1896	3034.7536	3082.8015
3143.1544	3241.6620	3282.7212

i49 – p16

C 0.958754 -0.606218 0.113919
C 2.108348 0.353674 -0.028203
C -0.319488 -0.267167 -0.018140
C -1.376026 0.693613 -0.268072
C -1.725861 -0.559335 -0.033638
H 1.191824 -1.642760 0.340207
H 1.756115 1.364438 -0.249151
H 2.789557 0.055719 -0.834456
H 2.708772 0.404831 0.888103
H -1.679283 1.681596 -0.569734
H -2.117481 1.727348 1.773599
H -2.523871 -1.278573 0.056234

Frequencies

-219.0073	130.4663	149.0230
200.4396	205.6424	262.9366
454.1131	511.9230	670.6861
779.3569	783.8639	876.9637
896.7305	951.0620	1053.4480
1060.2340	1102.8105	1115.4633
1357.1624	1416.1946	1482.5918
1499.7746	1575.0873	1833.6993
2999.3759	3034.7447	3084.0124
3140.8984	3240.7706	3282.9692

i48 – p5

C	0.957507	-0.601821	-0.042655
C	2.043137	0.166277	-0.209885
C	-0.385597	-0.083944	-0.020137
C	-1.843094	-0.452038	0.078996
C	-1.216489	0.910707	-0.056833
H	1.069075	-1.672748	0.093837
H	1.955032	1.233411	-0.382744
H	3.034902	-0.267309	-0.255138
H	2.611974	0.764772	1.912975
H	-2.342038	-0.901742	-0.780979
H	-2.257920	-0.759226	1.040386
H	-1.403811	1.967757	-0.125252

Frequencies

-426.1206	69.9842	162.1120
222.5127	246.3862	330.2804
473.3637	662.1642	727.6685
792.6884	945.2726	971.7307
1019.1112	1033.9614	1039.8936
1070.7833	1105.5029	1120.4224
1170.6179	1326.5077	1445.8133
1524.4530	1658.0829	1833.3100
3056.6158	3125.3664	3163.3033
3189.7498	3260.5298	3302.3276

i49 – p26

C	0.982515	-0.634075	-0.061692
C	1.952714	0.281181	-0.201066
C	-0.405020	-0.278986	-0.007657
C	-1.365939	0.879992	-0.051472
C	-1.658287	-0.589954	0.097043
H	1.227791	-1.688124	0.029603
H	1.710457	1.330989	-0.326250
H	2.994022	-0.006820	-0.279570
H	2.479267	0.835955	1.904844
H	-1.565706	1.374520	-1.003524
H	-1.452508	1.536451	0.815830
H	-2.429224	-1.331914	0.208129

Frequencies

-483.1314	131.6926	164.0107
208.8396	262.9535	338.1793
541.2791	680.1883	692.0379
783.9809	952.1295	975.4549
989.3969	1011.0201	1028.8260
1071.5130	1100.4850	1109.0480
1231.3445	1313.3159	1429.8224
1518.8734	1645.0938	1846.1678
3057.0496	3126.8278	3165.2241
3186.2628	3263.4480	3296.6654

i16 – i60

C	1.063394	-0.573053	0.076050
C	2.075411	0.288810	-0.139591
C	-0.305230	-0.197082	0.308076
C	-1.670851	-0.485472	-0.228323
C	-1.217380	0.915129	0.064493
H	1.278499	-1.637315	0.139335
H	1.906951	1.358553	-0.204854
H	3.096192	-0.057711	-0.246213
H	-1.689639	-0.744450	-1.284623
H	-2.441347	-0.970410	0.364334
H	-0.698397	0.529742	1.253381
H	-1.124315	1.831597	-0.505588

Frequencies

-1883.8599	128.3771	211.7486
300.5748	498.1335	650.8468
694.6845	720.5205	875.2792
889.0542	909.0296	994.0207
998.5593	1032.6512	1040.2244
1087.3114	1106.5319	1206.2332
1308.5558	1404.2401	1471.6769
1550.1052	1614.0721	2255.9937
3087.1439	3130.0929	3136.5647
3160.1524	3167.7381	3222.7816

i60 – p26

C 1.111201 -0.581011 -0.063844
C 2.078451 0.324508 0.088874
C -0.278240 -0.222770 -0.085372
C -1.537234 -0.533755 -0.194266
C -1.234633 0.934403 -0.022196
H 1.350346 -1.634066 -0.180913
H 1.841385 1.376342 0.209325
H 3.124025 0.040229 0.097800
H -2.295097 -1.255922 -0.440421
H -2.105700 -1.071570 1.919447
H -1.442558 1.411847 0.935539
H -1.309673 1.604889 -0.879956

Frequencies

-461.2082	134.0597	173.5394
205.2696	265.8362	325.7227
541.9222	674.5487	686.6515
781.6282	946.4775	975.1559
989.4072	1017.1224	1036.8887
1072.2654	1095.7543	1107.9264
1228.8580	1322.0568	1435.9031
1516.8097	1683.8260	1814.3903
3061.7663	3133.5018	3160.2037
3185.9326	3256.2033	3306.4579

i60 – p5

C	1.097832	-0.565665	0.056175
C	2.134820	0.269726	-0.017633
C	-0.273726	-0.135837	-0.048316
C	-1.709066	-0.574504	0.039483
C	-1.156903	0.792010	-0.280710
H	1.262651	-1.626676	0.215696
H	1.990221	1.334740	-0.165042
H	3.153121	-0.089469	0.074020
H	-2.128659	-1.186066	-0.760988
H	-2.162393	-0.749858	1.015443
H	-1.279220	1.824948	1.765828
H	-1.393467	1.778001	-0.638947

Frequencies

-426.9728	88.2841	145.0027
222.9659	235.0569	335.3281
473.9400	650.0093	723.5217
786.4685	935.5816	981.5402
1017.9755	1036.8906	1044.7930
1070.7517	1102.9549	1118.5626
1168.7895	1339.4376	1445.9669
1522.9260	1695.6114	1802.7729
3059.8491	3130.1013	3160.7018
3189.2769	3256.2314	3304.9707

i61 – i62

C	-1.251695	0.798198	-0.000590
C	-1.372946	-0.671833	0.000502
C	-0.042032	0.056881	-0.000046
C	1.248287	-0.025627	-0.759759
C	1.248292	-0.024413	0.759795
H	-1.757809	1.746085	-0.001303
H	-1.684457	-1.183361	-0.911490
H	-1.684456	-1.182036	0.913238
H	1.479040	-0.958141	-1.263664
H	1.594600	0.866135	-1.270536
H	1.594582	0.868181	1.269129
H	1.479063	-0.956102	1.265213

Frequencies

-463.3751	285.7685	306.9357
325.6560	607.6383	791.0573
801.7720	861.6938	883.0110
899.3862	973.6540	1000.1884
1042.7636	1047.5991	1060.1188
1067.1688	1133.2600	1170.1717
1180.5508	1432.5746	1457.8323
1479.2222	1522.3261	3037.6891
3100.6138	3108.2196	3111.2584
3187.4961	3202.3949	3284.1088

i60 – i61

C	-1.135269	-0.660066	-0.480061
C	-1.741135	0.436282	0.295082
C	0.099879	-0.208042	-0.104825
C	1.463464	-0.539001	0.363569
C	1.146301	0.823861	-0.264840
H	-1.433542	-1.699249	-0.393786
H	-2.092419	0.259840	1.305915
H	-1.824253	1.439542	-0.103379
H	1.654750	-0.561253	1.431894
H	2.035146	-1.263836	-0.209267
H	1.500056	1.018196	-1.274242
H	1.160824	1.688559	0.389310

Frequencies

-784.3341	237.6881	274.3946
351.8715	556.8177	592.2428
676.4163	697.7159	753.4779
853.5375	898.6583	994.0773
1027.1838	1034.3646	1065.6616
1071.4309	1124.4224	1168.0206
1267.5028	1434.6847	1441.2028
1457.9234	1604.1210	3094.9497
3098.5753	3117.2647	3156.9817
3172.0650	3185.2580	3220.6316

i62 – p25

C -1.281292 -0.485144 -0.597112
C -1.351319 0.079360 0.579469
C 0.006307 -0.062610 -0.005196
C 1.336285 -0.629700 0.334375
C 1.196232 0.760077 -0.327416
H -1.788787 -0.957178 -1.422054
H -1.941259 0.329783 1.444531
H -2.020575 2.266342 0.049073
H 1.647620 -0.657468 1.374048
H 1.739167 -1.434189 -0.273252
H 1.509333 0.852626 -1.362777
H 1.417220 1.628186 0.285718

Frequencies

-261.1418	135.5661	195.2630
298.0772	350.2915	401.1568
622.9328	636.3795	775.0216
791.0333	854.1458	897.5302
922.4402	956.2348	1006.1412
1034.8377	1041.2874	1066.9487
1146.2999	1166.1967	1415.6095
1454.2554	1504.8634	1679.0423
3097.2876	3100.9205	3172.7033
3187.0576	3239.2178	3281.9115

i46 – i48

C	0.739606	-0.634086	0.065984
C	2.032554	0.100659	-0.023634
C	-0.518883	-0.009709	0.097985
C	-1.772833	-0.671302	-0.018070
C	-0.759905	1.351816	-0.126420
H	0.767437	-1.717562	0.142716
H	2.627085	-0.257250	-0.873413
H	2.647385	-0.063229	0.870817
H	1.870005	1.172439	-0.145202
H	-2.660001	-0.253925	0.439569
H	-1.908587	-1.505652	-0.701193
H	-1.666562	1.800915	0.291639

Frequencies

-258.4809	112.1244	179.7080
248.2513	436.5759	504.2131
547.3374	663.1375	705.4715
764.1514	834.2980	888.7644
1006.0283	1013.5154	1059.6507
1128.0478	1254.8034	1361.0045
1404.0887	1444.9330	1474.7014
1479.5390	1508.3083	2996.8313
3031.0708	3079.1118	3108.8386
3118.9033	3150.4866	3230.4778

i69 – p17

C -1.180849 -0.669620 -0.223319
C 0.310263 -0.578808 -0.603366
C 1.476383 -0.415476 0.323449
C 0.469762 0.636636 -0.040866
C -0.999317 0.721061 0.420455
H -1.385290 -1.481495 0.478263
H -1.858139 -0.749008 -1.072869
H 1.497195 -0.878603 1.313260
H 2.446945 -0.321550 -0.147103
H 1.493143 2.969347 -1.329504
H -1.096124 0.744592 1.508217
H -1.555185 1.553963 -0.008381

Frequencies

-253.7570	55.8680	61.1866
214.5404	302.7262	315.3402
727.2478	729.1507	853.0099
864.6256	946.0982	1005.0463
1022.2991	1080.6010	1131.9838
1178.8921	1205.7540	1206.6292
1230.6352	1243.7854	1454.5374
1469.6846	1482.3995	1555.0051
3077.1021	3083.9345	3089.5090
3146.6896	3160.7746	3204.7453

i23 – i69

C	-0.788753	-0.972682	-0.073557
C	0.508370	-0.322159	-0.584856
C	1.690465	-0.172395	0.279334
C	0.034919	0.957360	-0.257128
C	-1.282923	0.470537	0.304075
H	-0.667763	-1.658840	0.768241
H	-1.382875	-1.461757	-0.847477
H	1.634854	-0.426743	1.333590
H	2.564214	0.365008	-0.067312
H	0.468455	1.944649	-0.365075
H	-1.414821	0.626029	1.378898
H	-2.174534	0.847684	-0.208065

Frequencies

-856.8697	229.0141	344.3194
511.6580	573.6937	698.8600
765.3626	838.2870	855.6423
889.8886	945.0430	956.4248
1036.0789	1066.7118	1158.8119
1173.6718	1201.2430	1237.3387
1276.0570	1353.6167	1440.3272
1454.5148	1482.9615	3023.9294
3049.8559	3067.8920	3100.5707
3110.0683	3182.2702	3223.2449

i52 – i69

C	-1.102676	-0.987913	0.022861
C	0.195315	-0.778410	-0.440899
C	1.326433	-0.296813	0.363186
C	0.472624	0.690024	-0.454981
C	-0.740938	1.173275	0.281094
H	-1.328410	-1.725946	0.793734
H	-1.939533	-0.732448	-0.616553
H	1.278365	-0.278100	1.450547
H	2.320740	-0.461826	-0.040333
H	0.947455	1.262563	-1.245546
H	-0.641185	1.497572	1.314864
H	-1.541974	1.637211	-0.284278

Frequencies

-712.0898	313.0404	388.7739
513.9260	584.0079	722.7342
746.5889	802.1295	891.6088
904.1738	938.3522	985.8203
997.8125	1037.4175	1055.4849
1087.6274	1112.0297	1144.9381
1284.6096	1415.0966	1440.6979
1489.5283	1527.2017	3078.8954
3088.9422	3096.0969	3138.7856
3167.4617	3191.4570	3202.7434

i71 – p35

C	-0.930642	0.261038	0.001300
C	-2.218472	0.007375	-0.001643
C	0.315367	0.527875	0.000584
C	1.419275	1.298593	-0.002482
C	1.113255	-1.668443	0.003317
H	-2.768216	-0.117846	-0.929392
H	-2.780242	-0.078012	0.923429
H	1.929732	1.544436	-0.928213
H	1.901699	1.590552	0.924895
H	0.182879	-2.198622	0.153707
H	1.798763	-1.615250	0.839043
H	1.542687	-1.683886	-0.989931

Frequencies

-486.0436	33.8149	84.4261
154.3585	231.3428	247.2474
370.3355	473.0153	511.7482
516.7609	683.7283	780.0350
834.1560	858.4949	891.8915
1017.1228	1038.2740	1389.9372
1418.0205	1418.5143	1458.6286
1579.5618	2124.0531	3094.0266
3114.3772	3116.9073	3189.5954
3196.8514	3256.5004	3265.0002

i66 – p33

C	2.137029	0.064243	-0.332088
C	1.228741	-0.388858	0.496665
C	-1.485471	-1.148559	-0.201221
C	-1.030613	0.083227	-0.002067
C	-1.021188	1.390881	0.090232
H	1.886108	0.718474	-1.163787
H	3.194369	-0.188505	-0.222181
H	1.268808	-1.052995	1.349791
H	-2.067945	-1.656100	0.561547
H	-1.183365	-1.728068	-1.066977
H	-1.870028	1.955293	-0.287288
H	-0.198935	1.946294	0.519767

Frequencies

-436.1275	51.8144	97.0727
165.7788	187.3616	316.5746
329.7266	392.3433	783.4428
807.0453	814.6022	876.7672
890.7226	933.5420	1002.9391
1020.9169	1055.0364	1088.8859
1389.3541	1426.5554	1470.7328
1637.4432	1925.8488	3050.6566
3118.1448	3122.0136	3143.8716
3198.6443	3210.3581	3221.6311

i47 – i51

C	-0.667496	-0.483000	-0.358149
C	-1.890193	0.156065	0.212326
C	0.666842	-0.032400	-0.132964
C	1.078595	1.303635	-0.047968
C	1.435349	-1.117586	0.316735
H	-0.795047	-1.441078	-0.851519
H	-1.675820	1.128096	0.658910
H	-2.347546	-0.477754	0.983621
H	-2.651425	0.287255	-0.566503
H	0.430626	2.116997	-0.351576
H	2.082066	1.535384	0.284757
H	1.218563	-2.109187	-0.097573

Frequencies

-92.0859	92.3297	261.2155
373.5514	436.0425	492.5318
556.4835	643.8088	728.1727
756.7835	831.5347	876.0079
985.6605	1008.9980	1056.5642
1112.3158	1270.2358	1365.5316
1398.5190	1421.7688	1472.1350
1483.2860	1494.9086	2995.9679
3034.8685	3060.1407	3108.1475
3144.4097	3164.7191	3247.6634

i70 – p12

C	-0.452789	-0.095968	-0.040793
C	-1.916994	0.106876	-0.040938
C	1.599708	-0.149983	-0.083623
C	0.393753	-1.102242	0.180717
C	0.765625	0.865630	-0.307613
H	-2.440494	-0.822701	0.192346
H	-2.261058	0.467040	-1.016977
H	-2.203197	0.864792	0.696960
H	2.674480	-0.269907	-0.093500
H	0.284962	-2.145887	0.441468
H	0.877227	1.902551	-0.592113
H	0.732261	2.258230	2.125320

Frequencies

-304.2264	57.8764	103.5502
204.6341	240.4084	311.5955
546.1202	595.2437	645.1740
744.1661	773.7984	871.8025
897.8851	1003.6399	1046.8526
1072.5646	1175.2069	1176.1627
1265.3569	1408.1767	1471.4473
1487.3846	1538.9318	1722.5595
3030.8568	3086.3777	3133.4510
3226.1186	3247.1749	3263.9418

i60 – i64

C	-1.149543	-0.607420	-0.073535
C	-1.832815	0.549704	0.108509
C	0.222881	-0.583293	-0.435578
C	1.428201	-0.572938	0.278036
C	0.993791	0.973845	-0.095618
H	-1.592039	-1.606781	-0.091476
H	-0.144057	1.232504	-0.247453
H	-2.812344	0.537334	0.588867
H	1.464914	-0.772921	1.352762
H	2.356210	-0.801214	-0.241645
H	1.609867	1.350683	-0.902674
H	1.142355	1.501011	0.850737

Frequencies

-705.9078	187.3930	285.9422
319.4797	503.9211	556.6976
632.8879	655.8428	701.3533
881.3680	916.9308	918.0686
951.8675	1046.7827	1087.8999
1143.1987	1150.3607	1293.0212
1399.5328	1420.4764	1450.8688
1498.4662	1529.4144	1931.8529
3027.0126	3044.9704	3067.7477
3111.6528	3127.5488	3193.8876

i68 – p30

C -0.451308 0.130670 -0.002625
C -1.270465 -1.132411 0.100971
C -0.988387 1.355801 -0.021801
C 2.169957 -0.046519 0.190145
C 0.981299 -0.032304 -0.068598
H -0.990403 -1.702832 0.991677
H -1.091865 -1.776697 -0.764796
H -2.335310 -0.901002 0.153796
H -0.373980 2.243425 -0.103112
H -2.061828 1.491513 0.044327
H 3.227681 -0.121643 0.266648
H 0.979136 -0.884190 -1.777098

Frequencies

-733.6522	93.7942	177.8918
234.6960	309.3471	397.5157
480.2107	549.7609	573.0878
634.7180	680.9287	741.3463
778.1327	935.2023	964.2899
1030.7067	1070.6449	1277.4465
1408.3359	1435.3600	1476.4113
1495.8690	1678.0403	2103.5279
3027.5592	3080.4315	3114.8104
3143.8154	3234.3544	3461.9669

i50 – i65

C	0.623526	0.108402	0.381601
C	1.809688	-0.618127	-0.157225
C	-0.800702	0.070967	0.156188
C	-1.858588	-0.695652	-0.069249
C	-0.164082	1.339289	-0.099749
H	0.617637	1.264932	0.935497
H	2.046254	-1.497568	0.446963
H	2.692825	0.026394	-0.175456
H	1.613170	-0.955435	-1.183929
H	-2.777658	-0.279544	-0.463682
H	-1.832443	-1.758317	0.140132
H	-0.018836	1.970263	-0.968923

Frequencies

-1831.4879	160.0262	194.7533
274.8326	376.0016	498.6186
642.9094	661.6805	729.7321
804.2748	836.3572	930.7497
992.9328	998.9306	1061.0733
1086.8214	1157.6748	1334.8561
1403.2827	1463.5557	1470.9960
1489.3775	1825.4029	2252.5169
2992.0334	3063.8863	3089.9089
3138.2568	3166.8505	3221.8877

i52 – i66

C	0.748876	-0.000491	0.489243
C	1.760365	-0.599603	-0.267037
C	-0.666830	0.019899	0.113170
C	-1.669281	-0.831486	-0.031979
C	-0.289070	1.381270	-0.209073
H	0.988292	0.344636	1.490850
H	1.546962	-1.043695	-1.231614
H	2.790662	-0.569372	0.063710
H	-2.622588	-0.510956	-0.437857
H	-1.565059	-1.871364	0.256817
H	-0.075301	1.660268	-1.233606
H	-0.367321	2.172955	0.525755

Frequencies

-553.4084	147.2366	310.3703
321.7607	450.5944	492.0404
639.2342	689.4875	718.4953
768.8430	853.3667	921.6037
932.4257	958.6351	1022.0341
1074.0522	1171.6213	1229.7675
1370.7090	1423.6451	1461.8365
1485.8357	1799.7156	3128.9831
3131.4933	3139.8730	3143.9113
3217.7787	3231.7993	3239.0803

i55 – i56

C 1.025404 -0.374044 -0.057448
C 2.249382 0.090396 -0.089882
C -0.279916 -0.111147 0.507590
C -1.541570 -0.627005 -0.179137
C -1.249671 0.840029 -0.192445
H 2.528547 1.028068 0.401971
H 3.051205 -0.427419 -0.610715
H -0.318239 -0.113757 1.594367
H -1.400231 -1.182227 -1.098145
H -2.336134 -0.993882 0.459147
H -1.837845 1.494436 0.439781
H -0.909081 1.285414 -1.118471

Frequencies

-106.6473	204.2624	298.6047
420.4119	572.5518	756.6217
802.1924	811.8616	848.4565
887.9355	944.3286	1005.9346
1048.4454	1071.8870	1102.2085
1121.1504	1200.9970	1206.0822
1338.0215	1423.9657	1466.5150
1496.6422	1746.9351	3022.6554
3110.8065	3125.7252	3130.2723
3135.4217	3208.0875	3223.1459

i56 – p27

C -1.060828 -0.000016 -0.051501
C -2.364649 0.000005 -0.073053
C 0.227668 -0.000008 0.102358
C 1.484335 0.761614 -0.104823
C 1.484350 -0.761602 -0.104835
H -2.940956 0.000002 0.848565
H -2.919652 0.000018 -1.006334
H 0.187160 -0.000025 2.146692
H 1.603283 1.279580 -1.050451
H 1.920786 1.263312 0.751574
H 1.920812 -1.263304 0.751554
H 1.603309 -1.279549 -1.050471

Frequencies

-522.7637	182.7645	200.9105
292.5556	390.8713	468.9564
536.0151	565.5549	659.5325
776.2230	851.0658	927.0713
932.4084	1000.8813	1004.5161
1050.0530	1075.4689	1078.3851
1172.7627	1357.1072	1451.9749
1461.4070	1525.5031	2050.3531
3107.4674	3113.1803	3113.2444
3179.9081	3191.6470	3203.5443

i73 – p33

C	1.559101	0.020745	0.564551
C	2.349405	-0.477747	-0.354772
H	1.601972	0.009783	1.646482
H	2.134859	-0.388540	-1.417836
H	3.268894	-1.010564	-0.101070
C	-1.418040	0.210915	-0.076135
C	-2.302612	-0.737205	0.023132
C	-0.421905	1.081313	-0.130734
H	-3.345078	-0.580921	-0.241979
H	-2.028857	-1.729786	0.376097
H	0.067337	1.295613	-1.074773
H	-0.294819	1.816287	0.656829

Frequencies

-327.9283	22.9875	107.8199
169.6419	250.3638	339.2289
367.4767	379.4073	794.5197
850.1649	872.0135	872.8810
881.0343	934.8126	999.3580
1031.5405	1060.3622	1091.2476
1397.7565	1420.2789	1466.4312
1640.5715	1970.8349	3050.8367
3091.1607	3122.8526	3134.2764
3159.8259	3197.6003	3199.2879

i65 – i71

C	-0.548085	0.032063	-0.049205
C	-1.845540	-0.694864	0.022663
C	0.727748	-0.180868	0.005642
C	2.027616	-0.587809	0.020917
C	-0.114597	1.437174	-0.019296
H	-1.689581	-1.773941	0.072017
H	-2.460390	-0.466422	-0.854395
H	-2.413775	-0.379397	0.903897
H	2.648669	-0.433289	0.895680
H	2.500365	-0.974116	-0.875204
H	0.067278	1.990793	-0.934874
H	-0.135418	2.002194	0.908552

Frequencies

-613.0317	142.2569	148.9800
217.5080	227.6962	387.0282
427.8505	644.4050	672.2896
748.8384	790.9052	953.6876
989.0216	1019.7992	1085.2261
1155.6251	1286.2206	1403.2753
1443.5432	1469.9160	1477.2527
1486.3586	1953.5569	3017.7204
3066.6181	3088.2659	3110.2806
3126.6888	3185.3866	3211.5082

i74 – i75

C	-1.340393	0.394787	-0.122632
C	-2.107770	-0.653949	0.029648
H	-1.777465	-1.536598	0.586779
H	-3.109979	-0.703169	-0.388788
C	1.111176	0.105675	-0.455570
C	2.084341	-0.550526	0.166937
C	0.014722	0.877536	0.242016
H	1.064449	0.102060	-1.541800
H	2.156051	-0.573955	1.250195
H	2.847607	-1.087593	-0.384860
H	0.101194	1.942240	-0.014507
H	0.145689	0.815874	1.330585

Frequencies

-125.1940	92.9678	248.3051
343.9002	413.2132	533.3675
647.6009	868.8819	889.3459
900.6713	942.0881	946.8429
1015.0439	1033.7354	1116.9831
1220.8198	1297.2570	1323.7173
1411.0244	1447.5176	1461.5147
1703.4408	1733.9701	2987.4066
3015.1355	3027.8825	3125.2710
3140.5983	3142.2162	3209.7931

i53 – i55

C	0.836739	-0.462126	0.258172
C	2.052806	-0.189303	-0.144535
C	-0.572260	-0.038892	0.448718
C	-1.609775	-0.855799	-0.252177
C	-0.594870	1.314215	-0.142201
H	2.379118	0.762183	-0.562438
H	2.826391	-0.952915	-0.064626
H	-0.785706	0.000481	1.522188
H	-1.398579	-1.281411	-1.225490
H	-2.641591	-0.761398	0.061965
H	-0.612498	2.209245	0.469177
H	-0.442983	1.415248	-1.208644

Frequencies

-408.9476	138.9993	210.3578
259.3440	312.2556	407.7817
457.9203	556.3860	574.8288
634.8585	768.3934	902.9292
910.8549	978.4022	1023.4939
1113.2636	1134.5416	1274.0331
1303.7957	1426.8314	1443.3144
1457.2988	1742.5732	3031.5342
3064.7634	3119.2259	3133.1213
3139.7411	3249.0685	3253.0151

i50 – p32

C	0.305418	0.630177	0.639286
C	2.182844	-0.689935	-0.240403
C	-0.883430	0.042311	0.051463
C	-1.784526	-0.932842	-0.042051
C	-0.327251	1.295712	-0.333514
H	0.920515	0.731776	1.516621
H	2.499365	-1.171900	0.675882
H	2.808879	0.092022	-0.649242
H	1.535981	-1.241108	-0.908555
H	-2.577979	-0.888354	-0.777623
H	-1.753132	-1.787774	0.621496
H	-0.391955	2.192800	-0.927262

Frequencies

-366.3699	47.5227	93.6431
190.5475	358.7608	404.3740
422.0295	467.4418	621.1263
710.6017	732.0517	770.6013
813.5730	836.1168	883.6167
1015.9049	1059.9683	1126.0778
1409.0255	1415.8009	1441.8655
1487.4430	1803.8577	3092.6137
3140.5835	3224.1866	3240.9121
3257.7333	3270.1865	3274.2169

i66 – i67

C	0.695342	-0.876469	-0.000094
C	1.807585	-0.146477	0.000119
C	-0.525720	-0.056022	-0.000033
C	-0.109024	1.394795	-0.000042
C	-1.778433	-0.520484	0.000060
H	0.657173	-1.962853	-0.000267
H	1.200005	1.106925	0.000271
H	2.861593	-0.391406	0.000145
H	-0.320952	1.959455	0.906981
H	-0.320284	1.959202	-0.907383
H	-2.635319	0.143248	0.000139
H	-1.980715	-1.586628	0.000055

Frequencies

-1827.2461	124.8427	356.1871
368.4837	568.8788	602.0908
651.7690	681.7763	758.0500
829.7374	902.5960	919.6259
943.6569	985.0882	1028.4223
1039.5013	1218.2933	1238.6962
1302.2741	1424.6835	1448.8056
1597.6792	1665.7123	1737.5146
3080.6006	3130.1533	3142.9045
3156.1473	3211.6601	3213.6108

i51 – p32

C	-0.305418	0.630177	0.639287
C	-2.182843	-0.689936	-0.240404
C	0.883430	0.042311	0.051463
C	1.784526	-0.932842	-0.042051
C	0.327250	1.295712	-0.333514
H	-0.920515	0.731776	1.516622
H	-1.535960	-1.241148	-0.908504
H	-2.808845	0.092017	-0.649302
H	-2.499414	-1.171857	0.675888
H	2.577979	-0.888353	-0.777624
H	1.753133	-1.787773	0.621496
H	0.391954	2.192800	-0.927262

Frequencies

-366.3715	47.5327	93.6441
190.5474	358.7614	404.3748
422.0311	467.4419	621.1259
710.6016	732.0514	770.6015
813.5728	836.1166	883.6169
1015.9048	1059.9683	1126.0780
1409.0262	1415.8011	1441.8653
1487.4426	1803.8575	3092.6133
3140.5834	3224.1864	3240.9122
3257.7324	3270.1868	3274.2170

i42 – i53

C	-0.741233	-1.172957	0.281108
C	0.472553	-0.690223	-0.454806
C	1.326526	0.296621	0.363148
C	0.195495	0.778384	-0.441005
C	-1.102494	0.988016	0.022886
H	-0.641577	-1.497821	1.314713
H	-1.542263	-1.636633	-0.284482
H	0.947120	-1.262875	-1.245444
H	1.278392	0.278212	1.450517
H	2.320897	0.461407	-0.040299
H	-1.328298	1.726348	0.793447
H	-1.939355	0.732315	-0.616447

Frequencies

-712.0968	313.0360	388.7617
514.2665	584.0531	722.8968
746.7294	802.4845	891.6560
904.0793	938.4273	985.8245
997.8517	1037.4673	1055.5175
1087.6344	1111.9946	1144.9377
1284.6682	1415.0097	1440.7240
1489.5083	1527.1408	3078.8721
3088.9542	3096.0720	3138.8230
3167.4621	3191.3442	3202.7070

i75 – p33

C	-1.417699	0.210744	0.076365
C	-2.301572	-0.737833	-0.024740
C	1.559512	0.023430	-0.564243
C	2.347931	-0.479803	0.354118
C	-0.422128	1.081686	0.132639
H	-3.344184	-0.582813	0.240534
H	-2.027020	-1.729566	-0.379471
H	1.604386	0.017636	-1.646138
H	2.131452	-0.395614	1.417197
H	3.267678	-1.011757	0.099541
H	-0.295457	1.818150	-0.653598
H	0.066880	1.294621	1.077106

Frequencies

-328.0112	22.5060	107.7764
169.6110	250.5106	339.2182
367.4842	379.3794	794.5449
850.1629	872.0082	872.8760
881.0564	934.8240	999.3605
1031.5290	1060.3541	1091.2644
1397.7360	1420.2823	1466.4325
1640.5729	1970.8240	3050.8462
3091.1568	3122.8522	3134.2989
3159.8324	3197.5736	3199.2613

i65 – p29

C	-0.636317	0.047452	-0.115324
C	-1.821586	-0.543161	-0.211687
C	0.772512	-0.017425	-0.011492
C	1.895617	-0.712144	0.028021
C	0.118481	1.327209	0.040052
H	-2.355333	-0.841903	1.948773
H	-1.901617	-1.618722	-0.322257
H	-2.734170	0.039312	-0.267245
H	2.855628	-0.221694	0.143548
H	1.885207	-1.793390	-0.055085
H	0.211366	1.983409	-0.822895
H	0.066675	1.841404	0.997741

Frequencies

-480.2512	147.6789	178.1501
237.4148	300.1324	357.8908
426.3493	632.3915	740.1274
801.3669	825.9895	937.9421
941.5637	960.0123	1005.5557
1036.9592	1049.5656	1111.1154
1175.6165	1432.3904	1436.9871
1474.9559	1709.0980	1876.9089
3101.9520	3154.3018	3156.3516
3183.5648	3245.2220	3248.2751

i67 – p30

C	-0.969955	-0.183034	-0.000007
C	-2.131750	0.168582	0.000041
C	0.473017	-0.105694	0.000002
C	1.007614	1.305681	-0.000028
C	1.262255	-1.179221	0.000042
H	-1.261332	-2.113246	-0.000378
H	-3.184498	0.323791	0.000068
H	0.652953	1.847283	-0.880916
H	2.098700	1.307001	-0.000044
H	0.652980	1.847313	0.880853
H	2.340579	-1.067677	0.000053
H	0.853534	-2.182350	0.000066

Frequencies

-779.2434	62.4774	168.3281
253.6983	286.0917	422.1806
544.8838	559.7959	563.7297
668.0662	687.6487	747.8666
790.8396	947.4886	965.5932
1030.0822	1073.2977	1280.4017
1407.5576	1436.9741	1475.5780
1496.6228	1721.4361	2130.7970
3054.5558	3123.4077	3150.1805
3165.9294	3261.3859	3467.8998

i67 – p34

C	-0.781891	-0.046951	0.000021
C	-0.859724	1.422473	0.000099
C	-1.625579	-1.050862	-0.000154
C	2.274040	0.137026	-0.000190
C	1.444155	-0.750878	0.000228
H	-0.361839	1.839664	-0.880583
H	-0.362030	1.839566	0.880934
H	-1.904089	1.763643	0.000002
H	-1.304542	-2.089969	-0.000187
H	-2.706649	-0.888637	-0.000282
H	2.869396	1.017998	-0.000602
H	1.063740	-1.747113	0.000694

Frequencies

-363.7660	31.5097	132.8697
150.0702	239.0398	260.8732
306.3164	532.0964	551.2869
637.6380	755.7449	767.5504
882.4440	908.4070	955.5400
1054.9699	1102.8721	1393.1739
1425.4651	1459.1533	1477.2473
1733.2180	1934.6333	2987.7590
3047.2284	3058.6452	3076.1013
3134.4385	3380.9662	3477.8356

i71 – p30

C	0.920397	0.032494	-0.147664
C	2.124135	-0.078716	-0.164372
C	-0.500620	0.120128	-0.028511
C	-1.102086	1.312259	0.028383
C	-1.244919	-1.189323	0.030026
H	2.653961	-0.048485	1.836520
H	3.161388	-0.170828	-0.383864
H	-2.179679	1.385835	0.123944
H	-0.534883	2.233796	-0.016536
H	-1.069289	-1.770127	-0.879393
H	-2.317452	-1.021316	0.138163
H	-0.895491	-1.789928	0.874001

Frequencies

-633.3737	73.5872	161.6107
191.8368	208.9584	369.5397
406.5662	554.6345	579.8332
690.0515	746.3322	771.4998
790.4698	951.1681	974.7107
1041.1668	1074.5867	1301.8880
1416.6889	1440.4355	1484.2630
1499.2080	1699.8741	2167.9401
3054.2666	3123.1670	3148.4349
3164.4705	3260.1485	3466.3036

i53 – i74

C	0.888762	0.069168	0.071854
C	1.998493	-0.611974	-0.038062
C	-0.964116	0.124432	0.459328
C	-1.818088	-0.682847	-0.256969
C	-0.032866	1.152039	-0.155365
H	2.884982	-0.190801	-0.520937
H	2.100652	-1.623566	0.347824
H	-1.014362	0.132971	1.542096
H	-1.842979	-0.656464	-1.340407
H	-2.431291	-1.423745	0.239589
H	0.115386	2.052015	0.444283
H	-0.245496	1.404675	-1.197173

Frequencies

-570.8008	130.7408	206.7914
373.1290	387.7959	502.0076
526.1992	742.6072	855.9445
876.2733	899.1009	933.2591
964.5878	1020.3352	1066.0617
1175.3392	1191.8009	1267.2778
1406.5721	1432.0004	1455.6319
1516.0824	1798.8604	3032.8300
3036.5889	3096.7715	3132.9429
3138.9953	3170.2675	3232.0366

i51 – i65

C	-0.623530	0.108403	0.381634
C	-1.809650	-0.618149	-0.157232
C	0.800698	0.070983	0.156179
C	1.858584	-0.695636	-0.069250
C	0.164042	1.339282	-0.099762
H	-0.617624	1.264929	0.935531
H	-1.613313	-0.954910	-1.184156
H	-2.692940	0.026176	-0.174927
H	-2.045851	-1.497937	0.446592
H	2.777651	-0.279540	-0.463704
H	1.832442	-1.758293	0.140170
H	0.018771	1.970272	-0.968919

Frequencies

-1831.5277	160.0960	194.7505
274.8467	375.9923	498.6141
642.9215	661.6819	729.7333
804.2809	836.3619	930.7453
992.9159	998.9405	1061.0814
1086.8335	1157.6657	1334.8653
1403.2928	1463.5551	1471.0034
1489.3743	1825.4054	2252.5147
2991.9946	3063.8739	3089.9113
3138.2563	3166.8620	3221.8874

i51 – p28

C	-0.603084	0.140959	0.049841
C	-1.880702	-0.589716	-0.125741
C	0.843364	0.053703	-0.008519
C	1.982183	-0.635443	0.002474
C	0.094866	1.264231	-0.124820
H	-1.012565	0.481560	2.082744
H	-1.887600	-1.039495	-1.125621
H	-2.740674	0.075467	-0.033481
H	-1.974864	-1.400690	0.597958
H	2.937896	-0.135134	-0.091911
H	1.981275	-1.713056	0.107141
H	0.076768	2.328949	-0.296240

Frequencies

-555.3199	169.1643	200.1409
243.9718	332.1992	423.7957
443.6362	514.8404	693.9433
707.8959	774.1629	783.0855
849.6002	989.2163	1033.3143
1052.0093	1095.4797	1183.4245
1403.4287	1449.7352	1472.4545
1486.6737	1616.1329	1843.7328
3022.1157	3088.8776	3121.8275
3140.6505	3224.2858	3246.4680

i14 – i51

C	-0.780683	0.192653	0.513515
C	-1.841705	-0.602881	-0.191188
C	0.949986	0.221830	-0.086855
C	2.003171	-0.630794	-0.033183
C	0.069619	1.172236	-0.173216
H	-0.792634	0.185291	1.600743
H	-1.625852	-0.690756	-1.259098
H	-2.825207	-0.120732	-0.094391
H	-1.939110	-1.610706	0.226078
H	2.883944	-0.383586	0.548201
H	1.954412	-1.608836	-0.495879
H	-0.057874	2.111058	-0.700093

Frequencies

-644.3968	119.8824	136.5588
249.2765	311.6242	396.1446
417.3517	634.1528	722.5548
792.0149	884.2140	960.0488
1006.9574	1031.4229	1084.6609
1142.6605	1225.9812	1371.2744
1404.8076	1438.9351	1480.1967
1488.8092	1875.2870	2982.3984
3040.5420	3086.8509	3118.5632
3133.4372	3156.1103	3219.8281

i53 – p29

C	-1.839185	-0.655629	-0.153028
C	-0.688972	-0.006751	0.077629
C	0.021528	1.309104	-0.080166
C	0.731152	-0.006307	-0.014859
C	1.885006	-0.652823	-0.041856
H	-1.874748	-1.739191	-0.177444
H	-2.775859	-0.118510	-0.251121
H	-0.793367	-0.002494	2.063630
H	-0.063240	1.817980	-1.038443
H	0.098543	1.972474	0.777569
H	2.822888	-0.125859	-0.178695
H	1.928611	-1.729963	0.078181

Frequencies

-702.2332	208.2809	260.5380
310.3000	373.2842	431.8277
449.6890	591.1073	729.8035
745.5496	816.4495	891.9495
918.2328	954.6623	996.0304
1026.5656	1048.1005	1105.1899
1160.7044	1428.8317	1435.4337
1472.7336	1646.5505	1839.7117
3079.6393	3129.1401	3130.0696
3156.3487	3212.7400	3218.6721

i53 – i66

C	-1.760306	-0.599646	-0.267042
C	-0.748921	-0.000315	0.489209
C	0.289210	1.381276	-0.209174
C	0.666831	0.019933	0.113334
C	1.669136	-0.831616	-0.031926
H	-1.546753	-1.044036	-1.231448
H	-2.790650	-0.569320	0.063550
H	-0.988478	0.345072	1.490693
H	0.075739	1.660166	-1.233800
H	0.367196	2.173039	0.525597
H	2.622466	-0.511235	-0.437872
H	1.564773	-1.871478	0.256873

Frequencies

-553.4096	147.3074	310.3660
321.7832	450.6168	492.0604
639.2515	689.4982	718.4870
768.8525	853.3793	921.5869
932.4318	958.6479	1022.0293
1074.0437	1171.6224	1229.7678
1370.7220	1423.6562	1461.8401
1485.8274	1799.6833	3128.9878
3131.4960	3139.8712	3143.9082
3217.7804	3231.8026	3239.0859

i3 – i74

C	-1.282350	0.261692	0.112293
C	-2.519898	-0.071565	-0.227934
C	1.244883	0.408961	-0.048767
C	2.453426	-0.162768	-0.146707
C	0.019259	-0.311059	0.269344
H	-2.705376	-0.874791	-0.944455
H	-3.388110	0.470895	0.130081
H	1.136026	1.475957	-0.228263
H	2.595328	-1.227240	0.009161
H	3.331771	0.419044	-0.396515
H	-0.563444	0.370844	1.230159
H	0.101885	-1.386280	0.450456

Frequencies

-1861.4903	134.9465	179.9112
257.5086	378.6421	468.3008
581.8192	686.4452	845.1512
867.6259	897.9602	910.9726
1000.0684	1012.8410	1077.8645
1117.9481	1185.3833	1267.8523
1315.1784	1431.7004	1460.7472
1652.9577	1669.4743	2095.8368
3051.6566	3057.8736	3134.5581
3141.8779	3174.0672	3224.2905

i4 – i79

C	-1.056260	0.045601	0.252715
C	-2.276133	0.377682	-0.133510
C	0.033537	-0.842824	-0.023104
C	1.433013	-0.431752	-0.057869
C	1.863095	0.839410	-0.037143
H	-2.589153	0.247097	-1.172128
H	-2.995597	0.835606	0.536995
H	-0.432483	-0.683118	1.189115
H	-0.210190	-1.830720	-0.417421
H	2.155996	-1.242021	-0.091307
H	1.167227	1.670914	-0.025181
H	2.920686	1.073543	-0.026609

Frequencies

-1910.6384	131.4994	223.9230
254.4126	319.2680	537.6844
596.5165	678.1336	850.2973
867.3379	894.0182	910.0600
1002.1263	1014.3707	1029.9315
1086.7266	1148.5241	1317.9956
1330.0043	1438.6318	1444.0066
1637.0374	1700.8911	2107.5495
3051.6619	3079.1163	3137.6369
3149.4977	3170.4157	3227.2483

i74 – i79

C	-1.129076	0.206873	-0.361009
C	-2.168907	-0.506802	-0.011559
C	0.015811	0.900615	0.260253
H	-2.376859	-0.737835	1.038395
H	-2.875227	-0.902440	-0.736401
H	-0.043164	1.969731	0.031141
H	-0.080901	0.820343	1.356734
C	1.375679	0.365840	-0.169789
C	1.803933	-0.868961	0.064060
H	2.018865	1.062212	-0.700667
H	1.187893	-1.599975	0.579075
H	2.784753	-1.197427	-0.260017

Frequencies

-132.3410	101.6842	253.5177
322.6397	418.2182	536.7970
658.3971	865.5763	883.5275
890.6113	942.0027	954.6284
1019.7840	1040.2884	1108.6726
1218.0932	1318.6815	1333.4519
1412.8264	1442.8575	1455.2939
1704.2418	1734.7464	2935.2619
3025.8891	3043.2858	3127.9929
3146.4773	3146.8697	3213.2106

i66 – i71

C	-0.823998	-0.302419	-0.150202
C	-2.067158	0.104272	0.058219
C	0.552489	0.150083	-0.013423
C	1.113978	1.359868	-0.009222
C	1.143235	-1.236957	0.059522
H	-2.282081	1.130676	0.357611
H	-2.916258	-0.559126	-0.060002
H	2.186997	1.485498	0.081193
H	0.516308	2.259798	-0.104812
H	1.486822	-1.600725	1.026171
H	1.708909	-1.593278	-0.799763
H	-0.211972	-1.571930	-0.169757

Frequencies

-2143.0898	103.2097	237.2795
247.8007	384.2287	437.2761
588.8724	611.9867	744.0994
802.2438	894.8823	911.2791
916.3942	954.6515	1038.9627
1062.9814	1201.5909	1218.6996
1403.1673	1411.3303	1448.1507
1653.5346	1702.6542	1857.1259
3077.7926	3079.5553	3133.7991
3173.5220	3189.8824	3216.6503

i67 – i68

C	0.443811	0.126284	0.065452
C	1.102589	-1.225964	-0.031705
C	1.096475	1.272121	-0.120728
H	0.627910	-1.824429	-0.815992
H	0.988461	-1.786100	0.903006
H	2.167815	-1.135606	-0.254214
H	0.595038	2.230513	-0.049574
H	2.155491	1.284130	-0.356867
C	-1.996306	-0.104668	-0.416787
C	-1.014877	0.116510	0.418299
H	-3.074389	-0.162175	-0.390815
H	-1.250474	0.287974	1.477271

Frequencies

-146.6161	211.1108	263.5307
320.4367	409.2349	543.1060
667.4163	722.4027	740.6217
825.7603	888.8837	930.2338
976.6577	1031.5086	1071.7729
1235.4048	1272.3282	1408.3562
1437.3108	1477.9063	1493.3711
1660.4731	1707.9076	2994.1854
3016.3775	3064.8869	3102.7597
3130.1353	3213.5840	3237.3079

i23 – i66

C	0.559970	-0.920992	0.181461
C	1.669088	-0.172457	-0.254532
C	-0.555722	-0.037457	0.074049
C	0.134552	1.255980	0.167961
C	-1.888352	-0.279554	-0.136682
H	0.600239	-1.883454	0.681265
H	2.674483	-0.345447	0.134356
H	1.658804	0.292596	-1.233666
H	-0.149331	2.105070	-0.456355
H	0.566845	1.517357	1.125017
H	-2.604126	0.530955	-0.202028
H	-2.264132	-1.290199	-0.242134

Frequencies

-808.0678	212.8775	359.5816
486.9683	559.6902	605.9900
638.0336	719.4544	733.4606
786.2795	891.7357	926.3656
947.2115	961.8819	1019.4874
1044.9459	1200.1466	1309.5034
1366.6776	1423.4468	1476.2242
1516.9622	1526.5370	3075.7084
3076.3266	3139.7724	3159.0658
3169.8309	3207.5922	3230.3335

i68 – i70

C -0.394917 0.015815 -0.144888
C -1.831042 -0.296088 0.136211
C 1.723758 -0.174212 0.321109
C 0.711289 -0.894814 -0.206876
C 0.205176 1.291928 -0.106311
H -1.943020 -1.082015 0.889881
H -2.338384 -0.646998 -0.771341
H -2.364352 0.594898 0.476978
H 2.796038 -0.314912 0.436809
H 0.725545 -1.917097 -0.578197
H 0.898236 1.589840 -0.880608
H -0.259651 2.120515 0.430999

Frequencies

-707.7491	75.7404	221.4500
348.8955	500.6217	627.4327
670.2623	755.1952	857.8364
889.1244	914.7817	933.3057
983.4625	1025.6434	1040.7639
1161.9991	1355.6203	1376.5117
1411.5121	1474.8342	1480.8490
1493.0121	1535.9075	3004.2092
3050.3604	3083.2545	3093.2963
3119.5900	3150.8077	3205.9866

i29 – i70

C	0.437762	0.039066	-0.182236
C	1.898832	0.067322	0.110632
C	-1.598633	0.011272	0.148525
C	-0.680367	1.013307	-0.009591
C	-0.564780	-1.037902	-0.013802
H	0.057550	-0.768210	-1.191870
H	2.402634	0.882431	-0.415742
H	2.378799	-0.872206	-0.177792
H	2.067080	0.211302	1.186271
H	-2.679106	-0.026955	0.150665
H	-0.747092	2.080115	-0.175448
H	-0.436745	-2.064865	0.302741

Frequencies

-2039.1794	193.6117	263.6317
317.9013	589.6054	666.2100
693.4778	771.8011	809.5596
931.2492	948.1608	972.1879
1034.2865	1073.2212	1175.6508
1219.9562	1253.0193	1288.8950
1374.9971	1408.9129	1476.5039
1490.3146	1502.9107	1863.9036
2994.6637	3058.7855	3089.5773
3191.4734	3201.7238	3223.1528

i28 – i70

C	-1.939671	-0.020004	0.113217
C	-0.481736	-0.045063	-0.120118
C	1.562989	-0.119057	0.084091
C	0.567766	-1.044072	-0.014538
C	0.591859	1.058314	-0.003478
H	-2.433714	0.933300	0.234525
H	-2.469641	-0.936589	0.332997
H	-1.302900	-0.060805	-1.086624
H	2.640801	-0.172306	0.145405
H	0.547868	-2.127383	-0.008164
H	0.703635	1.713279	-0.873483
H	0.506707	1.669797	0.900306

Frequencies

-1908.8799	225.5844	306.1801
355.7451	455.2559	627.1825
651.9523	682.5954	870.9442
878.0173	909.2700	954.5644
990.4904	1072.8091	1088.1536
1125.3050	1179.8692	1207.5922
1271.0262	1405.1671	1428.7960
1470.9565	1514.9611	2164.3180
3027.6797	3069.7793	3148.5426
3182.0652	3219.3978	3267.4488

i9 – i60

C	1.420124	-0.405629	0.012018
C	1.085630	1.034526	0.057056
C	0.093539	-1.115779	-0.071859
C	-1.164107	-0.681637	0.009630
C	-1.521939	0.711287	-0.020032
H	1.964354	-0.755435	0.893362
H	2.021379	-0.655703	-0.867369
H	-1.223364	1.336513	-0.848135
H	1.035425	1.608368	-0.857815
H	1.020810	1.563990	0.997776
H	-1.947867	-1.422234	0.174783
H	-2.350220	1.067889	0.586519

Frequencies

-505.5938	106.1355	295.1538
349.4050	399.8018	480.2219
633.3446	644.4990	686.9268
786.9896	797.9084	853.9982
1012.7812	1057.3999	1084.1352
1135.9681	1243.8537	1277.7608
1287.5729	1451.5305	1466.9310
1479.6018	1622.1665	3052.6627
3097.3443	3115.4299	3148.7155
3177.1548	3265.3877	3290.2141

i58 – i62

C	-1.262383	0.715067	-0.377729
C	-1.426089	-0.661777	0.188460
C	-0.169263	0.173199	0.171513
C	1.484102	-0.347962	-0.644508
C	1.207324	0.280643	0.677171
H	-1.753377	1.549836	-0.843939
H	-1.506398	-1.520639	-0.480497
H	-1.963604	-0.796078	1.130602
H	1.522599	-1.422546	-0.744586
H	1.702354	0.268181	-1.503862
H	1.571921	1.299590	0.802622
H	1.424366	-0.333366	1.550217

Frequencies

-636.8054	205.2110	242.1495
315.8719	410.1094	565.9135
637.1181	688.7394	813.8757
932.9503	946.7741	1003.2345
1054.0728	1061.1084	1075.3214
1109.0915	1170.8120	1205.8801
1234.3338	1447.3894	1476.5353
1496.3477	1608.1077	3018.2604
3065.9843	3077.4140	3130.5001
3164.8398	3278.2419	3278.9966

i46 – i50

C	-0.619061	-0.506072	-0.315878
C	-1.969091	-0.124850	0.188668
C	0.641402	0.061023	0.053005
C	1.848867	-0.644048	0.143861
C	0.388574	1.427578	-0.034612
H	-0.587966	-1.335816	-1.024777
H	-2.457698	-1.016295	0.607916
H	-2.623910	0.233450	-0.613321
H	-1.903205	0.656334	0.944033
H	2.781742	-0.120674	0.315821
H	1.874508	-1.726638	0.075133
H	1.172383	2.027858	-0.515075

Frequencies

-404.9086	193.9570	227.3874
309.1218	384.7042	447.8523
526.7491	671.1272	736.5198
760.7122	824.3772	859.6622
981.3555	1020.6171	1057.2170
1129.6602	1285.9592	1386.3885
1403.3359	1437.9891	1462.4830
1483.0948	1503.9040	2984.4595
3036.1431	3037.6749	3093.0101
3127.7070	3135.9945	3229.8445

i2 – i56

C	-0.867160	-0.078342	-0.147915
C	-2.182325	0.029542	-0.079243
C	0.341121	0.411322	0.517314
C	1.522641	0.464365	-0.440562
C	1.136441	-0.839377	0.143823
H	-2.650950	0.803155	0.528532
H	-2.842342	-0.628231	-0.632273
H	0.366429	0.937984	1.463413
H	1.360288	0.677722	-1.492135
H	2.419102	0.916435	-0.025743
H	1.689155	-1.522483	0.776340
H	-0.045987	-1.109645	-0.578639

Frequencies

-2123.1830	160.1660	308.7416
441.3353	533.9185	679.4775
765.2024	793.7429	797.8412
865.5840	900.9735	933.5475
985.6849	1034.9573	1062.6776
1092.6354	1135.5054	1172.0883
1215.1986	1295.8872	1428.4854
1474.7963	1719.4550	1853.0363
3087.5861	3099.8311	3170.9287
3177.2953	3188.0636	3192.7860

i60 – i66

C	-0.955182	-0.592382	-0.054245
C	-2.047700	0.211026	0.027406
C	0.375955	-0.138272	-0.204916
C	1.584927	-0.768364	0.059585
C	0.959507	1.176937	0.049950
H	-1.090980	-1.671686	-0.024109
H	-1.954514	1.290613	-0.009241
H	-3.044883	-0.201479	0.113025
H	1.686006	-1.585260	0.777907
H	2.491416	-0.492892	-0.467397
H	1.571266	1.692331	-0.681324
H	0.836648	1.634706	1.024463

Frequencies

-958.5197	184.8561	229.7031
306.3911	533.4217	568.0904
610.0450	629.3865	684.9607
832.3319	853.1414	885.5946
948.2364	992.8527	1033.9189
1050.5647	1278.2819	1311.5534
1388.6304	1436.8125	1469.6793
1534.2314	1565.3741	3058.8074
3123.0052	3128.5686	3141.2932
3174.8923	3223.9858	3231.5652

i57 – i58

C -1.049611 -0.494876 -0.389920
C -2.050855 0.309033 0.376820
H -1.153780 -1.558905 -0.147155
H -1.265201 -0.426028 -1.471439
H -1.804086 1.294824 0.747018
H -3.069768 -0.045408 0.472058
C 0.359205 -0.065697 -0.170320
C 1.708367 -0.480812 0.365978
C 1.281951 0.837157 -0.237749
H 1.862840 -0.559303 1.444347
H 2.332685 -1.164533 -0.213197
H 1.602973 1.830530 -0.500487

Frequencies

-90.0801	88.9572	196.5157
316.5762	437.4302	457.8677
668.4853	751.9851	853.4412
916.6718	1000.3385	1010.2004
1032.9310	1070.7440	1085.0908
1108.0100	1140.7177	1211.3960
1351.0457	1449.4098	1459.4586
1524.4899	1847.2801	2916.1765
3018.1054	3022.9980	3077.6993
3142.9260	3254.1295	3265.4877

i59 – i62

C	1.262405	0.714870	-0.378088
C	1.426054	-0.661717	0.188759
C	0.169266	0.173290	0.171405
C	-1.207314	0.281024	0.677019
C	-1.484108	-0.348294	-0.644321
H	1.753560	1.549531	-0.844318
H	1.963565	-0.795620	1.130960
H	1.506290	-1.520910	-0.479789
H	-1.424390	-0.332503	1.550402
H	-1.571905	1.300041	0.801915
H	-1.702398	0.267361	-1.504015
H	-1.522539	-1.422935	-0.743803

Frequencies

-636.7972	205.2197	242.1643
315.8692	410.1098	565.9162
637.1055	688.7358	813.8530
932.9344	946.7476	1003.2651
1054.0854	1061.1134	1075.3105
1109.0835	1170.8199	1205.8735
1234.3304	1447.3795	1476.5237
1496.3579	1608.0980	3018.2443
3065.9669	3077.3843	3130.4751
3164.8379	3278.2427	3278.9954

i47 – i49

C	-0.721855	-0.668074	-0.006864
C	-1.983654	0.127033	-0.010676
C	0.574697	-0.123576	-0.094110
C	0.933381	1.245774	0.021494
C	1.813978	-0.768135	-0.053214
H	-0.806036	-1.750357	0.035054
H	-1.805555	1.179236	-0.240710
H	-2.489549	0.074967	0.963132
H	-2.695747	-0.266386	-0.745550
H	0.377786	1.925484	0.662098
H	1.848761	1.596847	-0.429874
H	1.871050	-1.637920	0.616076

Frequencies

-415.9001	99.0787	162.9821
242.1264	432.1988	492.4347
597.3086	669.6698	698.5518
766.7721	834.1147	843.0414
994.5613	1012.7580	1056.8975
1121.6816	1308.5770	1355.5412
1405.7531	1451.4045	1472.4389
1481.9919	1503.3813	2992.6696
3028.8935	3033.5596	3099.0246
3127.1284	3151.8399	3261.4374

i46 – i51

C	0.619045	-0.506102	-0.315839
C	1.969073	-0.124867	0.188661
C	-0.641408	0.061031	0.053019
C	-1.848885	-0.644016	0.143852
C	-0.388516	1.427576	-0.034609
H	0.587943	-1.335835	-1.024752
H	1.903194	0.656273	0.944071
H	2.623825	0.233550	-0.613342
H	2.457760	-1.016331	0.607775
H	-1.874531	-1.726602	0.075075
H	-2.781758	-0.120642	0.315820
H	-1.172286	2.027852	-0.515146

Frequencies

-404.9029	193.9856	227.4403
309.1225	384.7090	447.8525
526.7514	671.1355	736.5217
760.7166	824.3908	859.6771
981.3573	1020.6333	1057.2194
1129.6855	1285.9658	1386.3837
1403.3452	1437.9929	1462.4753
1483.0994	1503.9159	2984.4583
3036.1187	3037.6158	3093.0016
3127.7104	3135.9993	3229.8504

i72 – i73

C -1.111170 0.105677 -0.455570
C -2.084333 -0.550527 0.166937
C -0.014719 0.877542 0.242015
H -1.064445 0.102064 -1.541801
H -2.156040 -0.573957 1.250196
H -2.847598 -1.087597 -0.384859
H -0.145681 0.815878 1.330584
H -0.101194 1.942245 -0.014508
C 1.340398 0.394794 -0.122631
C 2.107753 -0.653959 0.029648
H 3.109966 -0.703196 -0.388775
H 1.777418 -1.536603 0.586768

Frequencies

-125.1910	92.9676	248.3063
343.9064	413.2133	533.3684
647.6013	868.8819	889.3444
900.6718	942.0878	946.8426
1015.0463	1033.7365	1116.9834
1220.8200	1297.2565	1323.7174
1411.0230	1447.5174	1461.5143
1703.4407	1733.9678	2987.4089
3015.1392	3027.8859	3125.2713
3140.6028	3142.2152	3209.7934

i72 - p4

C	1.196913	0.151774	-0.424330
C	2.246533	0.338583	0.366514
C	-1.252168	-0.101501	-0.116298
C	-2.330997	0.435964	-0.029039
C	0.044168	-0.775034	-0.104902
H	1.127498	0.678444	-1.372514
H	2.337328	-0.165402	1.323872
H	3.054195	1.004713	0.085941
H	-2.913423	0.060258	1.919438
H	-3.250290	0.956310	-0.147006
H	0.199928	-1.239859	0.875597
H	0.018068	-1.593180	-0.837004

Frequencies

-478.0087	41.3272	87.3294
177.8809	252.2285	390.9784
409.5842	486.0012	645.3983
660.3918	763.2465	895.0065
924.7482	954.9388	981.4982
1028.9433	1124.6331	1241.8229
1313.1821	1328.9423	1449.8453
1459.6135	1709.7480	2170.4386
3001.1478	3039.6286	3128.9094
3146.8465	3214.7246	3462.9564

i74 – i76

C 1.216686 -0.253936 -0.047883
C 2.507502 -0.127593 -0.211189
H 3.137927 -0.964208 -0.502592
H 3.022104 0.827963 -0.064291
C -1.259751 -0.307718 0.326426
C -2.355199 -0.028267 -0.369996
C 0.005415 0.521087 0.306905
H -1.235890 -1.184414 0.969207
H -2.408379 0.833717 -1.028372
H -3.240208 -0.651178 -0.308593
H 0.154566 0.961735 1.304595
H -0.118044 1.354949 -0.395536

Frequencies

-123.6647	99.8099	197.8730
389.6719	412.4200	466.6280
630.9323	863.0496	879.5991
891.1323	949.1409	959.1281
1028.6471	1030.5318	1109.7429
1229.2601	1289.7177	1323.9850
1412.3512	1442.0914	1453.1994
1708.4621	1741.1314	2968.8495
3021.7381	3025.0830	3126.3132
3136.5738	3139.8992	3211.5699

i76 – p36

C	-1.232585	0.045951	0.173710
C	-2.318939	-0.482668	0.202451
C	1.162579	-0.150036	-0.439622
C	2.314546	-0.302781	0.202014
C	0.039293	0.749455	0.028105
H	-3.193015	-1.060794	0.380273
H	-3.397629	0.538649	-1.246552
H	0.978436	-0.685888	-1.367068
H	2.522117	0.211984	1.135246
H	3.094320	-0.949679	-0.183019
H	-0.103781	1.563739	-0.696594
H	0.310192	1.222459	0.977772

Frequencies

-461.0533	44.1133	86.5877
189.0922	233.1941	401.8854
407.3416	484.9180	645.3629
670.4801	754.6055	899.6689
919.7930	955.1083	982.2134
1030.5387	1125.8970	1242.6220
1313.2420	1329.6268	1450.7387
1459.9818	1709.6814	2170.8142
2991.9099	3050.1631	3128.4903
3147.6252	3214.1718	3462.9070

i78 – p7

C 1.071041 0.157635 -0.151911
C -0.094199 1.025130 -0.042878
C -1.628612 -0.991677 0.045560
C -1.431416 0.320547 0.045216
C 2.071610 -0.520056 -0.143044
H -0.109349 1.713539 -0.898323
H 0.029206 1.667702 0.840614
H -2.627705 -1.405717 0.114332
H -0.803300 -1.692036 -0.020626
H -2.281657 0.994787 0.114786
H 2.973285 -0.052781 1.656387
H 2.888974 -1.174974 -0.324828

Frequencies

-480.4163	51.7977	141.1729
163.3072	239.8037	371.8622
412.8412	567.5641	617.1432
670.0834	760.2268	865.8840
944.8440	963.0836	967.2724
1029.6802	1092.0453	1233.1699
1324.8494	1352.2866	1441.8594
1458.2940	1712.7929	2172.4979
2992.6569	3014.2012	3133.4502
3145.0805	3223.4693	3462.0916

i79 – p7

C -1.071022 0.157514 -0.151875
C -2.071679 -0.520040 -0.143097
C 0.094172 1.025082 -0.042902
C 1.431432 0.320586 0.045199
C 1.628701 -0.991627 0.045597
H -2.973446 -0.052502 1.656535
H -2.889066 -1.174951 -0.324802
H 0.109263 1.713451 -0.898380
H -0.029263 1.667684 0.840563
H 2.281638 0.994876 0.114724
H 0.803425 -1.692034 -0.020542
H 2.627817 -1.405612 0.114366

Frequencies

-479.9065	51.6262	141.1694
163.2999	239.7327	371.8467
412.7634	567.5622	617.1351
670.0934	760.1273	865.8846
944.8462	963.0847	967.2789
1029.6827	1092.0493	1233.1703
1324.8514	1352.2882	1441.8621
1458.2954	1712.7931	2172.5379
2992.6646	3014.2048	3133.4497
3145.0793	3223.4671	3462.1085

i78 – i79

C	1.020138	-0.190161	0.000005
C	2.314251	-0.371529	-0.000014
H	3.020053	0.466004	-0.000003
H	2.759427	-1.363664	-0.000036
C	-0.000698	0.877505	0.000021
C	-1.863911	-0.840093	0.000007
C	-1.442118	0.419222	-0.000025
H	0.156996	1.524820	-0.876197
H	0.156955	1.524753	0.876297
H	-2.921574	-1.077140	-0.000021
H	-1.167773	-1.671981	0.000063
H	-2.170061	1.227540	-0.000078

Frequencies

-128.0717	147.1497	168.1386
331.0343	448.9448	567.8864
569.1467	832.8949	880.9969
923.3154	952.6335	953.2985
999.8507	1033.2590	1099.6304
1207.9735	1313.7808	1333.1009
1414.8025	1434.0801	1447.3256
1709.6735	1746.7958	2965.1534
2989.3341	3021.5367	3128.4029
3135.3945	3139.2147	3217.8783

i72 – i74

C -1.077067 -0.167887 -0.126607
C -2.361980 -0.316510 0.120599
C 1.077067 -0.167887 -0.126607
C 2.361980 -0.316510 0.120599
C 0.000000 0.884255 -0.062501
H 0.000000 -1.049288 -0.344271
H -2.984839 0.528249 0.418194
H -2.855301 -1.278260 0.031309
H 2.984839 0.528249 0.418194
H 2.855301 -1.278260 0.031309
H 0.000000 1.514780 0.833242
H 0.000000 1.541766 -0.940877

Frequencies

-2194.9459	45.8650	182.9660
255.3279	384.3782	489.4688
561.9312	579.3113	850.3092
886.0514	903.5288	904.0271
919.5852	1034.2405	1086.3556
1113.6423	1131.9272	1230.0026
1414.6449	1420.5505	1448.0973
1710.4163	1738.6060	1843.3713
3008.5778	3048.2793	3075.4997
3075.5103	3181.7034	3181.8874

i77 – p37

C 1.332789 -0.402916 -0.168428
C 2.087331 0.715553 -0.049988
C -1.536010 -0.122080 -0.540078
C -2.403612 0.526575 0.047768
C 0.173401 -0.700219 0.611982
H 1.604684 -1.123179 -0.938570
H 1.861151 1.471967 0.694462
H 2.944571 0.891505 -0.688085
H -1.234216 -0.571302 -1.463919
H -2.922562 1.054119 0.814638
H -0.021427 -0.094249 1.488710
H -0.155595 -1.730334 0.685232

Frequencies

-643.0430	28.7996	122.0859
216.3889	276.7409	416.2094
518.5649	614.3284	636.1958
725.0226	773.2965	832.7655
875.8229	939.6179	954.7240
1000.4905	1032.6264	1208.4830
1303.3202	1428.7077	1490.2023
1577.0798	1838.3331	3117.7443
3130.8219	3135.6508	3220.8104
3224.7098	3328.9541	3432.4989

i57 – p31

C	1.647889	-0.712072	0.000131
C	2.358898	0.432703	-0.000106
H	1.439303	-1.245285	-0.919189
H	1.439248	-1.244869	0.919679
H	2.636234	0.928075	0.923510
H	2.636289	0.927656	-0.923931
C	-0.659084	-0.082399	-0.000026
C	-2.108843	-0.496612	-0.000079
C	-1.452137	0.925139	0.000078
H	-2.572429	-0.864640	-0.915449
H	-2.572437	-0.864843	0.915207
H	-1.726546	1.963349	0.000185

Frequencies

-221.4421	26.4219	89.1073
91.7224	220.8592	340.0000
666.8444	667.9819	828.6137
845.8882	905.5572	914.2556
951.6733	1018.3954	1023.9048
1050.9585	1087.8132	1236.4353
1327.5969	1468.8056	1510.4751
1601.3289	1751.8056	3042.5543
3114.0067	3133.8234	3147.1287
3210.1879	3238.4401	3303.0996

i63 – p22

C	-1.632368	-0.594953	-0.042089
C	-2.216577	0.450773	0.165398
C	0.602974	-0.332868	-0.609023
C	1.510081	-0.472100	0.546909
C	1.255510	0.886639	-0.109112
H	-1.490248	-1.648269	-0.121305
H	-2.568852	1.445011	0.300065
H	0.684840	-0.782547	-1.589339
H	1.079279	-0.626616	1.532539
H	2.474810	-0.953928	0.408301
H	2.046111	1.344602	-0.697366
H	0.656344	1.596799	0.454603

Frequencies

-392.3526	39.8706	133.0782
145.8626	268.8889	542.2855
645.1939	692.2523	738.0816
764.1068	788.1570	809.9714
854.4735	945.0335	1028.9694
1065.6558	1086.2302	1113.2309
1163.9777	1253.2187	1455.0767
1483.8287	1933.6264	3083.6222
3087.5771	3150.7136	3162.6526
3191.4452	3389.0649	3479.9497

i45 – i55

C	-1.086984	-0.305414	-0.162579
C	-2.222619	0.249395	0.158444
C	0.217251	-0.477675	-0.496743
C	1.349234	-0.510461	0.492606
C	1.510544	0.852240	-0.061451
H	-2.351269	1.334776	0.165569
H	-3.101308	-0.334032	0.426724
H	0.453834	-0.787991	-1.508800
H	1.035539	-0.569187	1.531902
H	2.137150	-1.226656	0.268878
H	2.171738	1.038663	-0.895888
H	1.049764	1.695914	0.429954

Frequencies

-629.0853	141.8133	189.4241
345.8739	441.3904	562.6878
604.8727	712.5644	811.5503
851.9951	882.7352	888.4331
997.6135	1046.2232	1114.0029
1159.0775	1200.5578	1220.4801
1346.3932	1449.1838	1453.4431
1490.0784	1868.4508	3041.5476
3085.1284	3121.8157	3148.4832
3158.8944	3164.2960	3273.0402

i65 – p28

C	-0.606925	0.071218	-0.076261
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C	-1.887943	-0.653143	0.022852
C	0.828511	0.011097	-0.044926
C	1.978003	-0.648595	0.078298
C	0.052897	1.206856	-0.262589
H	-1.919887	-1.458250	-0.717867
H	-2.741419	0.009157	-0.130680
H	-1.974138	-1.124286	1.007080
H	2.928508	-0.137036	-0.005933
H	1.990337	-1.714883	0.266584
H	0.022353	2.249702	-0.530969
H	-0.493008	2.251000	1.807534

Frequencies

-184.9817	129.2560	141.3105
183.5937	211.8604	298.7078
442.1807	515.3623	700.9576
711.0337	766.6140	779.1889
845.4299	985.0014	1032.8623
1045.3516	1090.3601	1193.5148
1401.1468	1450.0860	1474.9973
1478.9027	1643.4220	1863.1920
3026.3870	3078.1729	3113.6699
3140.2238	3223.2904	3259.4700

PRODUCTS

p17 including H

C	1.055514	0.773597	0.112131
C	-0.399082	0.677415	-0.412077
C	-1.567217	-0.000835	0.251486
C	-0.398739	-0.675158	-0.412202
C	1.055429	-0.774247	0.110820
H	1.116796	1.236602	1.100027
H	1.742761	1.282630	-0.563320
H	-1.698898	-0.001858	1.336979
H	-2.495378	-0.000535	-0.306331
H	1.117140	-1.239360	1.097717
H	1.742150	-1.282115	-0.566023

Frequencies

232.1378	299.7226	321.0509
716.4653	730.5756	830.5503
843.3159	927.3120	997.6101
1014.0198	1064.6582	1125.3238
1165.8373	1188.0135	1192.1451
1222.3167	1227.2205	1455.2667
1460.9780	1474.8241	1538.3533
3043.5783	3052.7374	3057.4514
3107.9396	3122.2911	3174.5231

p18 including r1

C	-0.863149	-0.000255	0.000147
C	0.501565	-0.644902	0.000406
C	0.501199	0.645112	-0.000399
H	-1.461896	-0.000097	0.911917
H	-1.459594	-0.000177	-0.913438
H	1.042377	-1.575439	-0.000667
H	1.041422	1.575985	0.001263

Frequencies

605.8807	786.6104	870.0370
923.3127	1014.7328	1031.7231
1069.0609	1109.9833	1154.0250
1521.0457	1733.1735	3032.0683
3094.5235	3246.7837	3293.9885

p19 including r2

C	0.789350	0.665865	-0.000064
C	-0.789260	-0.665858	0.000012
C	-0.789513	0.665706	0.000082
C	0.789422	-0.665722	0.000018
H	1.551255	1.433100	0.000149
H	-1.551134	-1.432861	-0.000081
H	-1.551738	1.432468	-0.000277
H	1.551625	-1.432656	-0.000079

Frequencies

539.9948	587.3575	601.7365
701.2288	851.7696	883.9145
888.8469	952.8305	1055.7548
1108.7252	1182.9346	1257.0100
1627.5345	1634.0515	3191.4190
3206.8397	3228.5290	3239.3338

p20 including H

C	1.537195	0.000011	0.473275
C	0.521793	-0.778236	-0.312875
C	0.521785	0.778224	-0.312889
C	-1.977839	0.000004	0.173844
C	-0.664134	-0.000008	0.004862
H	1.478955	0.000014	1.559687
H	2.551448	0.000010	0.080970
H	0.699773	-1.445995	-1.143275
H	0.699759	1.445982	-1.143290
H	-2.531359	0.928185	0.244296
H	-2.531379	-0.928165	0.244311

Frequencies

234.2365	344.5349	587.2249
698.2867	706.5560	738.3962
805.8360	839.8632	878.2600
985.5460	997.7140	1030.9245
1034.4146	1112.9649	1150.8836
1215.8184	1221.9401	1282.3894
1456.1479	1516.2098	1819.0335
3076.4996	3143.1732	3157.2291
3206.8683	3216.4759	3227.4940

p21 including H

C	-1.263507	0.000022	0.537054
C	-0.347006	0.761592	-0.405105
C	1.086566	-0.670348	0.098377
C	-0.347012	-0.761838	-0.404715
C	1.086340	0.670479	0.098460
H	-2.319790	0.000017	0.276953
H	-1.053110	0.000533	1.602196
H	-0.728394	1.399218	-1.191558
H	1.768851	-1.420970	0.479593
H	-0.728391	-1.399505	-1.191149
H	1.768544	1.421263	0.479546

Frequencies

424.4863	453.4097	738.0153
783.2125	803.7053	831.6818
860.8022	889.0190	947.0750
961.3585	1030.6132	1038.9125
1040.5472	1085.6107	1107.1401
1200.1762	1219.4183	1290.0445
1308.3606	1475.6617	1601.7960
3088.6417	3166.5615	3176.9022
3185.3218	3193.3810	3202.1917

p22 including r3

C	-0.599110	-0.000215	0.000226
C	0.599109	0.000887	-0.000093
H	-1.661885	-0.000825	-0.000745
H	1.661892	-0.003208	-0.000054

Frequencies

641.7117	707.2153	772.3881
2069.3801	3421.4943	3524.3083

p23 including r2

C	0.735469	0.110223	0.000086
C	-1.659547	-0.371443	-0.000057
C	-0.635848	0.488624	-0.000043
C	1.906556	-0.171716	-0.000032
H	-2.682927	-0.016566	0.000061
H	-1.500620	-1.443220	0.000192
H	-0.832585	1.557992	0.000100
H	2.936361	-0.432338	-0.000074

Frequencies

224.2867	316.4180	557.7143
647.7405	680.3845	703.4961
892.2675	954.7839	1009.9860
1111.4766	1320.9319	1443.5005
1668.4638	2205.6653	3136.5876
3147.5830	3236.4066	3476.2183

p24 including r4

C	0.663422	0.000006	0.000021
C	-0.663514	-0.000020	-0.000122
H	1.234985	-0.922431	0.000012
H	1.234746	0.922528	0.000061
H	-1.234596	0.922630	0.000243
H	-1.234582	-0.922640	0.000292

Frequencies

834.9037	973.0542	973.9308
1066.6751	1238.6866	1379.6577
1472.3233	1691.9537	3120.9179
3136.0676	3192.0523	3220.5232

p25 including H

C	-1.381646	-0.000130	0.650283
C	-1.381530	0.000239	-0.650316
C	-0.047841	0.000055	0.000011
C	1.216918	0.774001	0.000250
C	1.216887	-0.774045	-0.000246
H	-1.938224	-0.000909	1.572815
H	-1.938104	0.000336	-1.572866
H	1.534980	1.271433	-0.911084
H	1.534900	1.270729	0.912000
H	1.534899	-1.271369	0.911162
H	1.534819	-1.270937	-0.911919

Frequencies

296.3039	342.4564	389.2226
612.0420	635.4156	775.6041
791.7045	866.4682	895.8068
924.2113	958.2886	1007.1946
1035.8730	1041.2323	1068.3166
1145.0640	1165.6143	1419.1093
1455.0964	1514.5107	1710.3421
3094.3742	3098.2496	3168.7845
3183.1513	3234.7854	3279.9335

p26 including H

C	1.072620	-0.567465	0.000038
C	2.028337	0.369026	-0.000074
C	-0.329186	-0.261532	-0.000254
C	-1.340117	0.859826	0.000140
C	-1.575532	-0.628093	-0.000102
H	1.341132	-1.621068	0.000564
H	1.777655	1.424006	-0.000363
H	3.079049	0.105327	0.000445
H	-1.507685	1.433702	-0.913355
H	-1.507312	1.433280	0.913981
H	-2.319573	-1.405818	0.000241

Frequencies

154.3150	199.1404	290.5955
536.9667	661.8791	664.7532
762.7102	941.8074	953.3779
976.6528	1003.6049	1025.4875
1061.1745	1098.1850	1098.3421
1215.0004	1315.9591	1434.9939
1516.0940	1658.9325	1831.4768
3024.5605	3085.9443	3135.7712
3144.3381	3229.9792	3269.1571

p27 including H

C	-1.058302	0.000144	0.000172
C	-2.365327	-0.000043	0.000001
C	0.226869	0.000036	-0.000426
C	1.493452	0.762653	0.000105
C	1.493359	-0.762725	0.000103
H	-2.932055	-0.000086	0.926192
H	-2.931652	-0.000069	-0.926438
H	1.781329	1.273154	-0.913692
H	1.780540	1.273482	0.913955
H	1.780373	-1.273601	0.913950
H	1.781163	-1.273267	-0.913695

Frequencies

185.6954	187.5782	368.0694
561.7330	564.5100	651.2278
774.7607	853.0966	925.0419
936.3954	1007.2128	1021.1654
1047.0751	1070.6129	1079.4349
1170.5502	1366.7175	1454.0113
1468.3287	1538.2937	2106.4427
3101.0829	3101.4630	3113.9032
3175.4729	3185.2507	3189.1025

p28 including H

C	0.620624	0.149966	-0.000318
C	1.915250	-0.559424	0.000161
C	-0.819871	0.056128	-0.000374
C	-1.957250	-0.632744	0.000071
C	-0.061396	1.280740	0.000313
H	1.984554	-1.211777	0.876261
H	2.758177	0.134085	0.005336
H	1.989430	-1.204200	-0.881159
H	-2.916128	-0.129504	0.000712
H	-1.953261	-1.715673	0.000105
H	-0.046913	2.359071	-0.000374

Frequencies

135.1370	209.4820	265.7373
441.3254	512.6215	707.5685
711.6622	757.2871	785.4069
847.1494	987.1839	1042.5956
1046.0894	1089.1729	1190.2947
1403.2512	1451.9809	1475.8961
1480.4608	1672.8010	1878.6330
3025.3264	3077.1486	3108.9426
3138.0561	3219.4889	3248.1760

p29 including H

C	0.707530	-0.011918	-0.001161
C	1.867872	-0.651301	0.000478
C	-0.707608	-0.011746	-0.000812
C	-1.867957	-0.651197	0.000433
C	0.000115	1.308539	0.000233
H	1.912429	-1.735131	-0.000008
H	2.809097	-0.112584	0.001884
H	-2.809249	-0.112587	0.002039
H	-1.912428	-1.735032	-0.000382
H	-0.000158	1.901292	-0.913195
H	0.000596	1.899775	0.914639

Frequencies

237.5587	247.8358	327.5110
426.7044	606.8677	730.1638
775.5708	820.8731	913.6171
915.5215	956.5097	1005.2911
1027.7976	1038.8517	1106.2195
1164.5922	1432.9442	1436.1917
1474.4425	1696.7391	1869.9962
3066.8752	3127.9955	3128.6089
3139.3744	3211.2227	3211.5627

p30 including H

C	-1.004075	0.039682	-0.000023
C	-2.202667	-0.079851	-0.000040
C	0.424308	0.121973	0.000002
C	1.167364	-1.194836	0.000087
C	1.046741	1.308301	-0.000048
H	-3.261115	-0.169603	-0.000056
H	0.901453	-1.788033	0.879923
H	2.246492	-1.032930	0.000101
H	0.901489	-1.788125	-0.879698
H	2.129017	1.368606	-0.000029
H	0.492638	2.238473	-0.000109

Frequencies

176.0542	186.9003	268.6311
396.9905	546.3948	571.1248
650.0507	677.8309	743.9201
775.5743	931.9078	964.8473
1031.9442	1071.4830	1284.5910
1410.5281	1435.3005	1478.0144
1495.8336	1675.6068	2201.3420
3028.1446	3080.9802	3112.9291
3143.5745	3233.6641	3476.5419

p31 including r5

C	0.663422	0.000006	0.000021
C	-0.663514	-0.000020	-0.000122
H	1.234985	-0.922431	0.000012
H	1.234746	0.922528	0.000061
H	-1.234596	0.922630	0.000243
H	-1.234582	-0.922640	0.000292

Frequencies

834.9037	973.0542	973.9308
1066.6751	1238.6866	1379.6577
1472.3233	1691.9537	3120.9179
3136.0676	3192.0523	3220.5232

p32 including r2

C	1.019490	0.658632	0.000071
C	-0.263652	-0.000333	-0.000640
C	-1.590917	-0.000076	0.000260
C	1.019866	-0.658432	0.000073
H	1.592765	1.571609	0.000429
H	-2.148303	-0.928231	0.000126
H	-2.147728	0.928428	0.000316
H	1.594543	-1.570549	0.000537

Frequencies

359.0304	427.2792	686.9974
714.1929	767.6010	841.1038
844.1037	912.9016	1019.7216
1060.1267	1115.7996	1453.2831
1602.4224	1831.7810	3141.3245
3224.1986	3233.8654	3275.3713

p33 including r1

C	1.302452	0.000002	-0.000016
C	-0.000002	-0.000073	0.000117
C	-1.302448	0.000028	-0.000019
H	1.866971	0.663127	0.648052
H	1.866901	-0.663016	-0.648258
H	-1.867110	-0.648184	0.662825
H	-1.866772	0.648328	-0.663111

Frequencies

371.7987	371.8106	866.2426
866.2584	885.0895	1017.1692
1017.1764	1109.3233	1422.4951
1479.5973	2052.4143	3117.2859
3121.3263	3192.2676	3192.2929

p34 including r6

C	-0.599110	-0.000215	0.000226
C	0.599109	0.000887	-0.000093
H	-1.661885	-0.000825	-0.000745
H	1.661892	-0.003208	-0.000054

Frequencies

641.7117	707.2153	772.3881
2069.3801	3421.4943	3524.3083

p35 including r2

C	0.632670	-0.000004	-0.000033
C	1.946686	0.000001	0.000020
C	-0.632671	-0.000002	-0.000032
C	-1.946685	0.000000	0.000019
H	2.512982	0.926452	0.000039
H	2.512998	-0.926439	0.000039
H	-2.512977	0.926455	0.000039
H	-2.513001	-0.926437	0.000039

Frequencies

224.4326	229.4170	360.1807
571.3878	776.2276	884.2039
887.5899	903.2857	1021.5792
1042.3730	1407.7303	1465.6286
1682.2850	2204.9874	3113.5285
3116.3399	3189.8096	3190.0654

p36 including H

C	1.338364	0.111812	-0.043717
C	2.399674	-0.441361	-0.145081
C	-1.081490	-0.191863	0.413768
C	-2.193393	-0.313113	-0.301327
C	0.039087	0.772259	0.092273
H	3.338310	-0.929368	-0.240259
H	-0.931447	-0.806970	1.297257
H	-2.365269	0.279877	-1.194540
H	-2.973410	-1.011459	-0.020609
H	0.112779	1.523095	0.890368
H	-0.194414	1.318421	-0.827713

Frequencies

89.1871	187.4077	337.4265
408.6538	475.0295	644.9127
664.5444	680.3927	898.3509
925.9920	953.1322	982.0512
1030.8683	1127.9541	1245.4893
1314.0216	1330.0750	1450.5950
1464.4220	1709.6609	2223.9987
3001.8282	3049.6767	3127.9373
3146.1104	3213.3494	3477.6527

p37 including r7

C -0.599110 -0.000215 0.000226

C 0.599109 0.000887 -0.000093

H -1.661885 -0.000825 -0.000745

H 1.661892 -0.003208 -0.000054

Frequencies

641.7117 707.2153 772.3881

2069.3801 3421.4943 3524.3083

Radicals

r1

C	0.586665	0.029432	-0.000348
C	-0.706546	-0.142672	-0.000013
H	1.282549	-0.806960	0.001029
H	1.038849	1.025354	0.000631
H	-1.602110	0.461046	0.000505

Frequencies

710.0974	818.1174	921.1459
1045.3942	1390.9565	1649.7997
3038.3302	3135.2321	3236.1642

r2

C	-0.000035	-0.000090	0.000016
H	-0.998670	-0.412387	-0.000033
H	0.856880	-0.658119	-0.000033
H	0.142001	1.071048	-0.000033

Frequencies

505.2897	1402.6327	1403.3797
3104.1952	3282.8105	3283.7762

r3

C	-0.000157	0.871035	-0.168152
C	0.768282	-0.363223	0.030465
C	-0.768145	-0.363401	0.030502
H	-0.000558	1.815911	0.355956
H	1.255426	-0.826124	-0.824206
H	1.298172	-0.514318	0.968220
H	-1.298372	-0.515647	0.967887
H	-1.254546	-0.826288	-0.824745

Frequencies

560.3681	764.6115	779.9310
843.9405	928.9093	1023.6201
1059.5045	1082.0588	1096.7628
1157.0004	1261.1077	1454.1850
1483.0063	3079.3548	3080.1938
3142.3260	3155.2717	3209.4172

r4

C	-1.337790	-0.000036	-0.000137
C	1.251310	0.000077	-0.000077
C	-0.115777	0.000017	0.000412
H	-2.399972	0.000257	-0.000456
H	1.806292	-0.930175	-0.000367
H	1.807221	0.929569	-0.000368

Frequencies

351.7867	402.9866	468.4694
637.7994	681.7457	1031.4004
1089.4462	1455.3690	2011.5641
3139.3202	3229.8787	3468.0096

r5

C	-0.272240	0.832103	-0.000019
C	0.832537	-0.168913	-0.000013
C	-0.769850	-0.342844	0.000032
H	1.372890	-0.391750	-0.918342
H	1.372862	-0.391652	0.918414
H	-1.488434	-1.138670	-0.000072

Frequencies

631.3379	644.8185	767.3391
878.9779	1004.7353	1041.3574
1079.2310	1506.2047	1766.5213
3061.1181	3142.4166	3332.2150

r6

C	0.125534	-0.379785	-0.000033
C	-1.270821	0.076070	0.000004
C	1.342941	0.097836	0.000008
H	-1.807363	-0.286741	0.882302
H	-1.807689	-0.287412	-0.881808
H	-1.327268	1.175871	-0.000392
H	2.221110	-0.542458	0.000058
H	1.535283	1.176013	-0.000035

Frequencies

182.4273	315.2824	478.2545
882.4001	897.1193	936.0832
1051.6091	1099.4849	1392.0658
1416.0393	1456.0704	1473.1452
1747.2938	2961.0890	3023.5024
3048.5073	3073.2502	3143.7482

r7

C	0.000221	-0.441639	0.000043
C	1.227264	0.195641	0.000023
C	-1.227500	0.195766	0.000107
H	-0.000208	-1.529907	-0.000094
H	1.295914	1.278163	-0.000061
H	2.154946	-0.362143	-0.000227
H	-1.295986	1.278273	-0.000259
H	-2.154578	-0.362996	-0.000396

Frequencies

429.2335	531.6213	552.7482
786.2945	811.5630	936.5100
1014.1794	1036.9630	1207.5385
1270.3707	1423.2134	1511.1244
1517.1633	3127.8022	3133.8154
3140.2628	3231.8627	3234.8013