Electronic Supporting Information

Directed Gas-Phase Formation of the Propargyl Family of Resonance-Stabilized Radicals in the Reactions of Ground-State Carbon Atoms (C; ^3P_j) with Butene Isomers (C_4H_8): Dimethylpropargyl and Ethylpropargyl

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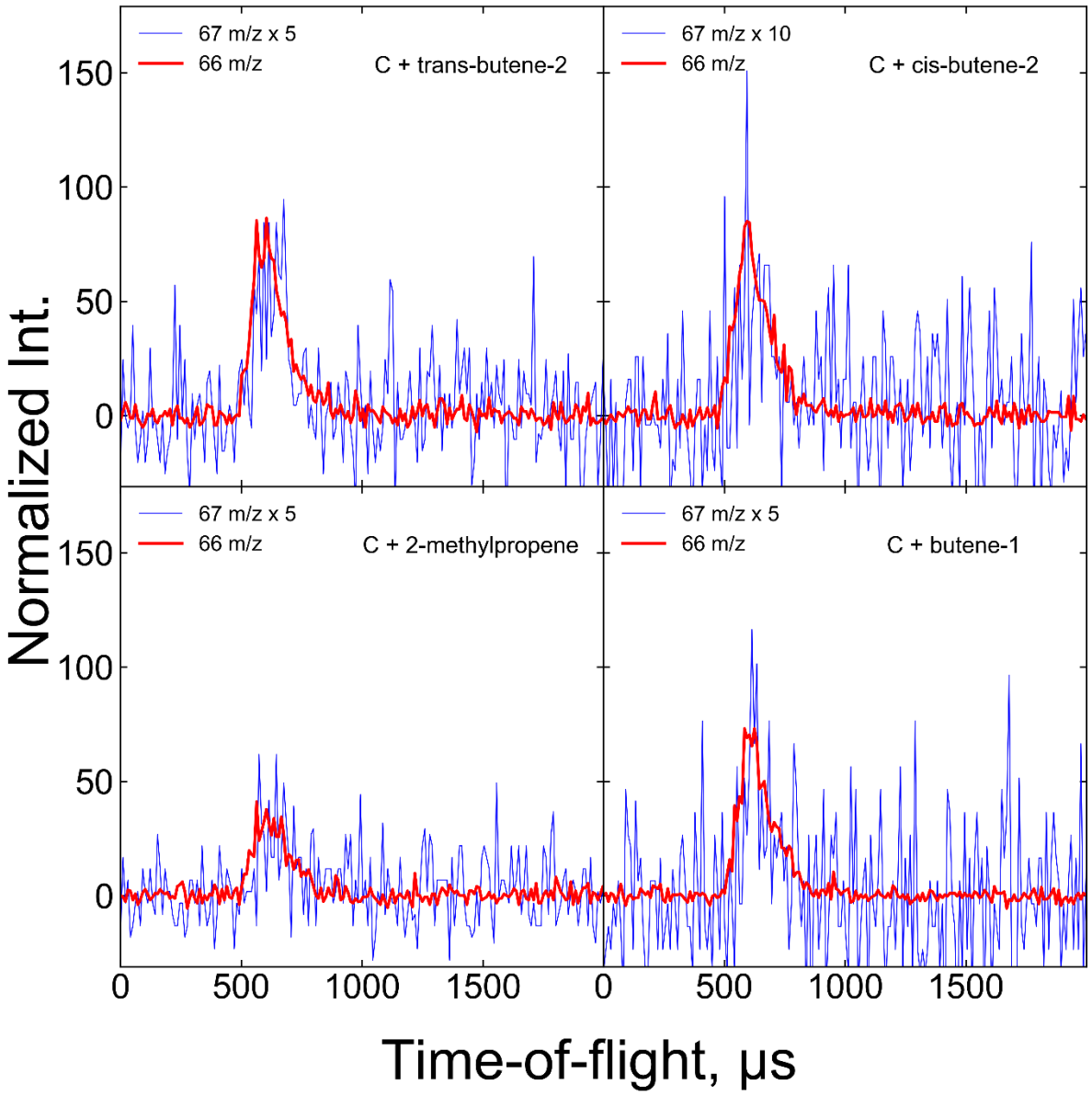

Figure S1. Time-of-flight (TOF) spectra recorded at mass-to-charge ratios *m/z*=66 ($C_5H_6^+$; red lines) and *m/z*=67 ($C_5H_7^+$; blue lines) for the reaction of atomic carbon (C; ^3P_j) with the four butene isomers (C_4H_8): *trans*-2-butene, *cis*-2-butene, isobutene, and 1-butene. The overlapping profiles of the TOF spectra at both mass-to-charge ratios suggest that the signal at *m/z*=66 originates from the fragmentation of the parent C_5H_7 product formed via H-loss channels (*m/z*=67) during electron impact ionization in the detector.

Alternative reaction pathways

C + isobutene

For **i11**, a [1,3]-shift from a methyl group to the non-branching bare carbon atom is also accessible, with an energy comparable to the H/CH_3 loss channels (Figure 10). This pathway produces the triplet 2-methyl-1,3-butadiene (isoprene) **i13**. A less favorable scenario involves two consecutive migrations: first, a [1,4]-H shift from a methyl group to the CH_2 moiety, affording **i12**, followed by a [1,2]-H shift from the new methyl group to the adjacent bare carbon atom in **i12**, also leading to **i13**. H-atom elimination from the methyl group attached to the branching bare carbon atom yields **p5** through a tight exit transition state lying 43 kJ mol^{-1} above the separated products **p5** + H. In turn, isomers **i11–i13** can form product **p8** (3-methyl-buta-1,3-dien-2-yl) via H-atom loss: from **i11**, abstraction from either of the two methyl groups proceeds through a tight exit transition state of 40 kJ mol^{-1}; from **i12**, elimination from the methyl group adjacent to the non-branching bare carbon occurs via a loose exit transition state of 9 kJ mol^{-1}; and from **i13**, loss from the methyl group adjacent to the branching bare carbon proceeds through a tight exit transition state of 22 kJ mol^{-1}.

A [1,3]-H migration from the methyl group to the non-branching bare carbon atom in **i12**, as well as an energetically more favorable by 90 kJ mol^{-1} [1,4]-H shift from the methyl group to the CH_2 moiety in **i13** lead to **i14** – a methyl-substituted trimethylenemethane. Finally, a [1,2]-H shift from a methyl group to the CH group generates an intermediate incorporating four methylene moieties. Intermediates **i13–i15** can reach product **p7** (2-vinylallyl) via an H-atom loss. Unlike 1-vinylallyl from the reactions with 2-butenes, **p7** lies higher in energy than product of the methyl loss channel. 2-Vinylallyl is formed through H-atom loss from the methyl group in **i13** and **i14** via tight and loose exit transition states located 50 and 3 kJ mol^{-1} above **p7** + H, respectively, and from **i15** via H-atom loss from the non-terminal CH_2 group through a tight exit transition state lying 19 kJ mol^{-1} above **p7** + H.

C + 1-butene

1-Butene represents the smallest alkene that exhibits hindered internal rotation about its central C–C single bond. Unlike the other butene isomers, 1-butene lacks a rigid, fixed molecular structure. Instead, it exists as a rapidly interconverting mixture of two distinct rotational conformers at room temperature. The equilibrium is dominated by the twisted, skew (gauche)

conformer, which possesses C_1 symmetry. The minor component is the planar cis conformer, characterized by C_s symmetry.[1,2] Although enthalpically less favorable compared to the [1,4]-H shift from the methyl group, several alternative hydrogen migration pathways exist: a [1,2]-H shift from the CH group to the bare carbon connecting **i17** and **i9**; a [1,3]-H migration from the non-terminal CH_2 group to the bare carbon atom linking **i18** and **i6**; as well as [1,2]-H shifts from the terminal CH_3 group to the adjacent CH moiety, connecting **i6** with **i19** and **i7** with **i20**. In addition, two rotational interconversions—**i6** ↔ **i7** and **i8** ↔ **i9**—proceed through moderate barriers of approximately 60 kJ mol^{-1}. Intermediates **i6** and **i7** lead to the thermodynamically most stable product **p3** in Figures 11, S6 via H-atom loss from the terminal CH_3 group through tight exit transition states located 39 and 41 kJ mol^{-1} above the separated products **p3** + H. Furthermore, **i6** and **i7** also yield **p13** via H-atom abstraction from the CH group adjacent to the terminal CH_2 group through tight exit transition states lying 23 and 21 kJ mol^{-1} above **p13** + H. In contrast, **i8** and **i9** afford the same product **p13** via H-atom loss from the terminal CH_3 group adjacent to the bare carbon atom through loose exit transition states located 11 and 9 kJ mol^{-1} above **p13** + H.

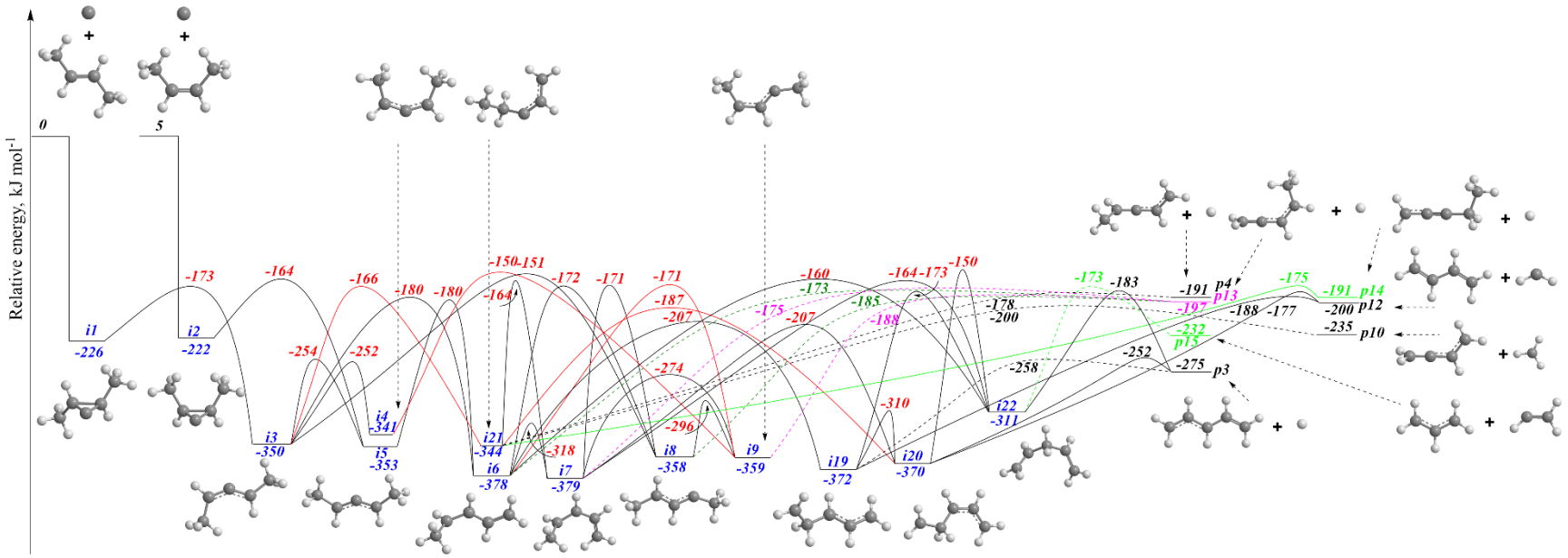

Figure S2. Potential energy surface for the bimolecular reaction of the ground-state atomic carbon (C, ^3P_j) with *cis*-2-butene (C_4H_8, X^1A_1) and *trans*-2-butene (C_4H_8, X^1A_g) leading to acyclic products **p3, p4, p10, p12–p15**. Relative energies were computed at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory.

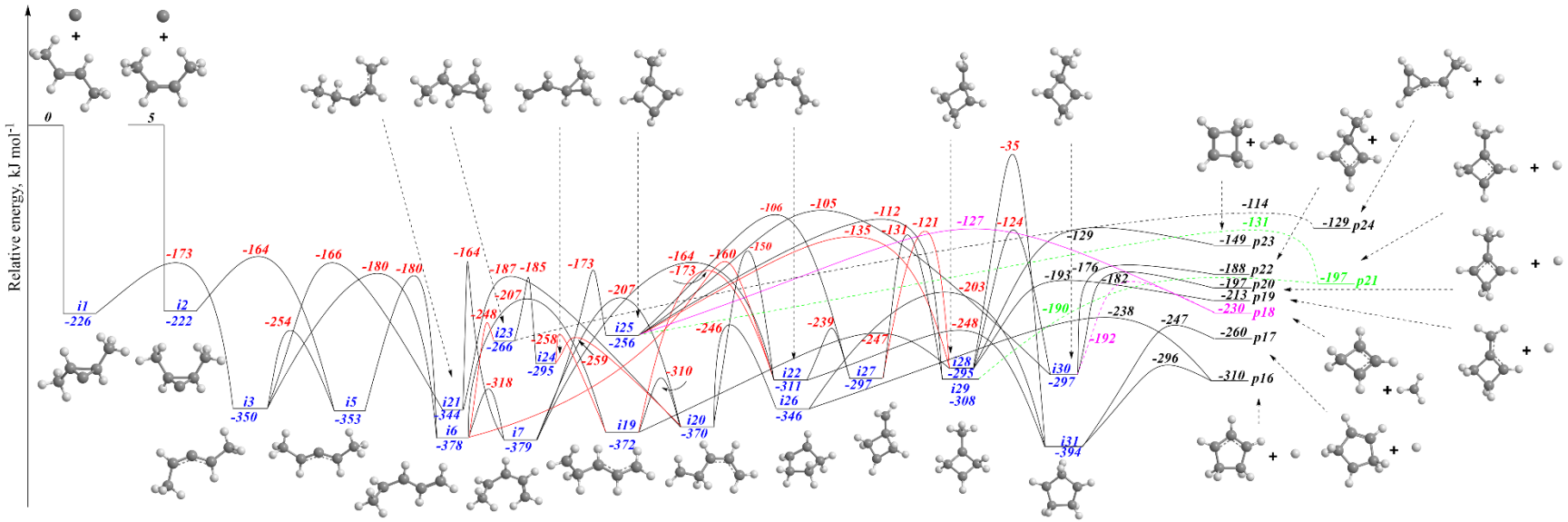

Figure S3. Potential energy surface for the bimolecular reaction of the ground-state atomic carbon (C, ^3P_j) with *cis*-2-butene (C_4H_8, X^1A_1) and *trans*-2-butene (C_4H_8, X^1A_g) leading to 3, 4 and 5-membered ring products **p16–p24**. Relative energies were computed at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory.

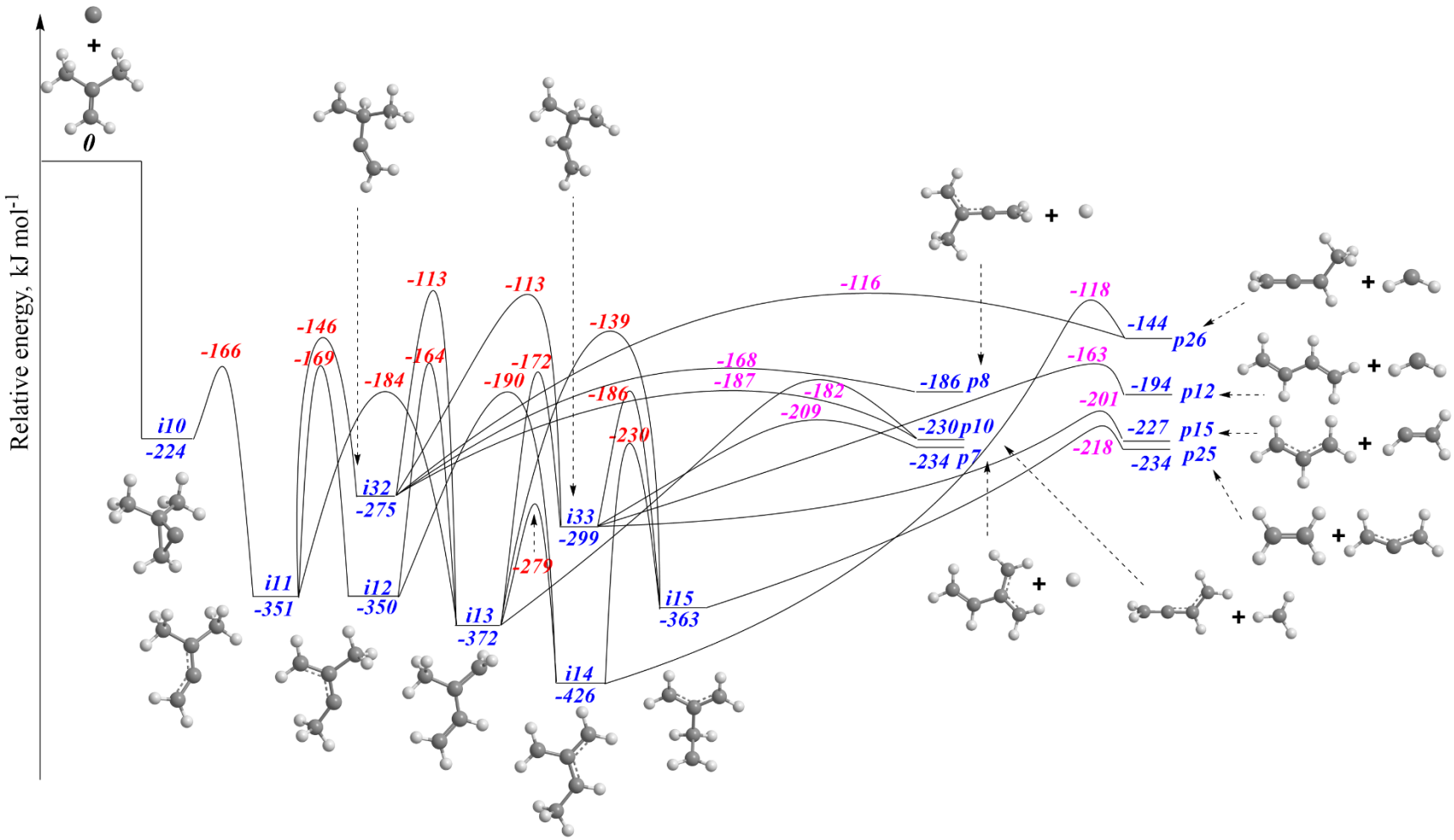

Figure S4. Potential energy surface for the bimolecular reaction of the ground-state atomic carbon (C, ^3P_j) with isobutene (C_4H_8, X^1A_1) leading to acyclic products **p7, p8, p10, p12, p15, p25, p26**. Relative energies were computed at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory.

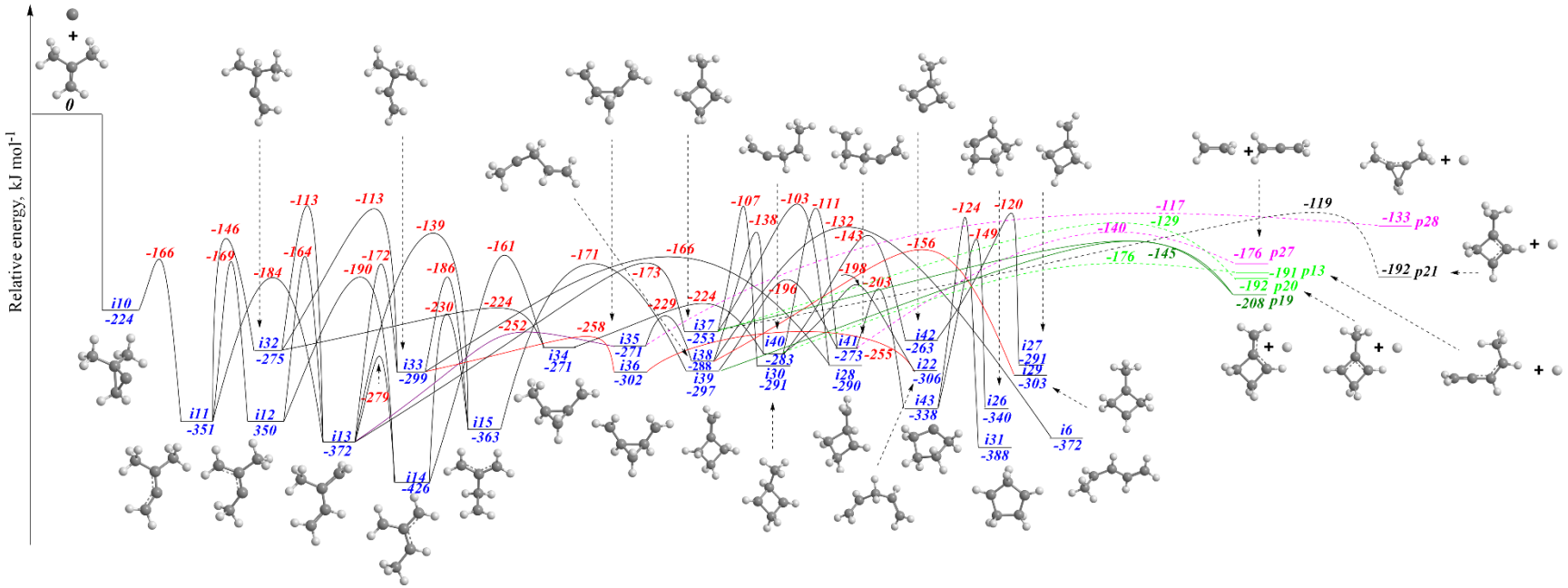

Figure S5. Potential energy surface for the bimolecular reaction of the ground-state atomic carbon (C, ^3P_j) with isobutene (C_4H_8, X^1A_1) leading to acyclic and 3- and 4-membered cyclic products **p13, p19–p21, p27, p28**. Relative energies were computed at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory. The channels terminating at intermediates **i6, i22, i26–i31** are associated with a transition to the potential energy surface for the reactions of the ground-state atomic carbon (C, X^3P_j) with *cis*-2-butene (C_4H_8, X^1A_1) and *trans*-2-butene (C_4H_8, X^1A_g).

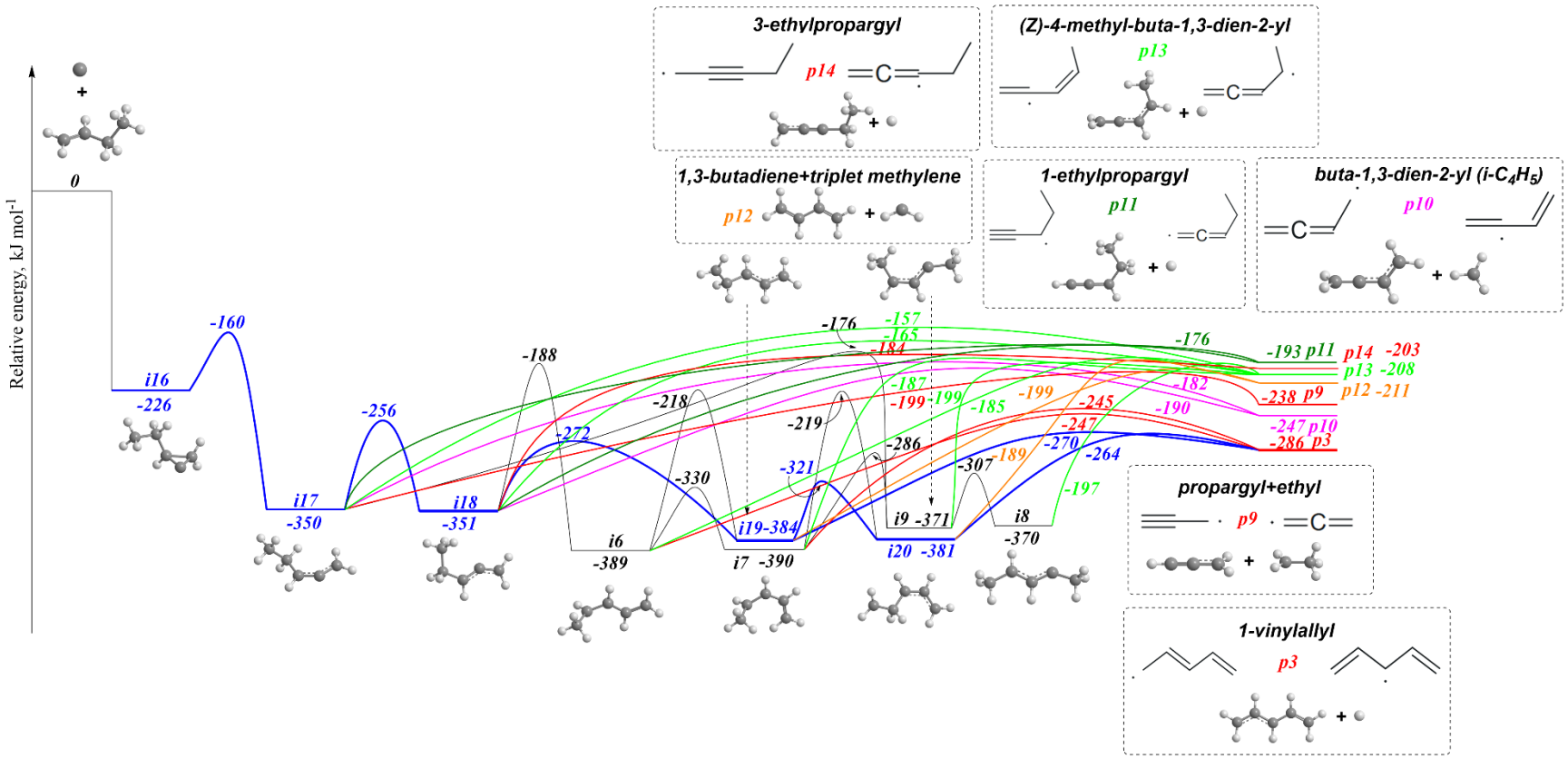

Figure S6. Potential energy surface for the bimolecular reaction of the ground-state atomic carbon (C, X^3P_j) with 1-butene (C_4H_8, X^1A) leading to acyclic products **p3, p9–p14**. Relative energies were computed at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory.

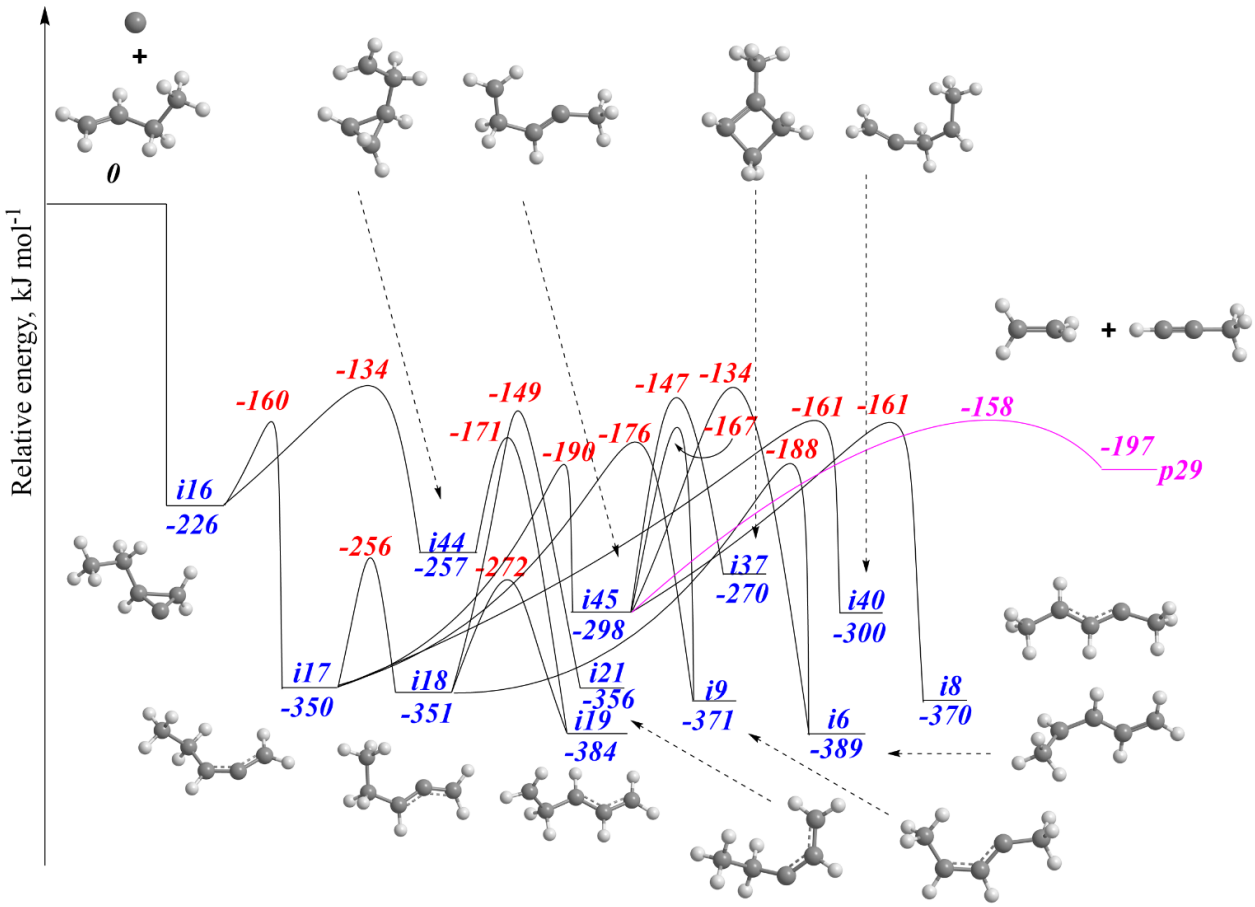

Figure S7. Potential energy surface for the bimolecular reaction of the ground-state atomic carbon (C, ^3P_j) with 1-butene (C_4H_8, X^1A) leading to acyclic product **p29**. Relative energies were computed at the CCSD(T)-F12/cc-pVTZ-f12//ωB97X-D/6-311G(d,p) + ZPE(ωB97X-D/6-311G(d,p)) level of theory. The channels terminating at intermediates **i6, i8, i9, i19, i21, i37, i40** are associated with a transition to the potential energy surface for the reactions of the ground-state atomic carbon (C, ^3P_j) with *cis*-2-butene (C_4H_8, X^1A_1), *trans*-2-butene (C_4H_8, X^1A_g), and isobutene (C_4H_8, X^1A_1).

Table S1. RRKM calculated rate constants (k(E), s^{-1}) of the reaction of the ground-state atomic carbon (C, X^3P_j) with *cis*-2-butene (C_4H_8, X^1A_1) for unimolecular reaction steps at the zero-collision-energy limit and at the experimental collision energy (E_C, kJ mol^{-1})

Step	E_C		Step	E_C		Step	E_C	
	0	28		0	28		0	28
i2 – i5	7.04E+11	1.07E+12	**i7 – i8**	4.95E+07	1.23E+08	**i32 – i13**	1.69E+07	5.20E+07
i5 – i2	9.73E+05	2.34E+06	**i8 – i7**	1.24E+08	2.95E+08	**i32 – i34**	5.43E+10	6.80E+10
i1 – i3	2.87E+12	4.18E+12	**i19 – p3**	1.12E+10	1.71E+10	**i34 – i32**	5.15E+11	6.43E+11
i3 – i1	4.61E+07	1.04E+08	**i20 – p3**	1.07E+10	1.69E+10	**i15 – i33**	1.10E+08	2.34E+08
i4 – p1	1.20E+11	2.53E+11	**i6 – i22**	1.41E+07	3.79E+07	**i33 – i15**	2.77E+08	4.83E+08
i3 – p1	2.86E+10	6.22E+10	**i22 – i6**	3.40E+08	7.54E+08	**i32 – p10**	7.90E+10	1.31E+11
i5 – p4	3.42E+07	9.84E+07	**i7 – i22**	2.11E+07	5.51E+07	**i37 – p19**	4.75E+10	9.94E+10
i3 – p4	1.74E+08	5.13E+08	**i22 – i7**	3.21E+08	6.89E+08	**i37 – p21**	2.39E+09	6.35E+09
i4 – p4	1.39E+08	4.38E+08	**i6 – i9**	3.30E+07	8.15E+07	**i37 – p20**	5.81E+09	1.42E+10
i5 – p2	3.60E+08	8.33E+08	**i9 – i6**	1.19E+08	2.83E+08	**i33 – i36**	2.22E+11	2.61E+11
i3 – p2	2.39E+09	5.47E+09	**i9 – p13**	2.02E+09	4.61E+09	**i36 – i33**	1.10E+12	1.31E+12
i5 – i6	3.25E+07	6.99E+07	**i9 – p2**	7.75E+09	1.78E+10	**i36 – i22**	9.50E+10	1.14E+11
i6 – i5	1.81E+07	4.14E+07	**i7 – i20**	9.92E+08	1.94E+09	**i22 – i36**	6.26E+10	7.65E+10
i3 – i6	1.46E+08	3.13E+08	**i20 – i7**	3.12E+08	5.94E+08	**i39 – p19**	1.22E+09	3.02E+09
i6 – i3	2.47E+07	5.66E+07	**i7 – p3**	1.40E+10	2.47E+10	**i39 – i41**	1.32E+10	2.10E+10
i3 – i4	1.07E+10	1.52E+10	**i7 – p4**	8.60E+07	2.24E+08	**i41 – i39**	3.80E+09	5.45E+09
i4 – i3	1.04E+11	1.44E+11	**i7 – p13**	1.33E+08	3.44E+08	**i38 – i6**	1.49E+08	3.78E+08
i3 – i5	1.43E+10	2.02E+10	**i27 – i29**	2.91E+07	7.87E+07	**i6 – i38**	1.13E+06	3.64E+06
i5 – i3	4.34E+09	6.15E+09	**i29 – i27**	3.53E+07	9.98E+07	**i33 – i32**	2.67E+06	8.67E+06
i3 – i8	5.18E+07	1.42E+08	**i28 – p19**	5.11E+09	8.74E+09	**i32 – i33**	8.92E+07	2.68E+08
i8 – i3	3.48E+07	9.78E+07	**i28 – i37**	2.57E+06	8.64E+06	**i33 – i28**	6.83E+07	1.34E+08
i3 – i21	1.24E+07	2.91E+07	**i37 – i28**	1.80E+08	5.36E+08	**i28 – i33**	2.11E+09	4.11E+09
i21 – i3	6.59E+07	1.53E+08	**i28 – p23**	3.87E+08	1.14E+09	**i35 – i38**	1.35E+11	1.61E+11
i6 – p4	5.44E+07	1.43E+08	**i28 – i30**	5.97E+06	1.66E+07	**i38 – i35**	1.97E+10	2.56E+10
i6 – i7	4.09E+11	4.89E+11	**i30 – i28**	1.05E+07	2.93E+07	**i38 – i29**	7.83E+07	1.59E+08
i7 – i6	6.49E+11	7.79E+11	**i24 – i19**	1.25E+12	1.48E+12	**i29 – i38**	3.01E+08	6.39E+08
i25 – p18	3.23E+09	8.36E+09	**i19 – i24**	1.48E+09	2.19E+09	**i41 – i40**	4.50E+07	1.35E+08
i6 – p3	1.02E+10	1.77E+10	**i24 – i20**	1.34E+12	1.57E+12	**i40 – i41**	1.20E+07	3.74E+07
i6 – p13	1.51E+08	4.00E+08	**i20 – i24**	1.93E+09	2.82E+09	**i41 – p27**	2.52E+09	6.21E+09
i7 – i25	1.16E+07	2.79E+07	**i29 – p21**	2.53E+10	4.72E+10	**i14 – i34**	1.40E+06	4.15E+06
i25 – i7	3.38E+11	5.60E+11	**i23 – i24**	1.09E+10	1.66E+10	**i34 – i14**	1.84E+10	3.52E+10
i6 – i8	2.42E+08	6.02E+08	**i24 – i23**	5.35E+08	9.14E+08	**i34 – i40**	1.55E+12	1.93E+12
i8 – i6	1.07E+08	2.54E+08	**i23 – p24**	1.03E+08	3.42E+08	**i40 – i34**	3.51E+10	4.56E+10
i6 – i19	6.71E+08	1.32E+09	**i30 – p20**	3.26E+09	6.08E+09	**i43 – i41**	2.87E+10	5.08E+10
i19 – i6	2.76E+08	5.33E+08	**i30 – p22**	4.41E+09	8.63E+09	**i41 – i43**	2.43E+09	3.30E+09
i25 – i27	2.08E+08	6.28E+08	**i30 – p18**	2.42E+10	4.18E+10	**i43 – i26**	2.56E+08	6.15E+08
i27 – i25	9.40E+05	3.23E+06	**i30 – i37**	3.74E+06	1.19E+07	**i26 – i43**	1.89E+07	4.50E+07
i27 – i28	1.34E+07	4.00E+07	**i37 – i30**	1.49E+08	4.19E+08	**i43 – i31**	1.35E+07	3.95E+07

i28 – i27	2.93E+07	8.77E+07	**i25 – i30**	1.33E+08	4.10E+08	**i31 – i43**	3.35E+04	1.08E+05
i31 – i28	8.99E-01	1.65E+01	**i30 – i25**	1.16E+06	4.09E+06	**i40 – p13**	1.70E+10	3.18E+10
i28 – i31	3.51E+01	4.79E+02	**i10 – i11**	1.23E+12	1.85E+12	**i40 – i22**	1.83E+10	2.78E+10
i21 – i20	1.34E+09	2.72E+09	**i11 – i10**	7.76E+06	1.80E+07	**i22 – i40**	8.31E+09	1.36E+10
i20 – i21	2.13E+07	4.54E+07	**i11 – p5**	7.10E+09	1.49E+10	**i38 – i40**	9.41E+06	2.19E+07
i21 – i7	3.05E+08	7.30E+08	**i11 – p8**	4.97E+07	1.49E+08	**i40 – i38**	7.61E+06	1.71E+07
i7 – i21	1.54E+07	3.99E+07	**i11 – p6**	5.72E+09	1.36E+10	**i41 – i22**	5.37E+07	1.60E+08
i21 – i18	3.45E+07	1.05E+08	**i11 – i13**	8.01E+08	1.65E+09	**i22 – i41**	6.49E+06	2.18E+07
i18 – i21	4.74E+07	1.42E+08	**i13 – i11**	1.16E+08	2.52E+08	**i42 – i40**	3.38E+09	7.09E+09
i26 – i20	2.40E+11	3.54E+11	**i11 – i12**	2.65E+07	5.97E+07	**i40 – i42**	5.78E+06	1.25E+07
i20 – i26	1.72E+08	2.61E+08	**i12 – i11**	1.20E+07	2.70E+07	**i42 – i27**	1.29E+08	3.14E+08
i31 – i26	5.63E+07	1.12E+08	**i13 – p8**	1.23E+08	3.34E+08	**i27 – i42**	4.32E+05	1.12E+06
i26 – i31	6.69E+09	1.20E+10	**i13 – p10**	2.05E+08	4.80E+08	**i16 – i17**	1.98E+11	3.29E+11
i31 – i22	3.77E+09	6.15E+09	**i13 – p7**	5.51E+08	1.26E+09	**i17 – i16**	7.54E+06	1.99E+07
i22 – i31	1.55E+10	1.98E+10	**i13 – i14**	2.63E+10	3.55E+10	**i17 – p9**	1.02E+10	2.15E+10
i25 – i28	7.07E+08	1.51E+09	**i14 – i13**	5.19E+09	7.96E+09	**i17 – p10**	3.52E+09	8.53E+09
i28 – i25	3.50E+06	8.49E+06	**i13 – i15**	3.88E+06	1.21E+07	**i18 – p10**	5.94E+09	1.36E+10
i19 – i20	5.88E+11	7.13E+11	**i15 – i13**	1.25E+07	3.83E+07	**i17 – p13**	1.22E+08	3.69E+08
i20 – i19	7.13E+11	8.60E+11	**i12 – i13**	4.06E+08	9.73E+08	**i18 – p13**	3.30E+08	9.28E+08
i4 – i9	7.82E+08	2.11E+09	**i13 – i12**	1.30E+08	3.28E+08	**i17 – p11**	3.11E+09	8.04E+09
i9 – i4	4.94E+07	1.40E+08	**i13 – i37**	7.27E+06	1.67E+07	**i18 – p11**	2.35E+09	6.09E+09
i22 – p15	2.22E+09	4.61E+09	**i37 – i13**	1.29E+11	2.06E+11	**i18 – p14**	1.57E+09	3.79E+09
i25 – i29	2.08E+08	5.85E+08	**i35 – i13**	1.41E+12	1.54E+12	**i18 – i6**	4.18E+08	8.90E+08
i29 – i25	2.28E+06	7.64E+06	**i13 – i35**	2.85E+09	4.25E+09	**i6 – i18**	9.66E+06	2.26E+07
i26 – p16	4.40E+11	6.83E+11	**i12 – p5**	1.25E+10	2.57E+10	**i17 – i9**	4.91E+07	1.13E+08
i31 – p17	1.67E+10	2.84E+10	**i12 – p8**	2.95E+09	7.01E+09	**i9 – i17**	5.47E+06	1.33E+07
i31 – p16	1.95E+11	2.67E+11	**i12 – i14**	4.47E+08	8.86E+08	**i18 – i19**	1.19E+11	1.60E+11
i8 – p2	4.48E+09	1.04E+10	**i14 – i12**	2.83E+07	6.68E+07	**i19 – i18**	1.13E+09	1.64E+09
i8 – p13	1.57E+09	3.65E+09	**i13 – i33**	5.09E+07	1.22E+08	**i17 – i45**	7.81E+07	1.61E+08
i22 – p3	7.02E+09	1.37E+10	**i33 – i13**	4.16E+08	7.94E+08	**i45 – i17**	1.38E+08	2.35E+08
i19 – i22	1.85E+07	4.50E+07	**i11 – i32**	9.96E+06	2.75E+07	**i16 – i44**	5.00E+09	1.01E+10
i22 – i19	2.18E+09	4.44E+09	**i32 – i11**	3.95E+08	8.45E+08	**i44 – i16**	5.22E+07	1.19E+08
i22 – i20	2.58E+08	6.39E+08	**i14 – p26**	1.11E+06	5.47E+06	**i17 – i40**	4.12E+07	1.09E+08
i20 – i22	2.66E+06	7.82E+06	**i14 – p7**	3.46E+09	6.93E+09	**i40 – i17**	1.35E+08	3.00E+08
i19 – p12	1.57E+09	3.61E+09	**i14 – i15**	3.18E+08	6.07E+08	**i45 – i20**	2.65E+06	1.02E+07
i20 – p12	5.31E+08	1.31E+09	**i15 – i14**	5.21E+09	8.57E+09	**i20 – i45**	2.30E+04	1.16E+05
i21 – p10	3.18E+10	6.36E+10	**i15 – p25**	7.72E+09	1.37E+10	**i45 – i6**	7.82E+06	2.26E+07
i21 – p4	3.35E+09	7.89E+09	**i15 – p7**	3.14E+09	5.82E+09	**i6 – i45**	1.36E+05	5.27E+05
i21 – p14	8.40E+09	2.05E+10	**i15 – i39**	1.38E+07	3.17E+07	**i45 – i37**	2.67E+06	6.52E+06
i8 – i9	5.02E+11	6.18E+11	**i39 – i15**	3.25E+09	6.28E+09	**i37 – i45**	1.49E+09	3.39E+09
i9 – i8	4.56E+11	5.64E+11	**i39 – i28**	2.92E+07	8.10E+07	**i45 – i9**	1.81E+08	3.77E+08
i7 – i9	2.55E+10	3.59E+10	**i28 – i39**	1.93E+07	5.17E+07	**i9 – i45**	1.14E+07	3.05E+07
i9 – i7	5.82E+10	7.81E+10	**i35 – p28**	9.46E+07	2.91E+08	**i45 – i8**	1.76E+08	3.90E+08

i23 – i6	2.66E+12	2.93E+12	**i33 – p15**	9.23E+09	1.48E+10	**i8 – i45**	1.22E+07	3.46E+07
i6 – i23	1.51E+09	2.37E+09	**i33 – p12**	1.98E+09	4.20E+09	**i45 – p29**	1.57E+09	3.93E+09
i19 – i28	2.96E+08	4.53E+08	**i33 – p7**	3.04E+09	4.73E+09	**i17 – i18**	4.35E+10	6.23E+10
i28 – i19	3.29E+11	4.04E+11	**i32 – p26**	6.69E+08	2.18E+09	**i18 – i17**	5.80E+10	8.32E+10
i27 – i22	1.76E+11	2.26E+11	**i32 – p8**	6.16E+09	1.19E+10	**i44 – i19**	3.50E+10	6.15E+10
i22 – i27	2.04E+10	2.74E+10	**i13 – i32**	6.19E+04	2.58E+05	**i19 – i44**	1.61E+06	4.35E+06
i25 – p21	2.22E+09	5.43E+09						

Table S2. RRKM calculated rate constants (k(E), s^{-1}) of the reaction of the ground-state atomic carbon (C, X^3P_j) with *trans*-2-butene (C_4H_8, X^1A_g) for unimolecular reaction steps at the zero-collision-energy limit and at the experimental collision energy (E_C, kJ mol^{-1})

Step	E_C		Step	E_C		Step	E_C	
	0	28		0	28		0	28
i2 – i5	6.47E+11	9.96E+11	**i7 – i8**	4.30E+07	1.10E+08	**i32 – i13**	1.35E+07	4.32E+07
i5 – i2	8.19E+05	2.02E+06	**i8 – i7**	1.09E+08	2.64E+08	**i32 – i34**	5.19E+10	6.55E+10
i1 – i3	2.77E+12	4.06E+12	**i19 – p3**	1.03E+10	1.59E+10	**i34 – i32**	4.80E+11	6.03E+11
i3 – i1	4.07E+07	9.39E+07	**i20 – p3**	1.01E+10	1.61E+10	**i15 – i33**	9.77E+07	2.13E+08
i4 – p1	1.03E+11	2.23E+11	**i6 – i22**	1.20E+07	3.32E+07	**i33 – i15**	2.57E+08	4.54E+08
i3 – p1	2.55E+10	5.64E+10	**i22 – i6**	3.02E+08	6.83E+08	**i32 – p10**	7.15E+10	1.20E+11
i5 – p4	2.77E+07	8.24E+07	**i7 – i22**	1.75E+07	4.69E+07	**i37 – p19**	4.27E+10	9.12E+10
i3 – p4	1.41E+08	4.28E+08	**i22 – i7**	2.76E+08	6.06E+08	**i37 – p21**	1.96E+09	5.40E+09
i4 – p4	1.10E+08	3.62E+08	**i6 – i9**	2.86E+07	7.24E+07	**i37 – p20**	5.07E+09	1.27E+10
i5 – p2	3.17E+08	7.48E+08	**i9 – i6**	1.04E+08	2.53E+08	**i33 – i36**	2.15E+11	2.54E+11
i3 – p2	2.03E+09	4.76E+09	**i9 – p13**	1.72E+09	4.01E+09	**i36 – i33**	1.03E+12	1.24E+12
i5 – i6	2.90E+07	6.35E+07	**i9 – p2**	6.57E+09	1.55E+10	**i36 – i22**	9.20E+10	1.11E+11
i6 – i5	1.59E+07	3.72E+07	**i7 – i20**	8.70E+08	1.73E+09	**i22 – i36**	6.19E+10	7.60E+10
i3 – i6	1.31E+08	2.85E+08	**i20 – i7**	2.75E+08	5.33E+08	**i39 – p19**	1.04E+09	2.63E+09
i6 – i3	2.18E+07	5.08E+07	**i7 – p3**	1.29E+10	2.31E+10	**i39 – i41**	1.17E+10	1.90E+10
i3 – i4	1.00E+10	1.44E+10	**i7 – p4**	7.13E+07	1.91E+08	**i41 – i39**	3.54E+09	5.13E+09
i4 – i3	9.72E+10	1.36E+11	**i7 – p13**	1.10E+08	2.93E+08	**i38 – i6**	1.29E+08	3.36E+08
i3 – i5	1.34E+10	1.90E+10	**i27 – i29**	2.38E+07	6.67E+07	**i6 – i38**	9.32E+05	3.10E+06
i5 – i3	4.06E+09	5.80E+09	**i29 – i27**	2.87E+07	8.39E+07	**i33 – i32**	2.11E+06	7.14E+06
i3 – i8	4.42E+07	1.25E+08	**i28 – p19**	4.64E+09	8.05E+09	**i32 – i33**	7.14E+07	2.24E+08
i8 – i3	2.96E+07	8.53E+07	**i28 – i37**	1.96E+06	6.90E+06	**i33 – i28**	5.97E+07	1.20E+08
i3 – i21	1.09E+07	2.61E+07	**i37 – i28**	1.45E+08	4.48E+08	**i28 – i33**	1.80E+09	3.59E+09
i21 – i3	5.79E+07	1.38E+08	**i28 – p23**	3.03E+08	9.34E+08	**i35 – i38**	1.26E+11	1.52E+11
i6 – p4	4.50E+07	1.21E+08	**i28 – i30**	4.74E+06	1.36E+07	**i38 – i35**	1.87E+10	2.45E+10
i6 – i7	3.95E+11	4.74E+11	**i30 – i28**	8.56E+06	2.47E+07	**i38 – i29**	7.06E+07	1.46E+08
i7 – i6	6.26E+11	7.55E+11	**i24 – i19**	1.21E+12	1.44E+12	**i29 – i38**	2.69E+08	5.83E+08
i25 – p18	2.66E+09	7.14E+09	**i19 – i24**	1.38E+09	2.05E+09	**i41 – i40**	3.60E+07	1.12E+08
i6 – p3	9.15E+09	1.61E+10	**i24 – i20**	1.30E+12	1.53E+12	**i40 – i41**	9.54E+06	3.10E+07
i6 – p13	1.30E+08	3.51E+08	**i20 – i24**	1.80E+09	2.64E+09	**i41 – p27**	2.20E+09	5.56E+09
i7 – i25	1.01E+07	2.49E+07	**i29 – p21**	2.24E+10	4.25E+10	**i14 – i34**	1.18E+06	3.58E+06

i25 – i7	3.17E+11	5.32E+11	**i23 – i24**	1.00E+10	1.55E+10	**i34 – i14**	1.63E+10	3.19E+10
i6 – i8	2.03E+08	5.16E+08	**i24 – i23**	4.81E+08	8.35E+08	**i34 – i40**	1.44E+12	1.81E+12
i8 – i6	9.04E+07	2.20E+08	**i23 – p24**	8.42E+07	2.93E+08	**i40 – i34**	3.34E+10	4.36E+10
i6 – i19	6.08E+08	1.21E+09	**i30 – p20**	2.88E+09	5.48E+09	**i43 – i41**	2.56E+10	4.61E+10
i19 – i6	2.51E+08	4.91E+08	**i30 – p22**	3.86E+09	7.71E+09	**i41 – i43**	2.28E+09	3.13E+09
i25 – i27	1.67E+08	5.23E+08	**i30 – p18**	2.17E+10	3.81E+10	**i43 – i26**	2.15E+08	5.31E+08
i27 – i25	7.33E+05	2.64E+06	**i30 – i37**	3.10E+06	1.03E+07	**i26 – i43**	1.59E+07	3.89E+07
i27 – i28	1.07E+07	3.34E+07	**i37 – i30**	1.27E+08	3.68E+08	**i43 – i31**	1.09E+07	3.30E+07
i28 – i27	2.29E+07	7.13E+07	**i25 – i30**	1.06E+08	3.41E+08	**i31 – i43**	2.66E+04	8.91E+04
i31 – i28	4.83E-01	1.04E+01	**i30 – i25**	9.03E+05	3.32E+06	**i40 – p13**	1.50E+10	2.86E+10
i28 – i31	1.94E+01	3.09E+02	**i10 – i11**	1.14E+12	1.73E+12	**i40 – i22**	1.69E+10	2.59E+10
i21 – i20	1.17E+09	2.41E+09	**i11 – i10**	6.57E+06	1.57E+07	**i22 – i40**	7.54E+09	1.25E+10
i20 – i21	1.83E+07	3.99E+07	**i11 – p5**	6.14E+09	1.32E+10	**i38 – i40**	7.95E+06	1.90E+07
i21 – i7	2.57E+08	6.30E+08	**i11 – p8**	3.99E+07	1.24E+08	**i40 – i38**	6.48E+06	1.49E+07
i7 – i21	1.28E+07	3.40E+07	**i11 – p6**	4.82E+09	1.18E+10	**i41 – i22**	4.31E+07	1.34E+08
i21 – i18	2.88E+07	9.07E+07	**i11 – i13**	6.95E+08	1.46E+09	**i22 – i41**	5.09E+06	1.78E+07
i18 – i21	3.98E+07	1.23E+08	**i13 – i11**	9.79E+07	2.16E+08	**i42 – i40**	3.03E+09	6.50E+09
i26 – i20	2.22E+11	3.31E+11	**i11 – i12**	2.25E+07	5.21E+07	**i40 – i42**	5.16E+06	1.14E+07
i20 – i26	1.58E+08	2.43E+08	**i12 – i11**	1.02E+07	2.36E+07	**i42 – i27**	1.08E+08	2.71E+08
i31 – i26	5.08E+07	1.03E+08	**i13 – p8**	9.84E+07	2.77E+08	**i27 – i42**	3.57E+05	9.56E+05
i26 – i31	6.17E+09	1.12E+10	**i13 – p10**	1.69E+08	4.07E+08	**i16 – i17**	1.79E+11	3.02E+11
i31 – i22	3.43E+09	5.66E+09	**i13 – p7**	4.58E+08	1.07E+09	**i17 – i16**	6.21E+06	1.69E+07
i22 – i31	1.48E+10	1.90E+10	**i13 – i14**	2.43E+10	3.31E+10	**i17 – p9**	8.79E+09	1.90E+10
i25 – i28	6.08E+08	1.33E+09	**i14 – i13**	4.78E+09	7.40E+09	**i17 – p10**	2.96E+09	7.35E+09
i28 – i25	2.86E+06	7.15E+06	**i13 – i15**	3.03E+06	9.81E+06	**i18 – p10**	5.04E+09	1.18E+10
i19 – i20	5.66E+11	6.90E+11	**i15 – i13**	1.01E+07	3.18E+07	**i17 – p13**	9.76E+07	3.06E+08
i20 – i19	6.88E+11	8.33E+11	**i12 – i13**	3.42E+08	8.40E+08	**i18 – p13**	2.69E+08	7.81E+08
i4 – i9	6.43E+08	1.79E+09	**i13 – i12**	1.06E+08	2.75E+08	**i17 – p11**	2.57E+09	6.85E+09
i9 – i4	4.02E+07	1.17E+08	**i13 – i37**	6.05E+06	1.42E+07	**i18 – p11**	2.02E+09	5.38E+09
i22 – p15	1.92E+09	4.08E+09	**i37 – i13**	1.17E+11	1.91E+11	**i18 – p14**	1.37E+09	3.38E+09
i25 – i29	1.68E+08	4.93E+08	**i35 – i13**	1.35E+12	1.48E+12	**i18 – i6**	3.74E+08	8.10E+08
i29 – i25	1.79E+06	6.25E+06	**i13 – i35**	2.58E+09	3.89E+09	**i6 – i18**	8.49E+06	2.03E+07
i26 – p16	4.16E+11	6.52E+11	**i12 – p5**	1.08E+10	2.28E+10	**i17 – i9**	4.16E+07	9.82E+07
i31 – p17	1.56E+10	2.67E+10	**i12 – p8**	2.49E+09	6.06E+09	**i9 – i17**	4.59E+06	1.14E+07
i31 – p16	1.83E+11	2.53E+11	**i12 – i14**	3.92E+08	7.89E+08	**i18 – i19**	1.12E+11	1.52E+11
i8 – p2	3.80E+09	9.04E+09	**i14 – i12**	2.40E+07	5.78E+07	**i19 – i18**	1.05E+09	1.54E+09
i8 – p13	1.33E+09	3.17E+09	**i13 – i33**	4.35E+07	1.07E+08	**i17 – i45**	6.78E+07	1.43E+08
i22 – p3	6.16E+09	1.22E+10	**i33 – i13**	3.79E+08	7.37E+08	**i45 – i17**	1.21E+08	2.09E+08
i19 – i22	1.56E+07	3.87E+07	**i11 – i32**	8.15E+06	2.32E+07	**i16 – i44**	4.53E+09	9.38E+09
i22 – i19	1.90E+09	3.94E+09	**i32 – i11**	3.39E+08	7.45E+08	**i44 – i16**	4.48E+07	1.05E+08
i22 – i20	2.16E+08	5.49E+08	**i14 – p26**	8.06E+05	4.20E+06	**i17 – i40**	3.40E+07	9.25E+07
i20 – i22	2.15E+06	6.53E+06	**i14 – p7**	3.12E+09	6.34E+09	**i40 – i17**	1.16E+08	2.63E+08
i19 – p12	1.38E+09	3.24E+09	**i14 – i15**	2.80E+08	5.44E+08	**i45 – i20**	1.96E+06	7.99E+06

i20 – p12	4.61E+08	1.17E+09	**i15 – i14**	4.73E+09	7.87E+09	**i20 – i45**	1.66E+04	8.88E+04
i21 – p10	2.78E+10	5.66E+10	**i15 – p25**	7.12E+09	1.28E+10	**i45 – i6**	6.15E+06	1.85E+07
i21 – p4	2.83E+09	6.83E+09	**i15 – p7**	2.79E+09	5.24E+09	**i6 – i45**	1.04E+05	4.21E+05
i21 – p14	7.32E+09	1.82E+10	**i15 – i39**	1.21E+07	2.85E+07	**i45 – i37**	2.26E+06	5.69E+06
i8 – i9	4.82E+11	5.97E+11	**i39 – i15**	2.89E+09	5.67E+09	**i37 – i45**	1.32E+09	3.07E+09
i9 – i8	4.38E+11	5.44E+11	**i39 – i28**	2.42E+07	6.93E+07	**i45 – i9**	1.58E+08	3.37E+08
i7 – i9	2.39E+10	3.38E+10	**i28 – i39**	1.61E+07	4.45E+07	**i9 – i45**	9.74E+06	2.68E+07
i9 – i7	5.50E+10	7.43E+10	**i35 – p28**	7.33E+07	2.36E+08	**i45 – i8**	1.46E+08	3.33E+08
i23 – i6	2.61E+12	2.88E+12	**i33 – p15**	8.40E+09	1.37E+10	**i8 – i45**	9.94E+06	2.90E+07
i6 – i23	1.38E+09	2.19E+09	**i33 – p12**	1.70E+09	3.71E+09	**i45 – p29**	1.27E+09	3.29E+09
i19 – i28	2.72E+08	4.21E+08	**i33 – p7**	2.88E+09	4.52E+09	**i17 – i18**	4.06E+10	5.86E+10
i28 – i19	3.08E+11	3.81E+11	**i32 – p26**	5.51E+08	1.87E+09	**i18 – i17**	5.41E+10	7.83E+10
i27 – i22	1.68E+11	2.17E+11	**i32 – p8**	5.41E+09	1.06E+10	**i44 – i19**	3.03E+10	5.45E+10
i22 – i27	1.93E+10	2.61E+10	**i13 – i32**	4.55E+04	1.99E+05	**i19 – i44**	1.33E+06	3.69E+06
i25 – p21	1.86E+09	4.68E+09						

Table S3. RRKM calculated rate constants (k(E), s^{-1}) of the reaction of the ground-state atomic carbon (C, ^3P_j) with isobutene (C_4H_8, X^1A_1) for unimolecular reaction steps at the zero-collision-energy limit and at the experimental collision energy (E_C, kJ mol^{-1})

Step	E_C		Step	E_C		Step	E_C	
	0	28		0	28		0	28
i2 – i5	5.89E+11	9.22E+11	**i7 – i8**	3.52E+07	9.23E+07	**i32 – i13**	1.04E+07	3.51E+07
i5 – i2	6.74E+05	1.71E+06	**i8 – i7**	9.01E+07	2.24E+08	**i32 – i34**	4.94E+10	6.27E+10
i1 – i3	2.45E+12	3.66E+12	**i19 – p3**	9.40E+09	1.47E+10	**i34 – i32**	4.57E+11	5.79E+11
i3 – i1	3.28E+07	7.79E+07	**i20 – p3**	9.20E+09	1.47E+10	**i15 – i33**	8.28E+07	1.85E+08
i4 – p1	8.75E+10	1.94E+11	**i6 – i22**	9.70E+06	2.76E+07	**i33 – i15**	2.28E+08	4.10E+08
i3 – p1	2.15E+10	4.88E+10	**i22 – i6**	2.53E+08	5.89E+08	**i32 – p10**	6.40E+10	1.09E+11
i5 – p4	2.19E+07	6.76E+07	**i7 – i22**	1.41E+07	3.92E+07	**i37 – p19**	3.62E+10	7.95E+10
i3 – p4	1.10E+08	3.50E+08	**i22 – i7**	2.33E+08	5.25E+08	**i37 – p21**	1.57E+09	4.51E+09
i4 – p4	8.53E+07	2.92E+08	**i6 – i9**	2.35E+07	6.11E+07	**i37 – p20**	3.96E+09	1.04E+10
i5 – p2	2.54E+08	6.18E+08	**i9 – i6**	8.65E+07	2.15E+08	**i33 – i36**	2.07E+11	2.46E+11
i3 – p2	1.69E+09	4.08E+09	**i9 – p13**	1.43E+09	3.44E+09	**i36 – i33**	9.93E+11	1.20E+12
i5 – i6	2.46E+07	5.50E+07	**i9 – p2**	5.47E+09	1.33E+10	**i36 – i22**	8.60E+10	1.04E+11
i6 – i5	1.33E+07	3.18E+07	**i7 – i20**	7.52E+08	1.53E+09	**i22 – i36**	5.76E+10	7.12E+10
i3 – i6	1.11E+08	2.47E+08	**i20 – i7**	2.39E+08	4.72E+08	**i39 – p19**	8.49E+08	2.22E+09
i6 – i3	1.82E+07	4.35E+07	**i7 – p3**	1.14E+10	2.07E+10	**i39 – i41**	1.06E+10	1.74E+10
i3 – i4	9.29E+09	1.34E+10	**i7 – p4**	5.78E+07	1.59E+08	**i41 – i39**	3.26E+09	4.80E+09
i4 – i3	9.06E+10	1.28E+11	**i7 – p13**	8.95E+07	2.45E+08	**i38 – i6**	1.04E+08	2.82E+08
i3 – i5	1.24E+10	1.78E+10	**i27 – i29**	1.90E+07	5.54E+07	**i6 – i38**	7.19E+05	2.50E+06
i5 – i3	3.77E+09	5.43E+09	**i29 – i27**	2.27E+07	6.92E+07	**i33 – i32**	1.61E+06	5.73E+06
i3 – i8	3.53E+07	1.03E+08	**i28 – p19**	4.13E+09	7.28E+09	**i32 – i33**	5.56E+07	1.82E+08
i8 – i3	2.35E+07	7.04E+07	**i28 – i37**	1.48E+06	5.51E+06	**i33 – i28**	5.14E+07	1.06E+08

i3 – i21	9.02E+06	2.23E+07	**i37 – i28**	1.13E+08	3.66E+08	**i28 – i33**	1.55E+09	3.17E+09
i21 – i3	4.81E+07	1.18E+08	**i28 – p23**	2.37E+08	7.63E+08	**i35 – i38**	1.22E+11	1.47E+11
i6 – p4	3.64E+07	1.01E+08	**i28 – i30**	3.77E+06	1.13E+07	**i38 – i35**	1.77E+10	2.33E+10
i6 – i7	3.80E+11	4.58E+11	**i30 – i28**	6.80E+06	2.04E+07	**i38 – i29**	6.03E+07	1.28E+08
i7 – i6	6.03E+11	7.29E+11	**i24 – i19**	1.17E+12	1.39E+12	**i29 – i38**	2.28E+08	5.07E+08
i25 – p18	2.14E+09	5.99E+09	**i19 – i24**	1.26E+09	1.91E+09	**i41 – i40**	2.80E+07	9.16E+07
i6 – p3	8.12E+09	1.45E+10	**i24 – i20**	1.26E+12	1.49E+12	**i40 – i41**	7.36E+06	2.51E+07
i6 – p13	1.05E+08	2.93E+08	**i20 – i24**	1.66E+09	2.46E+09	**i41 – p27**	1.79E+09	4.71E+09
i7 – i25	8.37E+06	2.11E+07	**i29 – p21**	1.95E+10	3.79E+10	**i14 – i34**	9.28E+05	2.92E+06
i25 – i7	2.84E+11	4.85E+11	**i23 – i24**	9.12E+09	1.43E+10	**i34 – i14**	1.41E+10	2.83E+10
i6 – i8	1.66E+08	4.35E+08	**i24 – i23**	4.28E+08	7.55E+08	**i34 – i40**	1.37E+12	1.74E+12
i8 – i6	7.48E+07	1.87E+08	**i23 – p24**	6.38E+07	2.35E+08	**i40 – i34**	3.15E+10	4.15E+10
i6 – i19	5.25E+08	1.07E+09	**i30 – p20**	2.51E+09	4.87E+09	**i43 – i41**	2.27E+10	4.14E+10
i19 – i6	2.18E+08	4.34E+08	**i30 – p22**	3.32E+09	6.80E+09	**i41 – i43**	2.13E+09	2.96E+09
i25 – i27	1.29E+08	4.27E+08	**i30 – p18**	1.92E+10	3.44E+10	**i43 – i26**	1.78E+08	4.50E+08
i27 – i25	5.53E+05	2.10E+06	**i30 – i37**	2.27E+06	7.94E+06	**i26 – i43**	1.31E+07	3.30E+07
i27 – i28	8.35E+06	2.72E+07	**i37 – i30**	9.56E+07	2.92E+08	**i43 – i31**	8.61E+06	2.70E+07
i28 – i27	1.79E+07	5.82E+07	**i25 – i30**	8.20E+07	2.77E+08	**i31 – i43**	2.05E+04	7.15E+04
i31 – i28	2.36E-01	6.10E+00	**i30 – i25**	6.77E+05	2.63E+06	**i40 – p13**	1.30E+10	2.55E+10
i28 – i31	1.01E+01	1.93E+02	**i10 – i11**	1.04E+12	1.60E+12	**i40 – i22**	1.54E+10	2.40E+10
i21 – i20	1.00E+09	2.11E+09	**i11 – i10**	5.46E+06	1.34E+07	**i22 – i40**	6.76E+09	1.14E+10
i20 – i21	1.56E+07	3.46E+07	**i11 – p5**	5.22E+09	1.14E+10	**i38 – i40**	6.59E+06	1.62E+07
i21 – i7	2.12E+08	5.35E+08	**i11 – p8**	3.13E+07	1.01E+08	**i40 – i38**	5.41E+06	1.28E+07
i7 – i21	1.03E+07	2.84E+07	**i11 – p6**	3.98E+09	1.00E+10	**i41 – i22**	3.36E+07	1.09E+08
i21 – i18	2.15E+07	7.09E+07	**i11 – i13**	5.94E+08	1.28E+09	**i22 – i41**	3.87E+06	1.42E+07
i18 – i21	2.98E+07	9.63E+07	**i13 – i11**	8.27E+07	1.87E+08	**i42 – i40**	2.57E+09	5.66E+09
i26 – i20	2.05E+11	3.08E+11	**i11 – i12**	1.89E+07	4.47E+07	**i40 – i42**	4.34E+06	9.89E+06
i20 – i26	1.45E+08	2.25E+08	**i12 – i11**	8.54E+06	2.02E+07	**i42 – i27**	8.86E+07	2.29E+08
i31 – i26	4.24E+07	8.77E+07	**i13 – p8**	7.88E+07	2.29E+08	**i27 – i42**	2.88E+05	8.00E+05
i26 – i31	5.26E+09	9.72E+09	**i13 – p10**	1.40E+08	3.47E+08	**i16 – i17**	1.59E+11	2.75E+11
i31 – i22	3.08E+09	5.16E+09	**i13 – p7**	3.82E+08	9.18E+08	**i17 – i16**	5.00E+06	1.41E+07
i22 – i31	1.41E+10	1.81E+10	**i13 – i14**	2.28E+10	3.12E+10	**i17 – p9**	7.46E+09	1.65E+10
i25 – i28	5.13E+08	1.15E+09	**i14 – i13**	4.37E+09	6.82E+09	**i17 – p10**	2.43E+09	6.23E+09
i28 – i25	2.34E+06	6.06E+06	**i13 – i15**	2.35E+06	7.92E+06	**i18 – p10**	4.20E+09	1.01E+10
i19 – i20	5.43E+11	6.65E+11	**i15 – i13**	7.85E+06	2.58E+07	**i17 – p13**	7.61E+07	2.49E+08
i20 – i19	6.61E+11	8.04E+11	**i12 – i13**	2.82E+08	7.13E+08	**i18 – p13**	2.14E+08	6.44E+08
i4 – i9	5.16E+08	1.48E+09	**i13 – i12**	8.67E+07	2.31E+08	**i17 – p11**	2.09E+09	5.74E+09
i9 – i4	3.20E+07	9.67E+07	**i13 – i37**	5.04E+06	1.22E+07	**i18 – p11**	1.57E+09	4.35E+09
i22 – p15	1.63E+09	3.56E+09	**i37 – i13**	1.06E+11	1.75E+11	**i18 – p14**	1.13E+09	2.87E+09
i25 – i29	1.33E+08	4.07E+08	**i35 – i13**	1.33E+12	1.45E+12	**i18 – i6**	3.17E+08	7.03E+08
i29 – i25	1.36E+06	4.99E+06	**i13 – i35**	2.36E+09	3.60E+09	**i6 – i18**	7.05E+06	1.73E+07
i26 – p16	3.79E+11	6.00E+11	**i12 – p5**	9.25E+09	1.99E+10	**i17 – i9**	3.46E+07	8.40E+07
i31 – p17	1.35E+10	2.35E+10	**i12 – p8**	2.06E+09	5.15E+09	**i9 – i17**	3.77E+06	9.69E+06

i31 – p16	1.71E+11	2.38E+11	**i12 – i14**	3.38E+08	6.94E+08	**i18 – i19**	1.05E+11	1.44E+11
i8 – p2	3.16E+09	7.72E+09	**i14 – i12**	1.99E+07	4.91E+07	**i19 – i18**	9.68E+08	1.43E+09
i8 – p13	1.10E+09	2.70E+09	**i13 – i33**	3.59E+07	9.05E+07	**i17 – i45**	5.78E+07	1.25E+08
i22 – p3	5.32E+09	1.08E+10	**i33 – i13**	3.29E+08	6.53E+08	**i45 – i17**	1.08E+08	1.90E+08
i19 – i22	1.28E+07	3.28E+07	**i11 – i32**	6.50E+06	1.92E+07	**i16 – i44**	3.86E+09	8.23E+09
i22 – i19	1.62E+09	3.45E+09	**i32 – i11**	2.86E+08	6.46E+08	**i44 – i16**	3.72E+07	9.01E+07
i22 – i20	1.76E+08	4.64E+08	**i14 – p26**	5.62E+05	3.12E+06	**i17 – i40**	2.74E+07	7.72E+07
i20 – i22	1.70E+06	5.34E+06	**i14 – p7**	2.69E+09	5.56E+09	**i40 – i17**	9.66E+07	2.27E+08
i19 – p12	1.15E+09	2.77E+09	**i14 – i15**	2.44E+08	4.81E+08	**i45 – i20**	1.43E+06	6.22E+06
i20 – p12	3.78E+08	9.85E+08	**i15 – i14**	4.25E+09	7.17E+09	**i20 – i45**	1.15E+04	6.57E+04
i21 – p10	2.39E+10	4.97E+10	**i15 – p25**	6.29E+09	1.15E+10	**i45 – i6**	4.83E+06	1.52E+07
i21 – p4	2.34E+09	5.82E+09	**i15 – p7**	2.44E+09	4.67E+09	**i6 – i45**	7.68E+04	3.27E+05
i21 – p14	5.79E+09	1.49E+10	**i15 – i39**	1.01E+07	2.44E+07	**i45 – i37**	1.77E+06	4.64E+06
i8 – i9	4.61E+11	5.74E+11	**i39 – i15**	2.50E+09	5.02E+09	**i37 – i45**	1.05E+09	2.54E+09
i9 – i8	4.19E+11	5.23E+11	**i39 – i28**	1.93E+07	5.74E+07	**i45 – i9**	1.34E+08	2.94E+08
i7 – i9	2.22E+10	3.17E+10	**i28 – i39**	1.29E+07	3.70E+07	**i9 – i45**	7.84E+06	2.23E+07
i9 – i7	5.16E+10	7.02E+10	**i35 – p28**	5.66E+07	1.91E+08	**i45 – i8**	1.22E+08	2.87E+08
i23 – i6	2.56E+12	2.83E+12	**i33 – p15**	7.57E+09	1.25E+10	**i8 – i45**	7.89E+06	2.39E+07
i6 – i23	1.26E+09	2.01E+09	**i33 – p12**	1.44E+09	3.22E+09	**i45 – p29**	1.03E+09	2.77E+09
i19 – i28	2.48E+08	3.89E+08	**i33 – p7**	2.53E+09	4.04E+09	**i17 – i18**	3.76E+10	5.48E+10
i28 – i19	2.94E+11	3.66E+11	**i32 – p26**	4.20E+08	1.51E+09	**i18 – i17**	5.00E+10	7.31E+10
i27 – i22	1.59E+11	2.07E+11	**i32 – p8**	4.68E+09	9.40E+09	**i44 – i19**	2.67E+10	4.90E+10
i22 – i27	1.81E+10	2.47E+10	**i13 – i32**	3.30E+04	1.53E+05	**i19 – i44**	1.06E+06	3.06E+06
i25 – p21	1.52E+09	3.97E+09						

Table S4. RRKM calculated rate constants (k(E), s^{-1}) of the reaction of the ground-state atomic carbon (C, ^3P_j) with 1-butene (C_4H_8, X^1A) for unimolecular reaction steps at the zero-collision-energy limit and at the experimental collision energy (E_C, kJ mol^{-1})

Step	E_C		Step	E_C		Step	E_C	
	0	28		0	28		0	28
i2 – i5	7.83E+11	1.17E+12	**i7 – i8**	6.24E+07	1.51E+08	**i32 – i13**	2.26E+07	6.60E+07
i5 – i2	1.22E+06	2.83E+06	**i8 – i7**	1.58E+08	3.64E+08	**i32 – i34**	5.75E+10	7.14E+10
i1 – i3	3.16E+12	4.53E+12	**i19 – p3**	1.24E+10	1.88E+10	**i34 – i32**	5.45E+11	6.75E+11
i3 – i1	5.67E+07	1.24E+08	**i20 – p3**	1.20E+10	1.86E+10	**i15 – i33**	1.33E+08	2.77E+08
i4 – p1	1.45E+11	2.97E+11	**i6 – i22**	1.85E+07	4.80E+07	**i33 – i15**	3.19E+08	5.45E+08
i3 – p1	3.49E+10	7.36E+10	**i22 – i6**	4.16E+08	8.95E+08	**i32 – p10**	8.98E+10	1.46E+11
i5 – p4	4.48E+07	1.24E+08	**i7 – i22**	2.69E+07	6.80E+07	**i37 – p19**	5.74E+10	1.16E+11
i3 – p4	2.29E+08	6.47E+08	**i22 – i7**	3.90E+08	8.13E+08	**i37 – p21**	3.07E+09	7.82E+09
i4 – p4	1.86E+08	5.61E+08	**i6 – i9**	4.24E+07	1.01E+08	**i37 – p20**	7.31E+09	1.71E+10
i5 – p2	4.45E+08	9.99E+08	**i9 – i6**	1.48E+08	3.41E+08	**i33 – i36**	2.31E+11	2.71E+11
i3 – p2	2.95E+09	6.55E+09	**i9 – p13**	2.49E+09	5.52E+09	**i36 – i33**	1.15E+12	1.37E+12
i5 – i6	3.95E+07	8.25E+07	**i9 – p2**	9.57E+09	2.14E+10	**i36 – i22**	9.94E+10	1.18E+11

i6 – i5	2.28E+07	5.06E+07	**i7 – i20**	1.18E+09	2.25E+09	**i22 – i36**	6.58E+10	8.00E+10
i3 – i6	1.77E+08	3.70E+08	**i20 – i7**	3.67E+08	6.84E+08	**i39 – p19**	1.54E+09	3.66E+09
i6 – i3	3.11E+07	6.92E+07	**i7 – p3**	1.61E+10	2.79E+10	**i39 – i41**	1.48E+10	2.33E+10
i3 – i4	1.17E+10	1.65E+10	**i7 – p4**	1.10E+08	2.76E+08	**i41 – i39**	4.16E+09	5.90E+09
i4 – i3	1.13E+11	1.55E+11	**i7 – p13**	1.69E+08	4.23E+08	**i38 – i6**	1.89E+08	4.61E+08
i3 – i5	1.56E+10	2.18E+10	**i27 – i29**	3.75E+07	9.74E+07	**i6 – i38**	1.55E+06	4.78E+06
i5 – i3	4.74E+09	6.64E+09	**i29 – i27**	4.61E+07	1.25E+08	**i33 – i32**	3.61E+06	1.11E+07
i3 – i8	6.70E+07	1.77E+08	**i28 – p19**	5.86E+09	9.83E+09	**i32 – i33**	1.18E+08	3.39E+08
i8 – i3	4.63E+07	1.25E+08	**i28 – i37**	3.51E+06	1.12E+07	**i33 – i28**	8.11E+07	1.55E+08
i3 – i21	1.54E+07	3.51E+07	**i37 – i28**	2.39E+08	6.74E+08	**i28 – i33**	2.50E+09	4.75E+09
i21 – i3	8.16E+07	1.85E+08	**i28 – p23**	5.12E+08	1.44E+09	**i35 – i38**	1.41E+11	1.67E+11
i6 – p4	7.10E+07	1.80E+08	**i28 – i30**	7.76E+06	2.06E+07	**i38 – i35**	2.11E+10	2.71E+10
i6 – i7	4.37E+11	5.19E+11	**i30 – i28**	1.37E+07	3.65E+07	**i38 – i29**	9.38E+07	1.85E+08
i7 – i6	6.79E+11	8.11E+11	**i24 – i19**	1.31E+12	1.53E+12	**i29 – i38**	3.64E+08	7.52E+08
i25 – p18	4.13E+09	1.02E+10	**i19 – i24**	1.64E+09	2.39E+09	**i41 – i40**	5.97E+07	1.70E+08
i6 – p3	1.16E+10	1.99E+10	**i24 – i20**	1.40E+12	1.63E+12	**i40 – i41**	1.61E+07	4.76E+07
i6 – p13	1.98E+08	5.04E+08	**i20 – i24**	2.12E+09	3.06E+09	**i41 – p27**	3.18E+09	7.52E+09
i7 – i25	1.45E+07	3.38E+07	**i29 – p21**	2.97E+10	5.41E+10	**i14 – i34**	1.85E+06	5.25E+06
i25 – i7	3.84E+11	6.24E+11	**i23 – i24**	1.21E+10	1.82E+10	**i34 – i14**	2.17E+10	4.05E+10
i6 – i8	3.12E+08	7.49E+08	**i24 – i23**	6.12E+08	1.03E+09	**i34 – i40**	1.63E+12	2.02E+12
i8 – i6	1.36E+08	3.14E+08	**i23 – p24**	1.40E+08	4.41E+08	**i40 – i34**	3.75E+10	4.83E+10
i6 – i19	8.14E+08	1.56E+09	**i30 – p20**	3.82E+09	6.96E+09	**i43 – i41**	3.31E+10	5.76E+10
i19 – i6	3.26E+08	6.16E+08	**i30 – p22**	5.23E+09	9.99E+09	**i41 – i43**	2.62E+09	3.53E+09
i25 – i27	2.77E+08	7.93E+08	**i30 – p18**	2.78E+10	4.71E+10	**i43 – i26**	3.08E+08	7.20E+08
i27 – i25	1.29E+06	4.20E+06	**i30 – i37**	5.04E+06	1.53E+07	**i26 – i43**	2.27E+07	5.26E+07
i27 – i28	1.77E+07	5.06E+07	**i37 – i30**	1.95E+08	5.21E+08	**i43 – i31**	1.78E+07	4.98E+07
i28 – i27	3.88E+07	1.11E+08	**i25 – i30**	1.78E+08	5.19E+08	**i31 – i43**	4.52E+04	1.40E+05
i31 – i28	1.95E+00	2.96E+01	**i30 – i25**	1.61E+06	5.33E+06	**i40 – p13**	1.99E+10	3.64E+10
i28 – i31	7.07E+01	8.06E+02	**i10 – i11**	1.37E+12	2.02E+12	**i40 – i22**	2.04E+10	3.05E+10
i21 – i20	1.60E+09	3.17E+09	**i11 – i10**	9.62E+06	2.17E+07	**i22 – i40**	9.42E+09	1.52E+10
i20 – i21	2.58E+07	5.36E+07	**i11 – p5**	8.28E+09	1.70E+10	**i38 – i40**	1.12E+07	2.53E+07
i21 – i7	3.81E+08	8.82E+08	**i11 – p8**	6.57E+07	1.89E+08	**i40 – i38**	9.01E+06	1.97E+07
i7 – i21	1.96E+07	4.90E+07	**i11 – p6**	7.13E+09	1.65E+10	**i41 – i22**	7.12E+07	2.02E+08
i21 – i18	4.58E+07	1.34E+08	**i11 – i13**	9.61E+08	1.93E+09	**i22 – i41**	8.86E+06	2.82E+07
i18 – i21	6.27E+07	1.80E+08	**i13 – i11**	1.41E+08	2.98E+08	**i42 – i40**	4.09E+09	8.31E+09
i26 – i20	2.64E+11	3.85E+11	**i11 – i12**	3.25E+07	7.13E+07	**i40 – i42**	7.05E+06	1.48E+07
i20 – i26	1.91E+08	2.87E+08	**i12 – i11**	1.47E+07	3.23E+07	**i42 – i27**	1.62E+08	3.79E+08
i31 – i26	6.70E+07	1.31E+08	**i13 – p8**	1.52E+08	4.02E+08	**i27 – i42**	5.51E+05	1.37E+06
i26 – i31	7.74E+09	1.36E+10	**i13 – p10**	2.54E+08	5.78E+08	**i16 – i17**	2.26E+11	3.66E+11
i31 – i22	4.26E+09	6.85E+09	**i13 – p7**	6.79E+08	1.51E+09	**i17 – i16**	9.66E+06	2.46E+07
i22 – i31	1.65E+10	2.08E+10	**i13 – i14**	2.84E+10	3.80E+10	**i17 – p9**	1.23E+10	2.53E+10
i25 – i28	8.58E+08	1.77E+09	**i14 – i13**	5.77E+09	8.76E+09	**i17 – p10**	4.41E+09	1.03E+10
i28 – i25	4.39E+06	1.03E+07	**i13 – i15**	5.19E+06	1.55E+07	**i18 – p10**	7.33E+09	1.62E+10

i19 – i20	6.17E+11	7.44E+11	**i15 – i13**	1.67E+07	4.88E+07	**i17 – p13**	1.62E+08	4.68E+08
i20 – i19	7.47E+11	8.97E+11	**i12 – i13**	5.07E+08	1.18E+09	**i18 – p13**	4.30E+08	1.16E+09
i4 – i9	1.01E+09	2.62E+09	**i13 – i12**	1.65E+08	4.01E+08	**i17 – p11**	3.96E+09	9.87E+09
i9 – i4	6.44E+07	1.75E+08	**i13 – i37**	8.98E+06	2.00E+07	**i18 – p11**	2.99E+09	7.49E+09
i22 – p15	2.67E+09	5.40E+09	**i37 – i13**	1.45E+11	2.28E+11	**i18 – p14**	1.97E+09	4.58E+09
i25 – i29	2.71E+08	7.29E+08	**i35 – i13**	1.44E+12	1.56E+12	**i18 – i6**	5.06E+08	1.05E+09
i29 – i25	3.11E+06	9.88E+06	**i13 – i35**	3.15E+09	4.65E+09	**i6 – i18**	1.22E+07	2.78E+07
i26 – p16	4.91E+11	7.53E+11	**i12 – p5**	1.50E+10	3.01E+10	**i17 – i9**	6.06E+07	1.35E+08
i31 – p17	1.91E+10	3.19E+10	**i12 – p8**	3.68E+09	8.47E+09	**i9 – i17**	6.85E+06	1.61E+07
i31 – p16	2.05E+11	2.80E+11	**i12 – i14**	5.32E+08	1.03E+09	**i18 – i19**	1.28E+11	1.71E+11
i8 – p2	5.68E+09	1.28E+10	**i14 – i12**	3.52E+07	8.07E+07	**i19 – i18**	1.24E+09	1.78E+09
i8 – p13	1.99E+09	4.48E+09	**i13 – i33**	6.35E+07	1.48E+08	**i17 – i45**	9.39E+07	1.89E+08
i22 – p3	8.32E+09	1.58E+10	**i33 – i13**	4.90E+08	9.14E+08	**i45 – i17**	1.58E+08	2.63E+08
i19 – i22	2.32E+07	5.45E+07	**i11 – i32**	1.29E+07	3.43E+07	**i16 – i44**	6.00E+09	1.18E+10
i22 – i19	2.61E+09	5.18E+09	**i32 – i11**	4.80E+08	9.95E+08	**i44 – i16**	6.45E+07	1.41E+08
i22 – i20	3.25E+08	7.77E+08	**i14 – p26**	1.67E+06	7.69E+06	**i17 – i40**	5.28E+07	1.34E+08
i20 – i22	3.50E+06	9.87E+06	**i14 – p7**	4.11E+09	8.08E+09	**i40 – i17**	1.66E+08	3.56E+08
i19 – p12	1.94E+09	4.33E+09	**i14 – i15**	3.74E+08	7.01E+08	**i45 – i20**	3.76E+06	1.36E+07
i20 – p12	6.68E+08	1.60E+09	**i15 – i14**	5.90E+09	9.56E+09	**i20 – i45**	3.49E+04	1.64E+05
i21 – p10	3.79E+10	7.40E+10	**i15 – p25**	8.92E+09	1.56E+10	**i45 – i6**	1.03E+07	2.84E+07
i21 – p4	4.16E+09	9.50E+09	**i15 – p7**	3.67E+09	6.67E+09	**i6 – i45**	1.97E+05	7.20E+05
i21 – p14	1.05E+10	2.48E+10	**i15 – i39**	1.70E+07	3.81E+07	**i45 – i37**	3.36E+06	7.88E+06
i8 – i9	5.41E+11	6.62E+11	**i39 – i15**	3.84E+09	7.23E+09	**i37 – i45**	1.84E+09	4.03E+09
i9 – i8	4.81E+11	5.91E+11	**i39 – i28**	3.79E+07	1.01E+08	**i45 – i9**	2.18E+08	4.42E+08
i7 – i9	2.78E+10	3.87E+10	**i28 – i39**	2.48E+07	6.38E+07	**i9 – i45**	1.46E+07	3.77E+07
i9 – i7	6.26E+10	8.34E+10	**i35 – p28**	1.26E+08	3.69E+08	**i45 – i8**	2.16E+08	4.63E+08
i23 – i6	2.73E+12	2.99E+12	**i33 – p15**	1.04E+10	1.64E+10	**i8 – i45**	1.63E+07	4.42E+07
i6 – i23	1.73E+09	2.67E+09	**i33 – p12**	2.31E+09	4.78E+09	**i45 – p29**	1.99E+09	4.77E+09
i19 – i28	3.29E+08	4.97E+08	**i33 – p7**	3.40E+09	5.21E+09	**i17 – i18**	4.76E+10	6.74E+10
i28 – i19	3.47E+11	4.23E+11	**i32 – p26**	9.08E+08	2.79E+09	**i18 – i17**	6.35E+10	9.01E+10
i27 – i22	1.88E+11	2.39E+11	**i32 – p8**	7.28E+09	1.36E+10	**i44 – i19**	4.04E+10	6.94E+10
i22 – i27	2.20E+10	2.92E+10	**i13 – i32**	8.93E+04	3.51E+05	**i19 – i44**	2.08E+06	5.40E+06
i25 – p21	2.80E+09	6.57E+09						

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm^{-1}) for all reactants, intermediates, transition states, and products involved in the $C+C_4H_8$ reactions.

Reactants

***cis*-2-butene**
Cartesian coordinates

C	1.581817	-0.522551	0.000006
C	0.665433	0.664411	0.000002
C	-0.665434	0.664410	0.000003
C	-1.581816	-0.522552	-0.000007
H	2.234153	-0.504873	-0.879180
H	1.047475	-1.473503	0.000863
H	2.235294	-0.503980	0.878315
H	1.164607	1.631207	-0.000040
H	-1.164611	1.631204	0.000030
H	-2.235178	-0.504063	-0.878404
H	-2.234265	-0.504788	0.879093
H	-1.047475	-1.473505	-0.000701

Vibrational frequencies

71.0900	99.0123	308.0764
399.4609	577.5713	695.8724
882.3668	992.8492	1012.4162
1041.1178	1064.4817	1067.8951
1164.2796	1308.3410	1396.4871
1424.1636	1450.3746	1485.1948
1490.3587	1492.6983	1502.1623
1771.0481	3039.3578	3042.2841
3093.5509	3094.0430	3134.5314
3148.8306	3153.2964	3176.8750

***trans*-2-butene**
Cartesian coordinates

C	1.955930	0.078849	-0.000024
C	0.534089	-0.394480	0.000032
C	-0.534089	0.394480	0.000032
C	-1.955930	-0.078849	-0.000024
H	2.493255	-0.290582	0.879494
H	2.013506	1.170081	0.000045
H	2.493117	-0.290455	-0.879681
H	0.385648	-1.474269	0.000094
H	-0.385648	1.474269	0.000094
H	-2.493119	0.290461	-0.879677
H	-2.493253	0.290575	0.879498
H	-2.013506	-1.170081	0.000038

Vibrational frequencies

160.8668	213.8687	242.5230
287.0935	507.5927	754.4090
882.1812	992.1040	997.1550

1067.2890	1073.1215	1090.4522
1171.6985	1339.8311	1348.4116
1416.7004	1416.9517	1479.4414
1479.9722	1494.8606	1502.7412
1777.6129	3038.7275	3039.4578
3098.2497	3098.5007	3122.3532
3123.5710	3142.4899	3147.5290

isobutene
Cartesian coordinates

C	1.271331	-0.677857	-0.000009
C	0.000000	0.125937	0.000047
C	0.000007	1.455470	-0.000020
C	-1.271337	-0.677846	-0.000008
H	1.315539	-1.329924	0.879257
H	2.156247	-0.039068	-0.000047
H	1.315441	-1.329954	-0.879254
H	-0.925739	2.021822	-0.000003
H	0.925758	2.021813	0.000017
H	-1.315558	-1.329894	0.879271
H	-1.315449	-1.329962	-0.879239
H	-2.156247	-0.039049	-0.000065

Frequencies

137.4018	193.1523	387.2596
447.2937	449.8529	711.4439
827.8437	932.6552	964.8126
991.2412	1024.6414	1083.9010
1112.1359	1305.6245	1413.1050
1418.7073	1446.2341	1476.4705
1480.8419	1496.3503	1501.4275
1753.6817	3030.2510	3034.4597
3089.0054	3091.6692	3130.6686
3132.9062	3147.4551	3233.1667

1-butene
Cartesian coordinates

C	-1.847298	0.013238	-0.282577
C	-0.719704	-0.287544	0.348059
C	0.539916	0.526620	0.304038
C	1.714636	-0.253025	-0.293883
H	-2.722711	-0.623503	-0.218455
H	-1.934954	0.912883	-0.885549
H	-0.672432	-1.201763	0.939391
H	0.799478	0.839364	1.322562
H	0.365149	1.440996	-0.271704
H	2.629158	0.345264	-0.287712
H	1.501874	-0.541334	-1.326505
H	1.909137	-1.167635	0.274151

Vibrational frequencies

92.8744	226.6089	315.0693

440.0740	655.4931	803.5339
867.8331	948.0332	993.7591
1032.1058	1044.6941	1102.5084
1204.6588	1297.3968	1325.0758
1353.9236	1418.1570	1455.5396
1486.4449	1503.0252	1507.7535
1739.7551	3041.2360	3044.6993
3085.9376	3120.4339	3125.8515
3136.8547	3150.5797	3235.3594

Intermediates

i10

Cartesian coordinates

C	-0.907046	-1.275378	-0.069305
C	-0.114246	0.000000	0.121719
C	1.392488	0.000001	-0.476495
C	-0.907046	1.275378	-0.069304
H	-1.695308	-1.337190	0.687483
H	-0.272776	-2.157587	0.034026
H	-1.384559	-1.294853	-1.054374
H	1.698109	0.915470	-0.984678
H	1.698109	-0.915469	-0.984679
H	-1.695311	1.337188	0.687480
H	-1.384555	1.294855	-1.054375
H	-0.272777	2.157587	0.034031
C	1.087363	-0.000001	0.932566

Vibrational frequencies

216.2040	246.7644	334.3522
352.3455	375.9933	392.7472
632.5054	805.3939	876.7304
935.7571	957.7574	995.4314
1002.7171	1027.0523	1111.7532
1154.4812	1240.6081	1352.6729
1402.2845	1414.7462	1477.4627
1478.1008	1491.9859	1498.5828
1512.5852	3039.2361	3042.6787
3073.0391	3107.5341	3110.5863
3138.6652	3141.0278	3148.6287

i11

Cartesian coordinates

C	0.632811	1.430997	0.000000
C	0.391093	-0.055388	0.000002
C	-2.169456	-0.189848	0.000000
C	1.604424	-0.937304	-0.000001
C	-0.874842	-0.570574	0.000000
H	1.215892	1.723485	0.881365
H	-0.296456	2.002046	0.000029
H	1.215836	1.723487	-0.881401
H	-2.452603	0.864290	0.000002
H	-2.977167	-0.913525	-0.000002

H	2.227556	-0.736681	0.880226
H	2.227559	-0.736674	-0.880221
H	1.335195	-1.993727	-0.000004

Vibrational frequencies

37.8846 88.2605 208.6255
253.2739 359.4918 410.6997
498.2178 574.6862 744.5707
753.6195 964.2901 974.3294
982.9335 1046.4243 1057.1332
1234.8562 1281.9073 1392.8601
1399.6693 1433.5521 1469.3000
1469.6167 1476.6202 1487.6444
1515.8866 3017.5901 3021.0601
3070.6030 3074.4827 3085.6839
3140.6530 3141.5127 3211.2847

i12
Cartesian coordinates

C	-1.775202	-0.775412	-0.002110
C	-0.504802	0.051405	0.005330
C	2.127210	-0.212365	-0.002399
C	-0.565845	1.427953	-0.000327
C	0.710944	-0.607141	0.006093
H	-2.650541	-0.146400	0.170483
H	-1.745827	-1.544658	0.772453
H	-1.901394	-1.278934	-0.964143
H	2.380687	0.337317	-0.918683
H	2.784433	-1.084730	0.050164
H	2.364379	0.432225	0.854751
H	-1.518772	1.944870	0.004112
H	0.333204	2.033666	-0.008653

Vibrational frequencies

23.0674 109.3855 187.0344
193.2501 391.5133 508.2846
515.8575 605.5291 785.8638
792.6380 933.4745 993.8071
1006.6841 1055.4278 1067.4245
1172.6546 1334.9020 1386.3159
1412.8005 1443.1732 1459.1360
1471.8004 1491.4683 1506.7793
1524.2794 2998.0600 3056.5408
3057.3177 3101.1445 3126.7754
3143.0802 3153.6089 3250.4815

i13
Cartesian coordinates

C	-0.657349	1.413061	-0.002518
C	-0.445360	-0.075228	-0.007086
C	2.040300	-0.046062	0.004462
C	-1.656628	-0.904706	0.005265

C	0.816490	-0.673902	-0.005549
H	-1.340382	1.705473	-0.807198
H	0.271269	1.971412	-0.125789
H	-1.123834	1.732127	0.937126
H	2.145075	1.032248	0.016581
H	2.954204	-0.626733	0.003067
H	-2.159776	-1.174266	-0.919270
H	-2.152795	-1.157267	0.938392
H	0.821519	-1.761978	-0.010359

Vibrational frequencies

70.5978	189.8912	285.8907
322.2968	337.5328	338.6333
493.2652	541.7380	578.4151
781.4921	784.2240	914.2865
994.5823	1000.7732	1038.0998
1050.8810	1232.3705	1266.7404
1323.7083	1404.8188	1445.4739
1451.7152	1480.6918	1498.6404
1534.5112	3032.8338	3086.4288
3126.7130	3146.9912	3159.2248
3170.0989	3223.2919	3259.5008

i14
Cartesian coordinates

C	-0.612332	1.402895	0.000091
C	-0.575779	-0.004810	0.001247
C	1.998375	-0.046898	-0.000335
C	-1.784533	-0.731052	-0.000838
C	0.658073	-0.703713	0.003201
H	-1.559475	1.928508	-0.000397
H	2.160949	0.535064	-0.916754
H	0.292043	1.997810	-0.001370
H	2.112539	0.649942	0.838764
H	2.798630	-0.784872	0.067884
H	-1.784955	-1.814568	-0.001283
H	-2.740651	-0.222100	-0.002396
H	0.618095	-1.788309	-0.004650

Vibrational frequencies

66.1819	163.2956	280.8857
431.0991	452.9168	472.3592
485.9062	532.9944	619.4785
685.1014	733.3783	856.8702
983.7326	1001.7888	1005.3080
1083.2341	1136.9369	1287.0248
1366.1711	1410.7871	1466.1243
1484.1665	1493.5028	1501.8302
1515.9626	3019.2347	3067.7581
3135.3771	3164.2704	3169.2602
3189.0059	3266.6464	3268.7194

i15

Cartesian coordinates

C	1.159593	-1.210606	-0.119255
C	0.536415	-0.000002	0.133126
C	-1.850436	0.000016	-0.494242
C	1.159576	1.210617	-0.119231
C	-0.900110	-0.000022	0.655724
H	2.161530	-1.247448	-0.531688
H	-1.054698	-0.881886	1.283986
H	0.663444	-2.152994	0.082148
H	-2.085417	-0.927993	-1.002868
H	-2.085312	0.928036	-1.002896
H	2.161509	1.247484	-0.531674
H	0.663420	2.152997	0.082192
H	-1.054704	0.881785	1.284069

Vibrational frequencies

67.4503	192.6402	223.9929
404.9039	437.1629	530.3289
548.5483	565.4774	630.0213
778.6127	781.8234	805.3164
857.4755	979.4438	1051.0248
1057.9019	1076.0627	1251.5990
1297.4506	1360.1978	1370.0598
1465.3615	1485.0083	1490.9974
1536.5294	3060.0294	3109.5708
3153.7275	3154.0631	3160.8395
3254.5187	3256.4242	3262.3960

i16
Cartesian coordinates

C	-1.867852	0.320998	-0.051124
C	-0.397710	-0.114641	0.444685
C	0.807731	0.614710	-0.106761
C	2.067594	-0.248344	-0.034627
C	-1.253898	-0.943101	-0.371885
H	-2.635865	0.392001	0.718861
H	-1.889905	1.131384	-0.780715
H	-0.340487	-0.327928	1.515197
H	0.957608	1.542421	0.457152
H	0.611497	0.894852	-1.146390
H	2.933526	0.286508	-0.431735
H	1.936361	-1.166636	-0.612303
H	2.292075	-0.530331	0.998206

Vibrational frequencies

98.2310	222.2499	236.3482
376.4117	437.8303	718.8386
794.6425	845.8391	901.3294
952.3213	1000.5307	1020.7307
1064.5621	1080.2666	1116.9367
1156.3811	1247.9938	1290.2423
1343.4296	1407.1987	1416.8551

1483.7266 1488.1612 1503.0570
1508.0592 3046.2091 3048.9445
3077.1162 3079.2763 3094.8783
3124.6128 3136.2709 3153.6149

i17
Cartesian coordinates

C	-2.282191	-0.503094	0.126333
C	-0.089587	0.791916	-0.112859
C	0.929572	-0.237689	-0.525864
C	2.159496	-0.236708	0.386418
C	-1.401755	0.522729	0.124290
H	-1.972783	-1.518338	-0.128424
H	-3.327155	-0.358990	0.378694
H	0.270435	1.813468	-0.000785
H	1.245232	-0.024341	-1.555487
H	0.472160	-1.230618	-0.539711
H	2.895838	-0.970214	0.048683
H	1.881841	-0.479033	1.415127
H	2.641219	0.745141	0.391991

Vibrational frequencies

37.4539 185.6540 259.7931
300.9065 444.3387 514.8893
528.0850 759.3901 774.8296
792.7597 889.1431 983.7555
1037.0595 1076.9352 1091.7639
1161.5470 1276.6017 1314.4782
1370.6208 1418.1615 1438.4509
1468.9293 1482.3347 1507.3330
1509.4026 3028.4884 3048.1373
3091.0673 3096.9904 3126.7352
3128.5748 3147.4950 3210.6708

i18
Cartesian coordinates

C	2.408936	-0.343529	0.000005
C	0.131192	0.817863	-0.000042
C	-1.353856	0.609731	0.000057
C	-1.786351	-0.852558	-0.000039
C	1.068472	-0.165946	0.000035
H	3.089315	0.509812	-0.000119
H	2.857502	-1.331011	0.000089
H	0.481026	1.854915	-0.000161
H	-1.778142	1.125952	-0.871485
H	-1.777998	1.125791	0.871767
H	-1.403131	-1.371519	0.882107
H	-1.403306	-1.371350	-0.882358
H	-2.875631	-0.935957	0.000057

Vibrational frequencies

95.2705 162.3429 223.8214

274.9869 321.8728 555.7328
577.6543 746.4569 764.7087
807.5665 847.8351 958.2932
1017.8627 1084.0311 1115.8456
1190.4426 1285.0822 1300.2504
1372.1504 1418.6970 1447.8498
1465.1056 1493.1490 1498.1418
1509.9461 3021.6591 3045.3293
3055.8095 3075.2423 3093.8606
3132.4056 3133.6357 3213.6041

i19
Cartesian coordinates

C	2.469579	-0.243182	-0.085218
C	1.224369	0.340217	-0.190873
C	-1.279705	0.482041	0.256386
C	-2.315275	-0.421056	-0.330480
C	0.066468	-0.156093	0.380542
H	2.610202	-1.162516	0.473423
H	3.339543	0.194942	-0.557666
H	1.142250	1.261809	-0.765987
H	-1.194501	1.402262	-0.343389
H	-3.354672	-0.115369	-0.356359
H	-1.625265	0.823756	1.246115
H	-2.032859	-1.337803	-0.833699
H	0.122691	-1.078643	0.955419

Vibrational frequencies

70.5811 93.1841 171.0492
272.8951 409.5819 452.9102
498.5732 563.6600 756.5302
802.7095 822.1653 936.0068
989.9687 1003.0469 1084.9181
1106.5646 1190.2159 1201.6392
1293.9314 1310.4704 1375.2494
1451.0375 1456.6689 1509.7072
1526.6287 2968.4015 2991.6179
3145.1633 3153.9471 3157.2834
3162.2064 3261.7354 3266.0007

i1
Cartesian coordinates

C	1.965213	-0.416729	-0.110213
C	0.663263	0.086731	0.465057
C	-0.663273	0.086763	-0.465061
C	-1.965212	-0.416731	0.110207
C	0.000008	1.282804	0.000020
H	2.035527	-1.505834	-0.036803
H	2.807615	0.012788	0.439998
H	2.069165	-0.125207	-1.157748
H	0.460517	-0.250272	1.484930
H	-0.460540	-0.250201	-1.484949
H	-2.035245	-1.505891	0.037302

H	-2.807612	0.012313	-0.440373
H	-2.069424	-0.124732	1.157582

Vibrational frequencies

169.1054 193.2498 215.8131
287.8202 397.1134 503.2908
672.8347 861.2269 930.6553
942.7624 947.8691 1061.3953
1082.7660 1094.5650 1124.0968
1143.5285 1233.5876 1338.4359
1409.2110 1410.7101 1429.2676
1485.6970 1486.4521 1497.3392
1501.1330 3043.1746 3044.3628
3078.6238 3084.3075 3113.8038
3114.1830 3135.6073 3136.4406

i20
Cartesian coordinates

C	-2.082540	-0.609652	-0.041776
C	-1.392098	0.578973	0.013946
C	0.943338	-0.448476	0.035159
C	2.374898	-0.054162	-0.032848
C	-0.009120	0.709349	0.049431
H	-1.573061	-1.566640	-0.061287
H	-3.164917	-0.626399	-0.068961
H	-1.971675	1.498700	0.034084
H	0.772085	-1.084654	0.917732
H	0.692016	-1.107990	-0.817789
H	3.153003	-0.757003	0.237258
H	2.667718	0.882139	-0.493932
H	0.417964	1.705657	0.109422

Vibrational frequencies

31.6706 169.6040 217.9257
298.1400 374.5430 483.1863
530.1200 603.0290 642.6501
795.3996 831.2926 925.5295
997.1809 1027.7787 1069.6263
1113.0629 1182.8561 1210.6556
1230.6301 1327.7187 1431.8771
1439.5478 1466.1274 1479.7027
1540.4900 2914.7436 2989.6060
3159.8594 3160.9422 3167.6122
3189.1726 3261.8738 3269.9367

i21
Cartesian coordinates

C	-1.902078	0.738042	0.178258
C	-1.403195	-0.459210	-0.296614
C	1.099681	-0.382369	0.535341
C	1.898650	0.563670	-0.374264
C	-0.119844	-0.905664	-0.105951

H	-1.283735	1.418193	0.753661
H	0.814543	0.143513	1.459398
H	-2.929726	1.025476	-0.005637
H	-2.074435	-1.101579	-0.865073
H	1.738535	-1.215618	0.848609
H	2.218865	0.048211	-1.282253
H	2.787792	0.934768	0.141469
H	1.288877	1.420218	-0.670801

Vibrational frequencies

49.1374	176.2254	221.4806
259.5576	440.3804	554.1790
620.4444	782.4636	791.2404
835.5808	944.4602	982.0802
1032.9073	1074.1570	1110.4342
1214.7206	1277.4561	1312.6531
1361.3730	1411.6341	1459.2101
1468.2282	1499.1264	1506.7891
1511.5604	2997.8101	3053.0814
3062.5595	3132.3763	3136.8646
3141.6097	3159.8462	3260.5355

i22
Cartesian coordinates

C	1.878083	-0.856363	-0.022528
C	1.304862	0.463290	-0.207618
C	-1.170895	0.302831	-0.343302
C	-1.979369	-0.657354	0.086301
C	0.000722	0.852906	0.435911
H	1.537899	-1.712596	-0.601915
H	2.634757	-1.044797	0.735635
H	1.708055	1.121371	-0.976645
H	-1.315584	0.721176	-1.337606
H	-2.791893	-1.031525	-0.526704
H	-1.856921	-1.101588	1.070058
H	-0.041553	0.471229	1.461796
H	-0.075181	1.944873	0.482796

Vibrational frequencies

71.7033	99.9938	235.1204
341.9596	395.4312	423.1405
498.2417	612.6232	671.0124
892.8930	919.6618	938.8630
962.2860	989.8409	1045.9287
1105.4955	1161.5766	1230.8212
1293.4385	1333.6295	1359.1437
1438.9396	1449.8369	1474.5337
1727.7124	3038.0494	3088.7891
3104.3978	3132.9546	3141.5336
3155.4148	3192.3625	3236.4609

i23
Cartesian coordinates

C	1.491137	0.738612	-0.282283
C	1.663529	-0.638083	0.175885
C	-0.860828	-0.466430	-0.241218
C	-2.171597	0.189863	0.018322
C	0.353190	-0.041427	0.463620
H	1.974169	1.547415	0.261726
H	1.355511	0.928312	-1.344116
H	1.940084	-1.554838	-0.325337
H	-0.742339	-1.065098	-1.140254
H	-3.005967	-0.423883	-0.330130
H	-2.251242	1.162338	-0.493015
H	-2.313799	0.386223	1.086648
H	0.191001	0.324323	1.478518

Vibrational frequencies

80.1813 155.7587 239.1424
304.1527 424.5580 483.7582
594.9678 747.4898 830.6621
876.1124 935.6884 981.3187
1007.3705 1034.8128 1087.0570
1092.9075 1126.3001 1188.0827
1249.4225 1301.3061 1404.9492
1438.2158 1470.1564 1485.2301
1494.7289 2979.0547 3063.2812
3097.7338 3101.2271 3117.5128
3177.2137 3183.7204 3236.8022

i24
Cartesian coordinates

C	2.314586	0.020182	0.118406
C	0.970287	-0.053183	-0.424975
C	-1.466763	0.759678	-0.073072
C	-1.497651	-0.733849	-0.030367
C	-0.236400	-0.003589	0.406248
H	2.821739	0.972515	0.262046
H	2.869530	-0.874959	0.392918
H	0.828598	-0.125020	-1.504269
H	-1.394913	1.241134	-1.041306
H	-2.032175	1.311700	0.668308
H	-2.087248	-1.217643	0.739195
H	-1.449675	-1.271130	-0.970475
H	-0.060214	0.027973	1.476134

Vibrational frequencies

37.2675 255.6052 278.4627
396.1415 420.8830 500.6209
611.6607 789.0521 800.1815
855.6736 863.4222 950.1992
957.2058 1051.3611 1073.6960
1115.0842 1119.1862 1204.0100
1206.0329 1217.2026 1292.1998
1436.6802 1455.1536 1467.4511

1507.5237 3098.3372 3115.8460
3142.5338 3148.2298 3178.5980
3183.5189 3228.3511 3244.1567

i25
Cartesian coordinates

C	1.842658	0.011468	0.097469
C	0.419350	0.010055	-0.433081
C	-1.643669	-0.142117	0.092692
C	-0.624324	0.993880	0.178583
C	-0.516519	-1.116946	0.023558
H	2.410059	-0.827947	-0.313240
H	1.849003	-0.075584	1.188065
H	2.358893	0.936907	-0.172892
H	0.413572	0.104602	-1.524370
H	-2.439992	-0.116006	-0.649784
H	-0.364840	1.257096	1.209632
H	-0.859009	1.903445	-0.380782
H	-0.232664	-1.720551	0.888039

Vibrational frequencies

200.4431 225.8816 316.6878
429.9583 488.7405 690.6397
744.6884 840.2192 875.9960
917.9150 954.6932 1013.4428
1052.8913 1089.2538 1132.3417
1143.2409 1196.8847 1222.2220
1252.2614 1262.0050 1357.5334
1405.1770 1468.2340 1493.8979
1500.1113 3040.5541 3043.9863
3055.2600 3103.2018 3105.5532
3120.7229 3125.9016 3144.3626

i26
Cartesian coordinates

C	1.197773	0.443135	0.006912
C	0.827575	-1.018570	-0.067120
C	-1.229163	0.150624	-0.287672
C	-0.159723	1.183147	0.163053
C	-0.623480	-1.134582	0.205590
H	1.883764	0.682519	0.828914
H	1.712085	0.741283	-0.914214
H	1.348718	-1.691028	-0.742288
H	-1.300928	0.153863	-1.383155
H	-2.221293	0.355751	0.118420
H	-0.329718	1.433917	1.213799
H	-0.200773	2.114529	-0.406689
H	-0.969748	-1.533353	1.160637

Vibrational frequencies

140.1107 297.1981 440.2821
582.9556 630.2157 749.5365

817.3506 871.7662 899.9416
944.9269 954.5273 995.1471
1047.7852 1098.4696 1119.9107
1186.2986 1220.7866 1256.5765
1289.9949 1298.8446 1331.7768
1348.4655 1471.4626 1482.8190
1506.4816 3027.6512 3029.5726
3058.3882 3068.9161 3101.2383
3115.3366 3126.0010 3174.1334

i27
Cartesian coordinates

C	1.848473	-0.020898	-0.236450
C	0.537480	-0.003181	0.435610
C	-1.511569	0.006781	-0.169713
C	-0.515182	-1.091694	0.021756
C	-0.503521	1.099442	-0.008800
H	2.769404	0.189097	0.293468
H	-0.216786	1.596911	-0.945923
H	1.902485	-0.169151	-1.310550
H	0.658735	0.020334	1.520464
H	-2.564983	0.010004	-0.418196
H	-0.235801	-1.617447	-0.902773
H	-0.735803	-1.853541	0.778162
H	-0.711339	1.881092	0.730927

Vibrational frequencies

103.5788 118.7861 236.9097
325.0187 408.7389 543.0454
699.2614 794.7591 843.4820
901.2911 926.1149 966.8720
997.8104 1025.6875 1045.5812
1116.5939 1210.4128 1221.5934
1234.5304 1272.6834 1297.6967
1371.3016 1462.4307 1471.4993
1481.6942 3002.1272 3008.7587
3053.0458 3057.4624 3102.6604
3147.8176 3217.0583 3255.8803

i28
Cartesian coordinates

C	-1.902466	0.046850	0.249163
C	-0.588451	0.041825	-0.431216
C	1.539180	0.070217	0.174317
C	0.473726	-1.046798	0.010824
C	0.444627	1.067770	-0.039212
H	-1.967042	0.319967	1.297307
H	-2.781156	-0.375372	-0.224643
H	-0.739595	-0.004272	-1.520120
H	2.305454	0.062924	-0.612893
H	0.203204	-1.521008	0.955284
H	0.684206	-1.818702	-0.730942
H	2.061876	0.106377	1.136771

H	0.433359	2.150908	-0.084017

Vibrational frequencies

122.0572 164.7692 275.1681
321.5770 428.2286 556.9718
703.1224 780.4081 861.3412
898.4809 936.8235 961.7841
982.3670 1042.5371 1068.5349
1155.7218 1197.9685 1220.9721
1227.5748 1268.4304 1297.7672
1344.9560 1463.2331 1474.2132
1501.1362 2991.7877 3012.1014
3057.6540 3087.0235 3146.0278
3148.8020 3204.1409 3255.4948

i29
Cartesian coordinates

C	1.921796	0.000002	0.046808
C	0.459396	0.000003	-0.183023
C	-1.587189	-0.000003	0.105071
C	-0.566427	-1.100209	-0.019269
C	-0.566434	1.100211	-0.019275
H	2.393597	-0.886818	-0.387197
H	2.393641	0.886695	-0.387402
H	2.164287	0.000108	1.122415
H	-2.668890	-0.000014	0.067845
H	-0.688710	-1.785614	-0.873403
H	-0.436034	-1.735165	0.874586
H	-0.688712	1.785680	-0.873354
H	-0.436034	1.735097	0.874633

Vibrational frequencies

106.8626 116.2533 201.7159
224.2739 310.1218 639.8051
743.8473 866.8620 913.5095
927.7075 949.4147 994.8797
997.3437 1005.4829 1078.6152
1188.8886 1215.6804 1240.8663
1298.4000 1361.0590 1415.9797
1429.0028 1451.8373 1481.2257
1482.6396 2941.9550 2948.8015
2968.1771 2978.5139 2979.0597
3067.7957 3114.8987 3224.9814

i2
Cartesian coordinates

C	1.574849	0.758577	-0.058780
C	0.814545	-0.502991	0.276151
C	-0.814524	-0.503015	0.276134
C	-1.574892	0.758540	-0.058774
C	0.000038	-1.235422	-0.664896
H	1.595976	1.445556	0.792638

H	1.144867	1.274742	-0.918096
H	2.608982	0.504750	-0.308579
H	1.230143	-1.052033	1.124541
H	-1.230102	-1.052120	1.124492
H	-1.596668	1.445175	0.792900
H	-2.608827	0.504640	-0.309312
H	-1.144467	1.275156	-0.917597

Vibrational frequencies

173.3698	175.2683	280.3681
303.4997	459.3498	479.6648
630.4987	858.4857	923.4178
950.2519	960.1398	1063.5737
1064.5045	1109.3414	1119.7859
1140.7301	1251.5598	1343.7021
1408.7982	1420.4066	1424.8424
1485.0466	1492.6567	1500.1776
1516.9432	3044.8794	3048.2890
3079.1615	3087.4946	3111.4646
3112.9941	3143.7062	3153.6207

i30
Cartesian coordinates

C	-1.829287	-0.003763	0.302448
C	-0.508696	0.026685	-0.477019
C	1.573973	-0.022759	0.252342
C	0.522935	-1.026618	-0.145537
C	0.538315	1.029372	-0.048354
H	-2.414841	0.898000	0.102302
H	-2.428276	-0.871275	0.010466
H	-0.746955	0.083563	-1.553849
H	2.479000	0.002890	-0.377160
H	1.924973	-0.077377	1.295804
H	-1.642263	-0.060604	1.377844
H	0.449936	-2.100027	-0.020489
H	0.594986	2.107328	-0.138198

Vibrational frequencies

121.3012	208.3119	216.6021
242.1883	347.4874	434.9963
752.2296	843.7692	893.0555
903.5140	948.1939	981.9197
1016.0574	1049.4591	1058.2548
1126.3015	1205.1272	1219.5543
1282.5943	1297.8190	1339.6964
1405.2646	1439.7357	1493.1126
1497.1282	2939.3194	2958.5803
2972.9555	3039.6313	3116.2962
3126.1465	3213.5388	3215.9943

i31
Cartesian coordinates

C	1.019713	-0.766206	0.104311
C	-0.406436	-1.169935	-0.084189
C	-0.406436	1.169935	0.084189
C	1.019714	0.766206	-0.104311
C	-1.331887	0.000000	0.000000
H	1.363918	-1.009854	1.121948
H	1.701882	-1.285782	-0.577125
H	-0.738794	-2.198142	-0.150117
H	-0.738793	2.198142	0.150116
H	1.701882	1.285782	0.577125
H	1.363918	1.009854	-1.121948
H	-2.011008	0.057970	-0.870465
H	-2.011007	-0.057970	0.870466

Vibrational frequencies

134.0101	143.6391	333.8330
337.2437	663.3670	743.4168
803.1143	871.2202	919.6981
920.6234	932.3561	962.7893
1051.6081	1058.4543	1095.7774
1118.2342	1222.7157	1285.7643
1291.7392	1298.2997	1359.2810
1383.7514	1442.5815	1467.6242
1487.1673	2924.0951	2929.8803
2978.0719	2983.2314	3063.4206
3067.4231	3219.7605	3222.2285

i32
Cartesian coordinates

C	0.687714	1.360754	-0.089971
C	0.511961	-0.092596	0.401985
C	-2.039720	-0.106282	-0.174288
C	1.470755	-1.025322	-0.265348
C	-0.888818	-0.551609	0.256883
H	1.719693	1.685199	0.065910
H	0.027142	2.037054	0.457141
H	0.460472	1.433442	-1.156056
H	-2.144440	0.899446	-0.590303
H	-2.941443	-0.711907	-0.142543
H	0.730612	-0.089707	1.485216
H	2.491000	-0.705278	-0.443284
H	1.205612	-2.057913	-0.451651

Vibrational frequencies

109.4076	152.4390	210.8414
270.2374	344.9200	369.3666
483.9743	500.5024	612.8066
797.8936	898.2720	905.8964
961.8139	1008.8576	1037.6163
1130.5731	1143.2085	1275.2848
1315.6993	1392.6814	1415.7659
1451.8235	1501.0344	1504.8322
1757.8708	2941.2687	3053.3494

3069.6154 3134.7178 3140.1214
3159.4728 3175.5679 3274.4585

i33
Cartesian coordinates

C	0.667866	1.415651	-0.021394
C	0.549059	-0.018313	0.408832
C	-1.884365	-0.000269	-0.304529
C	1.479856	-0.912903	-0.347870
C	-0.868088	-0.557572	0.340176
H	0.840089	-0.060735	1.474106
H	0.005969	2.161758	0.404797
H	1.459590	1.737148	-0.686155
H	-1.773765	0.938295	-0.838556
H	-2.861758	-0.469164	-0.321046
H	2.516268	-1.014135	-0.048094
H	1.164182	-1.347097	-1.289280
H	-1.016543	-1.505630	0.852937

Vibrational frequencies

75.6253 103.9159 122.7746
286.4135 336.3983 374.1985
467.1945 530.4293 598.0559
692.3652 802.4151 917.5716
970.0531 1006.5265 1044.2740
1058.2093 1116.4741 1156.9467
1267.0652 1309.3321 1339.9812
1438.3375 1445.2530 1460.0131
1728.3384 2937.9678 3150.5874
3151.9324 3155.3489 3166.7327
3246.0303 3267.5435 3269.1724

i34
Cartesian coordinates

C	1.527479	-0.815827	0.152504
C	0.686499	0.270284	-0.477903
C	-1.722878	-0.758164	0.064512
C	-0.039401	1.295092	0.374577
C	-0.796641	0.242729	-0.358456
H	2.546267	-0.462049	0.334478
H	1.581341	-1.694821	-0.495308
H	1.104812	-1.132365	1.110032
H	1.074662	0.658697	-1.418364
H	-1.531740	-1.360937	0.950582
H	-2.643321	-0.937912	-0.478056
H	0.024243	1.207973	1.458013
H	-0.086605	2.316730	0.007227

Vibrational frequencies

174.7024 198.5475 279.4486
340.7221 385.3128 475.0306
499.0794 744.6296 792.1409

849.7364 892.3670 930.5504
985.1598 1031.8660 1052.3450
1111.2932 1136.8582 1177.4700
1332.8709 1394.8896 1412.2468
1449.7890 1471.4399 1490.5845
1505.1869 3044.4469 3098.0158
3108.5415 3118.5750 3119.5431
3127.3920 3184.9634 3231.1211

i35
Cartesian coordinates

C	-1.729409	-0.631833	0.029289
C	-0.656830	0.309192	-0.353769
C	1.532349	-0.925742	0.208794
C	0.145051	1.303397	0.350205
C	0.815072	0.150343	-0.466619
H	-1.432173	-1.214783	0.915494
H	-1.929497	-1.349476	-0.770602
H	-2.657275	-0.108491	0.272189
H	1.192000	-1.295542	1.169607
H	2.475398	-1.290789	-0.175661
H	0.231326	1.236875	1.433552
H	0.228097	2.313559	-0.044484
H	1.254731	0.476502	-1.407497

Vibrational frequencies

100.4141 128.7272 174.0792
281.8764 356.0605 449.5847
521.2896 667.8318 825.4271
869.5063 887.1934 921.1399
995.8126 1039.1008 1063.1490
1110.5502 1129.7131 1164.2769
1328.3243 1395.7993 1427.9204
1466.1139 1472.6305 1482.3605
1492.3300 2982.9827 3083.9199
3090.8915 3126.3410 3128.3084
3155.6067 3173.1406 3264.3121

i36
Cartesian coordinates

C	1.537520	-0.849808	0.082860
C	0.772809	0.289263	-0.404370
C	-1.537526	-0.849797	0.082862
C	0.000003	1.178905	0.549801
C	-0.772807	0.289270	-0.404367
H	2.497801	-1.090139	-0.352799
H	1.182606	-1.453521	0.908252
H	1.203623	0.801821	-1.257766
H	-1.182639	-1.453500	0.908271
H	-2.497783	-1.090163	-0.352833
H	0.000005	0.888913	1.594505
H	0.000009	2.247767	0.369423
H	-1.203616	0.801830	-1.257766

Vibrational frequencies

101.4877 136.7385 253.5255
300.3941 402.7238 426.8251
472.4115 529.9499 738.6240
770.1632 883.8824 891.2672
940.3402 998.6493 1024.0800
1059.3086 1121.9581 1193.2205
1203.3611 1244.8536 1383.7116
1399.7183 1473.6653 1484.9761
1486.2665 3137.2331 3170.3282
3174.4402 3176.7431 3183.1348
3234.0881 3279.6477 3284.2508

i37
Cartesian coordinates

C	-1.976309	-0.019520	-0.011417
C	-0.517975	-0.022524	-0.246162
C	1.631446	-0.073219	-0.106998
C	0.524317	0.999866	0.147769
C	0.525444	-1.110524	-0.006291
H	-2.428073	0.926130	-0.324637
H	-2.203464	-0.146742	1.061756
H	-2.471146	-0.836886	-0.543595
H	2.454155	-0.144595	0.605439
H	2.031975	0.026349	-1.119835
H	0.455261	1.307670	1.201683
H	0.580761	1.901470	-0.473478
H	0.458994	-1.677866	0.931263

Vibrational frequencies

119.1492 155.9445 295.9369
303.6758 562.2465 674.3855
755.5708 887.4505 909.1941
928.1244 932.8717 989.7848
1060.8765 1072.8280 1147.5724
1194.6515 1226.5139 1238.7615
1263.2060 1350.4169 1411.6628
1441.1160 1471.1517 1481.1099
1485.5982 2952.8981 2992.6193
3037.6004 3053.6399 3068.0213
3069.3922 3117.9870 3135.9991

i38
Cartesian coordinates

C	-2.256049	-0.450231	-0.050643
C	-1.146875	0.437849	-0.429995
C	2.315143	-0.294291	-0.246346
C	0.111846	0.809442	0.250913
C	1.108384	-0.326415	0.301592
H	-1.929613	-1.495833	0.058820
H	-3.046676	-0.438235	-0.806430

H	-2.710553	-0.146152	0.905195
H	2.673806	0.585039	-0.773887
H	2.988568	-1.142238	-0.188580
H	-0.116109	1.133245	1.281678
H	0.568364	1.671169	-0.248560
H	0.777522	-1.225119	0.818637

Vibrational frequencies

33.9770	98.2509	132.3745
261.7405	368.9412	428.9527
655.7642	837.6513	880.2049
929.9268	957.0262	997.2574
1019.4225	1042.1892	1139.3982
1241.0270	1278.0666	1319.7484
1330.9977	1391.9866	1440.9906
1455.5416	1464.3767	1467.4306
1730.7880	2953.9147	2970.1804
3016.8073	3067.3138	3099.9786
3146.3593	3162.3704	3238.0815

i39
Cartesian coordinates

C	0.451029	-1.097263	0.029308
C	-0.584413	0.000000	-0.070215
C	1.549657	0.000000	-0.029832
C	-2.022556	0.000000	-0.003541
C	0.451030	1.097263	0.029309
H	0.455653	-1.833054	-0.783345
H	0.421669	-1.653377	0.976438
H	2.108299	0.000000	-0.966670
H	2.257662	-0.000001	0.799830
H	-2.549557	-0.000002	0.950235
H	-2.639527	0.000001	-0.899755
H	0.455655	1.833053	-0.783345
H	0.421671	1.653378	0.976437

Vibrational frequencies

88.2315	110.7597	296.0600
470.5785	500.4438	633.2842
752.6755	780.5522	866.7632
908.6669	955.4528	974.7545
1019.4464	1035.1829	1085.1656
1195.4680	1223.0774	1233.8106
1252.6548	1277.4763	1342.7111
1446.7567	1466.1278	1473.4511
1507.4416	3008.8645	3012.6362
3054.0809	3057.4321	3092.5732
3095.7526	3147.8916	3179.3658

i3
Cartesian coordinates

C	2.254269	0.503113	0.000846

C	1.317823	-0.674208	-0.002206
C	-1.028239	0.354123	-0.002167
C	-2.492650	0.042309	0.001610
C	-0.036165	-0.571128	-0.001189
H	2.851485	0.520637	0.919630
H	1.717151	1.450417	-0.071904
H	2.956791	0.443319	-0.837185
H	1.771144	-1.662656	0.004903
H	-0.750952	1.412527	-0.004984
H	-2.986508	0.471493	-0.877515
H	-2.982072	0.473458	0.882298
H	-2.667265	-1.034447	0.003398

Vibrational frequencies

49.1581	117.1450	154.6521
177.0824	342.4956	390.7362
598.5991	642.2150	770.8092
858.1840	958.8642	1017.2905
1028.7092	1062.4394	1126.4713
1171.4890	1287.0286	1401.8845
1411.9394	1415.4668	1446.4496
1478.7146	1479.5995	1502.1790
1514.2267	3029.8667	3031.1395
3070.8142	3083.9001	3087.4394
3134.3584	3143.5583	3163.6418

i40
Cartesian coordinates

C	1.761979	-0.857082	0.065870
C	1.260904	0.507967	-0.242879
C	-2.115053	-0.603062	-0.016395
C	-0.051783	0.968734	0.311401
C	-1.201047	0.280126	-0.324379
H	2.791984	-0.997495	-0.267508
H	1.146921	-1.629742	-0.420872
H	1.717016	-1.063069	1.142532
H	1.703163	1.070784	-1.057233
H	-2.183577	-1.015647	0.994450
H	-2.845708	-0.959599	-0.737243
H	-0.096857	0.764073	1.396907
H	-0.162946	2.050597	0.187258

Vibrational frequencies

67.3827	83.6613	122.6200
277.2181	326.5912	383.9793
443.4173	584.9467	867.8323
873.1524	897.6661	930.0178
993.6086	1016.2545	1116.3882
1155.2266	1232.5123	1304.0397
1378.1954	1413.7885	1419.1344
1450.6265	1477.8181	1487.4232
1753.1059	2935.7670	2986.0431
3047.3644	3062.1576	3073.9101

3122.3753 3177.4665 3194.3895

i41
Cartesian coordinates

C	-1.603142	1.036561	0.097717
C	1.136505	-0.261640	-0.336354
C	-1.376417	-0.397870	-0.216290
C	2.149481	0.488673	0.010490
C	-0.019896	-0.933247	0.280515
H	-0.771110	1.731300	0.114463
H	-2.607724	1.436092	0.161543
H	-1.430998	-0.562791	-1.304853
H	-2.176389	-1.010190	0.213998
H	2.308541	0.775369	1.054157
H	2.877156	0.852606	-0.709733
H	0.038471	-2.008504	0.080685
H	0.042869	-0.808753	1.373267

Vibrational frequencies

92.4531 146.8390 158.4316
276.4898 354.9602 402.3896
492.0403 576.1823 762.0829
877.0086 904.8309 912.1313
962.0849 1046.6686 1079.8037
1119.3266 1187.1852 1272.0235
1328.7987 1370.5693 1423.2884
1464.2716 1467.9832 1472.1008
1762.1017 2975.6102 2987.4251
3067.5977 3069.0719 3078.2481
3158.2281 3177.1121 3266.0031

i42
Cartesian coordinates

C	1.704111	0.000000	-0.213112
C	0.357873	0.000000	0.488437
C	-0.624296	-1.130406	0.025052
C	-0.624296	1.130406	0.025052
C	-1.501971	0.000000	-0.407922
H	2.285795	-0.886641	0.054357
H	2.285795	0.886641	0.054356
H	1.568656	0.000000	-1.299446
H	0.476606	0.000000	1.574299
H	-1.012656	-1.768835	0.826093
H	-0.230030	-1.774195	-0.770401
H	-1.012656	1.768835	0.826093
H	-0.230031	1.774196	-0.770400

Vibrational frequencies

114.9919 252.8285 342.7695
407.4770 703.9061 817.0885
819.8864 877.8475 921.9662
984.1842 998.8006 1045.3692

1087.2886 1101.0249 1137.6177
1179.8762 1204.6716 1257.1841
1259.0137 1353.4829 1421.3818
1463.0534 1480.8345 1497.5044
1497.5750 3027.7426 3032.5115
3037.2662 3067.1028 3072.1513
3093.4403 3116.5482 3118.4112

i43
Cartesian coordinates

C	0.737000	0.917116	-0.222196
C	-0.000001	-1.295084	0.000016
C	-0.737003	0.917111	0.222201
C	1.253398	-0.503221	0.121391
C	-1.253395	-0.503222	-0.121405
H	1.321496	1.705844	0.256428
H	0.795350	1.067207	-1.304535
H	-1.321505	1.705844	-0.256407
H	-0.795351	1.067183	1.304543
H	2.051297	-0.834550	-0.550737
H	1.661496	-0.536589	1.142345
H	-1.661454	-0.536589	-1.142375
H	-2.051320	-0.834549	0.550692

Vibrational frequencies

190.9750 230.5068 563.2576
660.9971 825.3769 841.7671
879.0258 902.6812 917.3312
950.6883 1015.2092 1030.3156
1100.8156 1172.8294 1203.8802
1219.8378 1232.7229 1284.4570
1313.1784 1331.2772 1349.6407
1477.7921 1479.3519 1494.4437
1511.4351 2996.5713 2999.0560
3060.7905 3061.0858 3074.0007
3075.9778 3114.3022 3125.7951

i44
Cartesian coordinates

C	-1.348709	-0.259325	-0.682294
C	-0.458311	0.689078	0.126922
C	1.058934	0.665581	0.020596
C	1.677145	-0.681044	-0.099465
C	-1.229668	-0.374878	0.777463
H	-2.252690	0.165967	-1.110589
H	-0.874057	-1.017574	-1.301796
H	-0.863647	1.695688	0.220730
H	1.467012	1.176663	0.910327
H	1.362519	1.289134	-0.829786
H	-0.930989	-1.205818	1.401420
H	2.676150	-0.787661	-0.503042
H	1.219355	-1.552869	0.353404

Vibrational frequencies

137.3678 153.6571 251.0413
330.2043 465.7035 518.0174
612.2063 768.9457 786.0915
871.0517 917.7829 955.6222
1007.7969 1031.2552 1054.9353
1099.4401 1114.9840 1150.5383
1228.1507 1252.6569 1364.8015
1396.3085 1460.9849 1470.1458
1480.4628 2950.9815 3039.7640
3099.7071 3115.0089 3156.0640
3179.8351 3223.7145 3261.1160

i4
Cartesian coordinates

C	-1.756052	0.805235	-0.000511
C	-1.302601	-0.633809	-0.002960
C	1.286165	-0.633512	0.002602
C	1.764397	0.794694	0.000406
C	-0.004842	-1.040390	0.000133
H	-1.260895	1.382445	-0.787433
H	-1.527788	1.292712	0.954577
H	-2.833724	0.873920	-0.158808
H	-2.076575	-1.397422	0.005944
H	2.063585	-1.395641	-0.004289
H	2.492074	0.955968	0.802729
H	0.948394	1.505542	0.131596
H	2.272527	1.029166	-0.942331

Vibrational frequencies

78.3884 132.4171 199.1557
216.4088 339.7523 419.2646
633.8192 644.3509 787.7016
841.1304 958.1772 1013.6163
1022.4838 1063.6383 1099.7457
1155.6514 1313.1752 1395.6997
1404.8018 1415.4300 1447.4690
1480.4223 1491.8175 1501.2206
1512.8924 3030.6091 3031.9296
3086.1737 3090.6258 3131.8301
3140.6406 3156.3695 3162.0960

i5
Cartesian coordinates

C	2.502127	-0.403976	-0.000021
C	1.277990	0.457371	0.000073
C	-1.277988	0.457365	-0.000043
C	-2.502128	-0.403976	-0.000007
C	0.000000	0.001661	0.000056
H	3.122458	-0.202221	-0.880689
H	2.241520	-1.463291	0.001367
H	3.124032	-0.200242	0.879064

H	1.433119	1.540412	-0.000047
H	-1.433123	1.540406	-0.000094
H	-3.123598	-0.200757	-0.879525
H	-3.122893	-0.201686	0.880230
H	-2.241522	-1.463292	-0.000653

Vibrational frequencies

29.7879	36.3408	145.5755
237.9331	274.3744	411.5091
459.8624	676.8383	766.9455
861.5934	966.9101	1016.6365
1025.8583	1072.0558	1130.3643
1217.0679	1243.3843	1400.0553
1404.7443	1421.6600	1449.1792
1477.7198	1478.1710	1503.1346
1510.3704	3025.7380	3026.7761
3078.3053	3079.5767	3079.6737
3084.2193	3136.2369	3136.4883

i6
Cartesian coordinates

C	-2.476358	-0.156386	-0.186589
C	-1.194733	-0.240136	0.311965
C	1.236695	0.427831	0.401613
C	2.256909	-0.430521	-0.269741
C	-0.125779	0.532891	-0.122144
H	-2.724611	0.548651	-0.973104
H	-3.270356	-0.788565	0.190395
H	-0.998005	-0.961657	1.102753
H	1.558011	1.124018	1.172424
H	3.182047	-0.487376	0.307522
H	2.511717	-0.045902	-1.269224
H	1.877530	-1.447841	-0.421944
H	-0.316740	1.256607	-0.919445

Vibrational frequencies

96.2217	125.2072	165.0688
296.4670	380.3275	413.0128
537.5758	571.4081	761.7407
812.4559	888.6007	979.7406
998.7386	1018.9082	1088.6489
1136.8577	1189.9128	1284.6761
1294.4792	1369.9628	1401.9525
1470.6889	1480.5512	1490.6817
1518.4373	2991.0872	3056.2782
3086.6805	3123.9183	3154.3651
3161.4335	3161.9162	3261.5383

i7
Cartesian coordinates

C	1.946855	-0.495415	-0.329208
C	1.002761	0.257770	0.547411

C	-1.397897	0.405420	-0.208430
C	-1.729095	-0.895418	0.102308
C	-0.144710	0.974921	-0.011299
H	2.560631	0.181924	-0.942485
H	1.401191	-1.135947	-1.031834
H	2.628547	-1.118691	0.253537
H	1.237751	0.381014	1.601373
H	-2.167927	1.038932	-0.642587
H	-2.725019	-1.280731	-0.076644
H	-0.997057	-1.566425	0.539223
H	-0.005602	2.016253	-0.305275

Vibrational frequencies

86.7346	166.4493	224.5268
265.8181	373.6444	456.7673
559.2733	629.8375	724.9486
813.2016	891.2246	984.4220
997.1587	1021.8942	1076.1780
1108.4086	1173.6423	1226.1455
1340.0770	1407.9830	1426.8923
1445.0084	1481.1913	1493.0555
1526.0886	2989.0669	3059.3254
3118.1883	3123.0867	3155.4773
3167.7402	3171.0513	3258.7165

i8
Cartesian coordinates

C	-2.638206	0.114036	0.000008
C	-1.246693	-0.355906	-0.000014
C	1.205757	-0.461199	-0.000005
C	2.536149	0.215197	0.000007
C	-0.002209	0.210046	-0.000015
H	-3.183917	-0.236225	-0.883002
H	-2.674225	1.213148	0.000440
H	-3.184091	-0.236900	0.882639
H	1.191671	-1.547577	0.000024
H	3.127881	-0.068039	-0.878535
H	3.127712	-0.067737	0.878762
H	2.432738	1.303290	-0.000189
H	0.033447	1.307006	-0.000022

Vibrational frequencies

78.0769	100.8926	163.4672
171.7593	242.4134	396.5214
469.9048	730.0678	874.9215
892.3160	956.3022	1013.2623
1026.7207	1031.9024	1138.8358
1236.8708	1270.4279	1390.4857
1415.2617	1449.7274	1450.1191
1474.7133	1479.5803	1494.7365
1522.5662	2997.1979	3017.9515
3047.8706	3067.5592	3069.5452
3084.0484	3117.6373	3179.5593

i9
Cartesian coordinates

C	-2.047160	-0.720618	-0.000262
C	-1.362752	0.605925	-0.002677
C	0.954248	-0.216035	-0.000921
C	2.420193	-0.299667	0.000184
C	0.009981	0.773735	0.000048
H	-1.326641	-1.537025	-0.087112
H	-2.761313	-0.800300	-0.827113
H	-2.617327	-0.868549	0.924617
H	-1.986597	1.494239	0.004225
H	2.794480	-0.839046	0.877161
H	2.864062	0.706338	0.013539
H	2.797757	-0.817433	-0.888366
H	0.388514	1.801738	0.004817

Vibrational frequencies

60.3991	89.8387	157.8629
175.9039	326.5951	364.7248
613.4014	666.0759	876.8342
884.0532	930.4236	1015.8647
1027.7199	1028.4019	1119.9789
1208.8014	1316.1742	1399.6657
1406.2855	1449.3964	1450.8430
1477.1224	1481.2383	1490.7613
1520.1184	2997.8820	3028.4203
3068.6440	3070.6300	3082.5018
3086.5259	3125.4219	3179.8991

Transition states

i10 – i11
Cartesian coordinates

C	0.517836	1.445690	-0.034698
C	0.259489	-0.024434	0.185445
C	-1.761090	-0.257398	-0.336285
C	1.405686	-0.935026	-0.170642
C	-0.883898	-0.508632	0.789125
H	1.379036	1.744584	0.574603
H	-0.337709	2.055837	0.251952
H	0.773896	1.649922	-1.078986
H	-1.792028	-0.954691	-1.169030
H	-2.380953	0.633738	-0.407871
H	2.268646	-0.688822	0.459505
H	1.711288	-0.778863	-1.209413
H	1.149686	-1.982901	-0.018421

Vibrational frequencies

-585.3159	77.5306	200.8093
271.3765	356.6601	367.7574
391.7117	521.4055	603.5245

781.5820 924.5250 942.7529
960.9069 1058.1677 1078.5937
1151.8337 1209.6752 1376.5094
1387.8410 1407.9839 1447.1386
1468.1049 1476.8952 1498.3348
1517.4407 3030.5892 3036.9932
3093.3432 3106.3954 3107.8273
3154.5696 3161.0272 3205.2015

i11 – i12
Cartesian coordinates

C	1.939882	-0.402905	-0.000018
C	0.481200	-0.079123	0.000021
C	-1.941131	-0.340010	-0.000013
C	-0.055942	1.323250	0.000013
C	-0.554664	-0.902560	0.000028
H	2.430610	0.023386	-0.881053
H	2.101745	-1.482181	0.000051
H	2.430680	0.023487	0.880929
H	-2.522092	-0.453732	0.913169
H	-2.521946	-0.453592	-0.913305
H	0.097992	1.901476	-0.912812
H	0.098109	1.901545	0.912775
H	-1.331168	0.947702	0.000059

Vibrational frequencies

-1776.0325 162.3767 216.7474
294.9326 322.5836 423.3416
511.7445 561.2834 617.1061
858.4076 928.2639 952.9639
969.4510 1024.1507 1056.9725
1101.2042 1126.1052 1262.0947
1343.1048 1420.3486 1425.0227
1436.2948 1480.8195 1492.1406
1622.6808 1742.0091 3041.9474
3079.3962 3101.6177 3112.2157
3140.9845 3164.8263 3199.1562

i11 – i13
Cartesian coordinates

C	-1.126893	-1.357756	-0.000034
C	-0.472978	-0.024557	0.002488
C	2.102217	-0.169981	-0.000613
C	-1.090200	1.337428	-0.000828
C	0.848970	0.363861	0.001286
H	-1.801636	-1.464168	0.856996
H	-0.391818	-2.164480	0.037925
H	-1.736559	-1.491414	-0.901382
H	2.242924	-1.249505	-0.000950
H	2.987641	0.452629	-0.001977
H	-1.572391	1.685671	0.915259
H	-1.570398	1.682442	-0.919174
H	0.275541	1.654854	-0.000492

Vibrational frequencies

-2243.0454 38.7343 212.2324
214.4293 264.0760 398.8087
500.7327 601.1849 664.2979
751.9749 772.2589 938.0367
949.1071 977.5793 1049.1404
1057.2432 1179.4052 1247.5674
1289.8290 1394.5446 1412.1466
1456.2650 1475.7074 1476.2330
1511.3568 1874.0545 3028.5934
3064.1210 3083.1202 3123.4339
3131.1239 3153.7512 3236.3059

i11 – i32
Cartesian coordinates

C	0.671176	1.410220	-0.038790
C	0.437869	-0.076534	0.109164
C	-2.136859	-0.148251	-0.035887
C	1.601617	-0.987407	-0.091028
C	-0.891901	-0.576627	0.016923
H	1.659497	1.688820	0.336608
H	-0.077115	1.986480	0.508962
H	0.618663	1.692187	-1.096151
H	-2.375979	0.916582	0.014209
H	-2.975629	-0.831225	-0.127945
H	1.042053	-0.587024	1.084274
H	2.583057	-0.553345	-0.219185
H	1.434039	-2.040876	-0.263071

Vibrational frequencies

-1908.4070 148.8666 188.1785
219.8406 357.8294 368.6259
440.7871 484.7801 585.5483
667.1225 757.4266 819.6117
946.5320 972.0209 1031.7919
1036.1730 1202.1373 1258.8255
1296.1762 1399.3068 1422.0961
1436.6368 1485.1732 1495.3026
1701.5485 2228.6967 3035.8683
3080.1178 3108.2212 3135.5759
3174.5073 3193.6504 3301.9941

i11 – p5
Cartesian coordinates

C	1.525590	1.155198	-0.001673
C	0.242407	0.439473	0.003513
C	-2.315083	0.015548	-0.001978
C	1.018663	-1.680839	0.000504
C	-1.001672	0.384150	0.002273
H	2.168151	0.818408	0.815953
H	1.360315	2.229742	0.101090

H	2.065299	0.973734	-0.935827
H	-2.593701	-1.034290	-0.011443
H	-3.108676	0.753402	0.003106
H	1.410020	-1.727414	1.010846
H	1.747425	-1.625176	-0.801025
H	0.131739	-2.269583	-0.198533

Vibrational frequencies

-596.9546	57.6490	120.8824
130.1729	214.2511	252.7149
343.6793	375.5723	444.6260
517.5537	532.2755	670.5883
766.7034	865.7419	1012.1573
1045.1184	1048.8743	1255.3024
1417.4052	1418.6075	1425.9128
1462.7946	1482.9228	1486.0245
1958.6011	3046.2636	3096.2240
3112.3500	3132.8230	3135.2385
3235.2808	3255.4137	3264.1315

i11 – p6
Cartesian coordinates

C	1.384097	-1.150508	0.002532
C	0.409732	-0.013270	-0.010013
C	-2.173296	-0.299432	0.001275
C	0.944794	1.386810	0.000634
C	-0.947033	-0.237823	-0.003947
H	2.078632	-1.072755	-0.842593
H	0.883261	-2.117239	-0.048565
H	1.993324	-1.124744	0.914959
H	-2.770094	1.571300	0.010602
H	-3.191061	-0.611311	0.005942
H	1.620975	1.546636	-0.847713
H	1.529691	1.567054	0.911281
H	0.145505	2.126391	-0.046796

Vibrational frequencies

-752.0510	43.8493	52.1720
153.8235	213.6299	262.7073
340.8640	371.4743	450.7586
460.6389	610.5592	734.0331
796.9782	962.2226	979.1226
1020.2325	1048.2116	1254.1835
1344.8145	1403.6038	1416.3318
1471.2806	1477.2516	1487.9973
1508.5003	1976.1243	3017.9389
3023.1158	3070.7461	3075.1448
3149.5919	3150.9148	3453.9746

i11 – p8
Cartesian coordinates

C	1.523758	-1.013508	-0.053070

C	0.432957	0.019467	-0.029371
C	-2.151206	-0.178847	-0.073700
C	0.676400	1.339256	-0.175062
C	-0.908869	-0.444194	0.241600
H	2.489773	-0.562940	-0.285806
H	1.307164	-1.787542	-0.794827
H	1.594748	-1.509479	0.920066
H	-2.985461	-0.738559	0.339587
H	-2.397594	0.620199	-0.778312
H	1.665847	1.697974	-0.436059
H	-0.130342	2.063156	-0.169813
H	1.017631	1.884146	1.742785

Vibrational frequencies

-777.0227	126.4766	153.7553
201.7562	218.8816	273.0484
386.2211	419.9111	522.4058
610.9645	782.4221	803.3171
903.2038	964.2224	967.0864
1006.6352	1038.0990	1067.1174
1277.7568	1401.5046	1421.9674
1433.1330	1479.7389	1496.4515
1631.6322	1756.8751	3042.3888
3068.0315	3107.8177	3141.4287
3153.8895	3182.5083	3248.6483

i12 – i13
Cartesian coordinates

C	-0.816258	1.379721	-0.000596
C	-0.553657	-0.114402	-0.002082
C	2.129778	-0.026231	0.001156
C	-1.589508	-1.015054	0.001714
C	0.774724	-0.521061	-0.005957
H	-1.886135	1.590713	-0.044983
H	-0.334302	1.857796	-0.857405
H	-0.410634	1.841623	0.903499
H	2.582651	0.310044	0.931719
H	2.608474	0.264684	-0.931655
H	-2.621302	-0.683402	0.001090
H	-1.395510	-2.080908	0.003779
H	1.786291	-1.318393	0.028547

Vibrational frequencies

-2067.1619	31.1172	76.1637
188.7952	201.3740	407.2268
484.7382	552.0834	576.6367
766.7085	800.0475	801.9798
930.8925	944.3405	1009.7986
1037.8808	1064.8483	1220.2029
1360.3481	1406.0312	1416.5192
1466.4113	1484.7452	1501.8027
1529.1336	2254.1852	3052.9908
3094.3316	3121.1699	3142.0234

3159.5734 3199.0276 3259.7867

i12 – i14
Cartesian coordinates

C	-1.370940	-1.135876	-0.000100
C	-0.586059	0.150766	0.000036
C	2.081342	-0.001237	0.000044
C	-0.996218	1.456066	-0.000079
C	0.667045	-0.445619	0.000326
H	-1.878874	-1.420810	0.920322
H	-0.055466	-1.634688	-0.001070
H	-1.880544	-1.420029	-0.919824
H	2.141223	1.090935	0.070443
H	2.594778	-0.313179	-0.915350
H	2.630771	-0.428649	0.844433
H	-2.047844	1.715876	0.000558
H	-0.275063	2.265943	-0.000877

Vibrational frequencies

-2177.7225 43.1453 203.2998
218.4867 362.5720 417.9464
485.8078 591.9101 592.9864
787.3572 798.9504 916.5170
972.7861 1009.4694 1042.8427
1060.0024 1095.0150 1145.8443
1363.9327 1389.2359 1412.5963
1451.7782 1462.4699 1491.9817
1521.3501 1893.9883 3022.6858
3095.7350 3098.3687 3100.9352
3157.6946 3198.4975 3253.8093

i12 – p5
Cartesian coordinates

C	-1.126765	-1.645111	0.000015
C	-0.387115	0.528201	-0.000012
C	2.227140	-0.039393	0.000007
C	-1.585621	1.205441	0.000000
C	0.860771	0.454924	-0.000023
H	-1.689949	-1.619834	0.925393
H	-0.221146	-2.239694	0.000153
H	-1.689692	-1.619882	-0.925521
H	2.773045	0.304818	-0.883811
H	2.242015	-1.135644	0.001638
H	2.773999	0.307471	0.882192
H	-1.583289	2.289220	0.000208
H	-2.535442	0.689171	-0.000180

Vibrational frequencies

-548.0986 68.3612 92.2917
118.9447 162.9744 213.0574
263.6384 363.2703 399.7392
510.3291 519.9554 691.8906

768.5044 844.8549 1021.8984
1031.3297 1032.5803 1252.2105
1410.9721 1421.4319 1424.6880
1469.7840 1472.2971 1476.5833
1919.9592 3019.0525 3087.2115
3096.8640 3098.0467 3159.5025
3260.2708 3263.7342 3264.2940

i12 – p8
Cartesian coordinates

C	-1.494697	-1.064365	-0.000080
C	-0.517029	0.097317	0.000201
C	2.103639	-0.344166	0.000031
C	-0.995833	1.407717	-0.000003
C	0.806556	-0.161544	0.000112
H	-2.139901	-1.015484	0.880556
H	-0.975405	-2.022771	0.006489
H	-2.130687	-1.022741	-0.887795
H	2.653996	-0.496628	-0.926366
H	2.654213	-0.496078	0.926389
H	2.901254	1.591978	-0.000681
H	-2.061947	1.601188	0.000210
H	-0.317340	2.250783	-0.000378

Vibrational frequencies

-511.9288 26.7655 148.5091
160.0610 203.3204 303.5523
376.1615 477.9901 519.9335
603.0505 627.5394 733.7501
776.8832 922.2351 962.8070
991.1417 1003.7178 1054.5980
1266.9295 1299.9994 1411.4231
1449.4655 1486.1417 1493.7902
1501.5075 1872.8325 3052.9793
3101.8961 3124.0973 3149.9735
3161.1198 3177.7275 3267.6230

i13 – i14
Cartesian coordinates

C	-0.119549	1.380852	-0.000011
C	-0.563545	-0.057276	-0.000031
C	1.836948	-0.170845	0.000000
C	-1.881956	-0.457849	0.000002
C	0.545907	-0.900367	0.000012
H	-0.318083	1.949085	-0.908333
H	1.203238	1.038334	-0.000114
H	-0.317958	1.948942	0.908428
H	2.444956	-0.235521	0.905191
H	2.445011	-0.235731	-0.905133
H	-2.140434	-1.511208	-0.000083
H	-2.691336	0.262138	0.000140
H	0.467774	-1.983130	0.000062

Vibrational frequencies

-1900.0898 145.8366 283.2210
363.0659 451.6823 556.3895
583.6374 647.5766 659.6039
702.5031 778.7007 880.1131
926.2921 991.0816 1006.8509
1020.6105 1050.3977 1119.5215
1245.4788 1374.0068 1375.7019
1396.6318 1435.6938 1445.7864
1516.7926 1669.7416 3068.0199
3100.4126 3138.9798 3154.4340
3182.7246 3188.3286 3255.6208

i13 – i15
Cartesian coordinates

C	-1.103870	1.223549	-0.169859
C	-0.580972	-0.153003	0.087046
C	1.964481	-0.114642	-0.294752
C	-1.103604	-1.360053	-0.054746
C	0.805627	0.300560	0.503734
H	-1.281715	1.506394	-1.205967
H	0.224860	1.530053	0.179607
H	-1.794800	1.650964	0.555492
H	2.249120	0.425780	-1.190152
H	2.427519	-1.082654	-0.123106
H	-2.124150	-1.497082	-0.396191
H	-0.526046	-2.252571	0.162990
H	0.935239	0.340646	1.588791

Vibrational frequencies

-2145.4751 81.6670 202.4214
287.7367 305.4423 393.2662
458.7566 563.9188 589.0421
698.3681 785.2160 862.3648
923.5151 929.6323 963.4160
1014.5617 1052.5025 1125.6077
1230.0624 1263.7621 1345.9401
1401.8137 1442.6785 1454.3557
1717.0893 1876.1785 3089.9442
3097.2548 3128.9640 3150.7164
3199.0119 3234.9439 3237.6006

i13 – i32
Cartesian coordinates

C	0.655888	1.396539	-0.033987
C	0.511287	-0.110755	0.055414
C	-2.098654	-0.125256	-0.065674
C	1.636112	-0.937209	-0.061143
C	-0.836648	-0.620106	-0.010768
H	1.682273	1.702863	0.173693
H	-0.006458	1.904926	0.669848
H	0.378970	1.720635	-1.041545

H	-0.162765	-0.556366	1.154609
H	-2.331734	0.879997	0.284176
H	-2.929643	-0.757278	-0.354434
H	2.624340	-0.499546	-0.098309
H	1.537111	-2.014513	-0.091087

Vibrational frequencies

-1812.2589 166.1121 177.2719
210.7949 318.2411 402.7135
468.2722 504.9162 591.7084
643.2677 660.9674 782.7651
938.7217 960.3546 1001.1801
1035.2010 1068.1012 1235.5687
1342.6956 1398.2502 1410.6338
1477.0851 1499.6286 1502.3950
1555.2878 1797.1229 3054.1145
3113.2969 3128.5447 3147.7162
3175.0381 3222.8646 3282.5095

i13 – i33
Cartesian coordinates

C	-0.650055	1.431539	0.042904
C	-0.475697	-0.040800	-0.137218
C	2.013945	-0.039230	0.112082
C	-1.656190	-0.876590	0.133621
C	0.844397	-0.652160	-0.130992
H	-0.648903	0.718795	-1.118849
H	0.208722	2.083865	0.116736
H	-1.639782	1.816037	0.244764
H	2.081108	1.010398	0.375683
H	2.946663	-0.587272	0.057331
H	-2.516370	-0.886362	-0.525942
H	-1.740678	-1.378300	1.091942
H	0.850842	-1.713717	-0.364052

Vibrational frequencies

-1873.3674 129.6691 232.5199
286.1367 354.7451 381.3661
451.2573 514.0458 532.3344
643.7059 682.5809 788.4732
871.9414 945.6712 998.2298
1009.8857 1055.4697 1203.0996
1252.6591 1313.2711 1327.1745
1417.4864 1458.2087 1461.7440
1645.5147 2230.3321 3140.1821
3161.6645 3170.8810 3179.3509
3244.2042 3251.8833 3301.2454

i13 – i37
Cartesian coordinates

C	1.907111	-0.182499	-0.061999
C	0.481107	0.040306	0.304946

C	-1.728210	-0.220113	-0.089369
C	-0.294159	1.221437	-0.078723
C	-0.558588	-0.990841	0.133633
H	2.521749	0.690212	0.172515
H	2.016798	-0.383776	-1.140659
H	2.318373	-1.045818	0.468305
H	-2.456309	-0.529773	-0.840926
H	-2.190114	0.312831	0.737485
H	0.075048	1.826786	-0.914186
H	-0.783235	1.825679	0.682413
H	-0.345882	-1.905884	-0.415872

Vibrational frequencies

-1037.0555 93.7557 116.9418
284.5214 329.7989 531.3885
583.8729 689.3552 832.5472
853.1552 912.5780 947.0035
965.0053 991.7951 1003.1932
1043.9904 1202.7667 1239.5543
1316.5269 1395.5074 1412.6909
1464.4680 1480.6524 1488.6492
1521.6709 2970.8271 3053.0469
3079.1780 3098.0935 3125.8974
3143.7095 3152.6601 3176.6410

i13 – p10
Cartesian coordinates

C	-0.612591	1.778895	-0.000006
C	-0.444075	-0.560454	-0.000002
C	1.976026	0.036115	0.000010
C	-1.726113	-0.900058	0.000007
C	0.890750	-0.823988	-0.000011
H	-1.686245	1.916363	-0.000044
H	-0.095339	1.993654	-0.927889
H	-0.095407	1.993652	0.927915
H	1.864652	1.110866	0.000049
H	2.979668	-0.368627	-0.000009
H	-2.291844	-0.968940	-0.926840
H	-2.291819	-0.968976	0.926867
H	1.112359	-1.891046	-0.000039

Vibrational frequencies

-524.3076 102.5798 174.9711
229.3578 243.0022 285.3170
459.2619 465.5330 510.7453
548.4382 550.6181 762.8182
804.6142 831.2028 899.2197
952.0698 983.3670 1080.7067
1213.2400 1383.3810 1417.7089
1433.0282 1449.1772 1510.7936
1735.2503 3096.5134 3103.3543
3133.2772 3181.0600 3181.3530
3265.8231 3267.5343 3283.3426

i13 – p7
Cartesian coordinates

C	0.701862	1.301709	-0.209304
C	0.472887	-0.039086	-0.135947
C	-1.999541	0.019318	0.149285
C	1.590668	-0.943893	0.134078
C	-0.869882	-0.615373	-0.173000
H	0.855513	1.656333	1.543284
H	-0.093973	1.996957	-0.447717
H	1.716069	1.677070	-0.289905
H	-2.000630	1.046772	0.498152
H	-2.957914	-0.482649	0.091374
H	1.423328	-1.999440	0.305860
H	2.604415	-0.565899	0.162468
H	-0.922770	-1.665195	-0.454191

Vibrational frequencies

-1586.6398 102.8314 179.4839
218.8542 280.2084 335.6211
425.1547 495.7012 524.8024
600.4636 730.7834 825.8870
840.1670 951.2834 981.2712
997.1419 1011.3077 1026.6869
1097.7819 1292.8140 1344.8048
1422.7294 1464.4148 1481.5770
1613.3490 1688.1545 3150.1309
3156.5599 3160.7460 3166.7083
3247.3870 3250.6469 3278.8363

i13 – p8
Cartesian coordinates

C	1.103348	-1.299416	-0.000019
C	0.486149	0.091883	0.000081
C	-2.146532	-0.146377	0.000014
C	1.332564	1.198874	0.000005
C	-0.866481	0.155275	0.000010
H	1.729532	-1.432497	-0.885754
H	0.338827	-2.075760	0.002684
H	1.734007	-1.430666	0.882794
H	-2.710251	-0.224252	0.927553
H	-2.710188	-0.224514	-0.927541
H	2.406887	1.059634	0.000135
H	0.937815	2.206587	-0.000182
H	-1.180915	2.120032	-0.000231

Vibrational frequencies

-813.7319 37.3055 99.7034
230.7141 260.2579 397.6849
486.3818 504.6365 558.4010
574.6319 590.4753 738.0228
784.8026 884.4969 961.6584

990.0383 1008.7921 1054.7519
1266.8625 1294.9029 1408.7742
1450.7870 1479.0818 1494.5787
1499.8248 1827.3832 3051.4365
3100.9119 3122.0745 3152.5680
3157.8587 3178.7919 3264.1209

i14 – i15
Cartesian coordinates

C	-0.690590	1.395082	-0.018121
C	-0.574112	0.005940	-0.015696
C	2.043836	0.033068	-0.027270
C	-1.725124	-0.790911	0.007130
C	0.727524	-0.649700	-0.026309
H	-1.667825	1.859777	0.029058
H	0.168159	2.050392	-0.084087
H	2.114333	1.103880	0.095615
H	1.398023	-0.534698	1.026463
H	2.922142	-0.528606	-0.310792
H	-1.662666	-1.872728	0.006322
H	-2.709043	-0.338744	0.015016
H	0.747670	-1.700145	-0.295995

Vibrational frequencies

-1852.9711 103.2488 295.3815
344.4736 438.8019 470.7683
500.9390 522.3059 564.5759
637.0558 689.3171 741.9667
814.5342 827.8186 986.7546
1024.1579 1049.5377 1179.2963
1239.6529 1294.2520 1363.2834
1435.9270 1476.3296 1498.2943
1536.8834 2252.1252 3164.4446
3172.5522 3181.4783 3187.7563
3266.5213 3269.0639 3300.5817

i14 – i34
Cartesian coordinates

C	1.739080	-0.461863	0.277260
C	0.729817	0.255179	-0.562876
C	-1.430317	-1.106403	0.026134
C	-0.699282	1.322087	0.337691
C	-0.724738	0.111834	-0.326177
H	2.619581	0.158047	0.476181
H	2.093306	-1.373772	-0.223532
H	1.312612	-0.765574	1.236361
H	1.078770	0.787709	-1.445389
H	-1.123417	-1.723012	0.868623
H	-2.214793	-1.495623	-0.614480
H	-1.106164	1.463521	1.344680
H	-0.347253	2.223698	-0.154636

Vibrational frequencies

-1068.2392 105.0546 169.3121
227.3949 288.5259 345.8394
430.0427 521.3433 656.7926
705.8774 837.9968 910.8190
969.2091 988.3746 1011.0578
1018.4489 1104.8445 1208.9272
1337.0977 1407.6337 1422.2838
1463.8103 1476.8453 1491.2507
1543.9228 3006.6910 3052.5152
3066.8471 3113.7917 3120.3485
3142.3639 3182.6854 3215.8706

i14 – p26
Cartesian coordinates

C	-0.972778	1.729273	-0.020137
C	-0.436067	-0.540941	-0.163931
C	1.930462	0.042224	0.378261
C	-1.574075	-1.081500	0.190731
C	0.832887	-0.422357	-0.531556
H	-1.644981	1.977528	0.794240
H	-0.658562	2.368446	-0.837086
H	1.597851	0.064659	1.416741
H	2.799417	-0.618075	0.300816
H	2.260152	1.050485	0.104355
H	-1.617050	-2.146927	0.397779
H	-2.486825	-0.508284	0.289451
H	1.067421	-0.548023	-1.586502

Vibrational frequencies

-445.4552 55.6159 76.2129
123.4747 188.0153 233.7345
319.4693 370.0768 403.9004
527.3494 594.2809 837.6313
879.0260 904.5508 1009.2917
1047.2935 1096.1220 1138.7635
1158.1068 1361.7791 1411.5857
1467.7157 1484.5330 1502.6523
1973.1876 3034.5376 3096.2912
3105.3005 3138.2806 3144.7039
3155.2209 3238.9615 3310.1358

i14 – p7
Cartesian coordinates

C	0.686239	1.399573	-0.020082
C	0.592254	0.011058	0.010637
C	-1.899898	-0.123021	-0.271116
C	1.729701	-0.782029	0.025567
C	-0.720448	-0.666357	0.041145
H	1.655385	1.881374	-0.066724
H	-0.187754	2.035862	0.031439
H	-1.992853	0.897411	-0.626586
H	-2.807804	-0.713383	-0.242990

H	-2.679580	0.778314	1.792897
H	1.662225	-1.862824	0.062735
H	2.718402	-0.339808	-0.004927
H	-0.695107	-1.712290	0.337252

Vibrational frequencies

-298.8390 61.0341 151.9615
209.6892 304.2485 432.5533
442.7240 514.6295 550.5165
556.2009 742.4872 767.2943
810.6467 829.2178 954.0002
984.4423 1026.8107 1039.5863
1077.2258 1301.1983 1349.5323
1376.1830 1461.2121 1494.5490
1535.6198 1681.2209 3155.2624
3157.8941 3164.3945 3168.9470
3248.7364 3257.4825 3264.9904

i15 – i33
Cartesian coordinates

C	0.692934	1.412086	-0.000371
C	0.527205	0.000917	0.065597
C	-2.031026	0.012987	-0.117578
C	1.672192	-0.828783	-0.119685
C	-0.832515	-0.621858	0.055523
H	-0.143329	2.093078	0.083851
H	1.687108	1.830414	-0.079476
H	-0.085450	-0.302212	1.221496
H	-2.105084	1.080613	-0.281965
H	-2.953460	-0.549244	-0.061373
H	2.662669	-0.394886	-0.092429
H	1.579098	-1.903504	-0.214327
H	-0.814294	-1.706358	0.123311

Vibrational frequencies

-1632.3047 189.4227 296.1085
387.3383 398.9920 424.6880
463.3451 539.1681 590.4515
609.4508 709.6417 755.5357
806.8574 905.5926 977.3533
1002.9058 1056.5347 1135.6348
1279.9455 1304.8287 1354.5935
1441.1006 1484.8054 1499.2488
1549.8155 1604.0810 3169.3582
3172.7262 3176.5140 3183.4138
3269.2176 3277.9527 3283.8456

i15 – i39
Cartesian coordinates

C	-0.093614	1.295160	-0.151736
C	0.547279	0.063001	-0.257207
C	-1.551810	-0.108085	0.472456

C	1.871838	-0.273348	0.238227
C	-0.599519	-0.926083	-0.391279
H	-0.853194	1.577729	-0.875519
H	0.388215	2.142070	0.337264
H	-2.569104	0.081262	0.133726
H	-1.435646	-0.225358	1.545625
H	2.015659	-0.653300	1.248093
H	2.739635	-0.265706	-0.414917
H	-0.969105	-1.032353	-1.417750
H	-0.361507	-1.928211	-0.019284

Vibrational frequencies

-936.4498	121.7958	299.1017
333.7839	346.2785	514.1042
537.7094	626.0713	771.6002
809.4322	847.5411	905.0928
949.9736	981.4743	992.2037
1021.0013	1056.4943	1191.5339
1220.4070	1255.3584	1402.7132
1448.8719	1456.8336	1484.4425
1546.6769	3037.9335	3078.9380
3107.1231	3110.5196	3111.3610
3187.0117	3202.8268	3221.6606

i15 – p25
Cartesian coordinates

C	1.803447	-0.916338	-0.000339
C	0.881845	0.082820	-0.000013
C	-2.173486	0.198410	-0.000616
C	0.904957	1.440650	0.000177
C	-1.274283	-0.805677	0.000794
H	2.870350	-0.693936	-0.000478
H	1.514581	-1.962061	-0.000477
H	-2.532958	0.634190	-0.926386
H	-2.533229	0.636570	0.923927
H	1.848289	1.985289	0.000044
H	-0.014600	2.016050	0.000425
H	-1.003544	-1.308817	-0.920836
H	-1.003772	-1.306482	0.923762

Vibrational frequencies

-341.0099	51.8102	153.3072
227.3588	247.3734	312.2306
384.4546	492.3253	688.4088
772.0577	785.9987	834.5095
886.4566	914.0317	926.3390
1031.7132	1036.4433	1162.1436
1241.4652	1327.0620	1357.8828
1463.8118	1465.6418	1476.0972
1607.3840	3101.1173	3111.2043
3142.9701	3155.6376	3208.4491
3214.3911	3226.6696	3251.6650

i15 – p7
Cartesian coordinates

C	1.597380	-0.880349	-0.167334
C	0.553568	0.006177	0.020028
C	-1.937413	0.042581	-0.297671
C	0.760503	1.377330	0.074344
C	-0.823407	-0.558369	0.155080
H	2.612701	-0.524131	-0.295090
H	1.431592	-1.950676	-0.195790
H	-2.898222	-0.455051	-0.245772
H	-1.919625	1.049176	-0.700865
H	1.752370	1.789253	-0.067181
H	-0.046225	2.065563	0.292948
H	-0.874709	-1.607282	0.434765
H	-0.961669	-0.291067	2.070309

Vibrational frequencies

-884.7672	99.5701	287.7944
335.2294	379.5657	435.9345
472.6856	533.8074	559.8598
568.3578	708.7543	776.2490
814.0494	818.9606	930.7690
982.5305	1043.2350	1047.0884
1072.4166	1286.5065	1324.7385
1369.3633	1460.0376	1488.2254
1538.3180	1655.9603	3155.5765
3157.0786	3163.6960	3169.1333
3251.9339	3257.2290	3263.4020

i16 – i17
Cartesian coordinates

C	-2.073032	0.414092	-0.040430
C	-0.245672	-0.509006	0.347743
C	0.799082	0.559714	0.136844
C	2.159788	-0.074784	-0.170906
C	-1.338328	-0.761714	-0.448397
H	-2.611821	0.423942	0.901938
H	-2.089848	1.325066	-0.635327
H	-0.002826	-1.205803	1.163843
H	0.880434	1.167697	1.044860
H	0.495744	1.221637	-0.676839
H	2.921726	0.697556	-0.298294
H	2.113524	-0.665315	-1.088939
H	2.482041	-0.734589	0.639642

Vibrational frequencies

-730.6839	85.9652	218.9433
228.6913	358.8975	394.9322
522.2787	613.2210	793.7408
869.1965	890.7677	960.5561
1020.5317	1085.9558	1114.0387
1141.1376	1220.8974	1279.4207

1334.4131 1406.8089 1418.5290
1469.2349 1480.5383 1501.0696
1506.7435 3016.5020 3048.1674
3049.2514 3107.8420 3112.2873
3129.4104 3134.7541 3212.5558

i16 – i44
Cartesian coordinates

C	1.458381	-0.295358	0.492616
C	0.505258	0.735628	-0.233789
C	-0.968200	0.756609	0.170984
C	-1.473379	-0.674365	0.052018
C	0.853043	-0.563358	-0.801358
H	2.499114	0.015749	0.547518
H	1.093517	-0.792271	1.391842
H	0.981356	1.671148	-0.511020
H	-1.511833	1.425079	-0.501693
H	-1.092098	1.149953	1.186968
H	-0.376780	-1.126561	-0.611712
H	-2.361888	-0.835467	-0.553302
H	-1.482005	-1.262564	0.968572

Vibrational frequencies

-1908.2695 163.5948 324.9509
454.4791 585.7490 637.0793
718.5531 832.8758 874.8080
903.1373 965.3161 1000.2191
1016.3166 1046.1183 1064.8604
1069.7001 1109.7161 1218.7960
1229.3953 1306.2269 1331.5195
1364.7957 1458.8530 1478.9768
1490.1943 1634.5255 3044.8282
3088.8467 3101.5651 3114.7899
3166.5103 3175.2203 3201.7071

i17 – i18
Cartesian coordinates

C	-2.126150	-0.448856	0.276246
C	-0.061533	0.949505	-0.347120
C	1.129612	0.481646	0.420139
C	1.756767	-0.797257	-0.141628
C	-1.210577	-0.011281	-0.550096
H	-2.156914	-0.122464	1.320576
H	-2.897387	-1.147413	-0.038393
H	-0.330564	2.002223	-0.294819
H	0.843334	0.301655	1.470783
H	1.869485	1.288281	0.449629
H	2.107379	-0.640780	-1.164586
H	1.028447	-1.612016	-0.155870
H	2.607502	-1.112032	0.467433

Vibrational frequencies

-429.3042 91.3882 187.1008
 247.4088 297.8624 386.9961
 512.5654 603.4966 765.2395
 849.8866 894.1978 918.9863
1021.6718 1061.8997 1093.1302
1129.1748 1274.7009 1307.7418
1364.0473 1392.0613 1422.3837
1463.6836 1499.1206 1511.3651
1727.4952 2959.0217 3053.0749
3058.6611 3076.0523 3130.1322
3134.4916 3156.8272 3181.7144

i17 – i40
Cartesian coordinates

C	2.340362	-0.476550	-0.096868
C	0.080104	0.746418	0.058371
C	-0.907121	-0.362540	0.242434
C	-2.330089	-0.190361	-0.176617
C	1.474515	0.518394	-0.059610
H	2.012274	-1.517711	-0.145087
H	3.412496	-0.306581	-0.105092
H	-0.335281	1.693961	-0.271830
H	-0.417837	0.486685	1.184374
H	-0.498369	-1.350527	0.416869
H	-2.993681	-0.875429	0.355086
H	-2.448769	-0.372861	-1.253515
H	-2.677451	0.830299	0.012933

Vibrational frequencies

-1894.7828 120.5691 174.9788
 191.3211 321.0965 386.1985
 489.0761 522.3701 669.8400
 797.7589 815.4640 885.7188
 981.1744 1026.6095 1059.4961
1110.6126 1168.1379 1235.5298
1318.9526 1394.9235 1419.4569
1429.9267 1486.6728 1498.6656
1691.9437 2216.0117 3009.8707
3077.0882 3080.8568 3128.4010
3173.1538 3193.3128 3209.2502

i17 – i45
Cartesian coordinates

C	-1.550322	-0.623433	0.154703
C	0.122157	1.222246	-0.123789
C	1.224720	0.276019	0.326809
C	0.974481	-1.104277	-0.274509
C	-1.104283	0.743504	-0.179852
H	-2.423673	-0.999626	-0.374705
H	-1.574720	-0.849681	1.221582
H	0.368823	2.229242	-0.446523
H	1.239602	0.205115	1.420563
H	2.208037	0.655628	0.026759

H	-0.355367	-1.229839	-0.146689
H	1.438994	-1.947433	0.235827
H	1.097790	-1.147765	-1.356986

Vibrational frequencies

-1921.7579 142.0691 336.7337
387.3219 499.9961 522.7561
638.1695 677.0890 739.9449
857.3070 892.4898 952.8294
977.2776 1033.3046 1067.2785
1091.6500 1098.2240 1245.6270
1278.5958 1320.4518 1387.7642
1449.6081 1455.2456 1483.7441
1512.3250 1697.8646 3036.7924
3074.6340 3092.9951 3096.5626
3177.1446 3179.5426 3181.9688

i17 – i9
Cartesian coordinates

C	1.612145	-0.847546	-0.005989
C	0.170592	1.113534	-0.023805
C	-0.699561	0.031278	0.547415
C	-1.877742	-0.427829	-0.279577
C	1.355781	0.599202	-0.299148
H	2.319418	-1.074521	0.788450
H	1.668863	-1.519853	-0.859320
H	-0.145222	2.137576	-0.187629
H	-0.904479	0.139248	1.615839
H	0.245842	-0.876289	0.499482
H	-2.352201	-1.310429	0.156472
H	-1.564272	-0.669606	-1.298721
H	-2.635244	0.362042	-0.347947

Vibrational frequencies

-1725.5351 132.2551 217.7601
262.2318 352.3326 471.1239
543.4443 706.5739 786.0035
845.1068 901.8108 929.9926
999.2455 1021.4383 1065.3522
1095.9412 1142.6703 1239.1326
1319.8446 1361.8578 1411.0755
1432.2164 1493.7258 1496.0447
1629.4700 1700.1092 3030.9995
3092.8448 3101.1163 3117.2299
3131.0691 3204.3741 3204.8800

i17 – p10
Cartesian coordinates

C	1.967008	-0.830240	0.177821
C	0.236525	1.032927	-0.305652
C	-0.742638	0.850714	0.613147
C	1.419640	0.229629	-0.373259

H	1.472773	-1.377952	0.985091
H	2.935296	-1.207996	-0.137883
H	0.106722	1.789912	-1.074466
H	-1.590775	1.523336	0.654698
H	-0.597117	0.192864	1.461835
C	-2.150399	-0.918639	-0.265275
H	-2.804882	-1.062034	0.586019
H	-1.350886	-1.630984	-0.422182
H	-2.551951	-0.413493	-1.133804

Vibrational frequencies

-372.0973	64.6959	91.2743
137.2661	222.1581	269.1612
437.2688	457.0040	488.0116
535.7576	712.4632	742.9624
876.7038	881.7432	916.2130
984.7267	1021.1222	1089.7070
1296.2658	1404.1136	1413.2135
1420.0077	1436.0321	1568.9043
1715.6953	3063.0441	3102.2956
3156.0028	3163.3225	3178.3952
3253.0989	3273.4081	3280.7079

i17 – p11
Cartesian coordinates

C	-2.462889	0.205604	-0.195275
C	-0.066169	-0.731698	0.129192
C	1.036615	0.183790	0.569162
C	2.187542	0.237012	-0.442528
C	-1.355194	-0.309408	-0.063832
H	-2.217807	2.094326	0.289087
H	-3.492653	0.400756	-0.382215
H	0.172485	-1.774478	-0.061749
H	1.425104	-0.169373	1.533201
H	0.633851	1.185304	0.736749
H	2.989082	0.885336	-0.080407
H	1.841639	0.624309	-1.403694
H	2.608873	-0.757978	-0.611285

Vibrational frequencies

-750.5293	29.1100	153.4284
208.6982	253.2071	357.8021
384.1995	406.6780	494.2084
566.1299	653.9121	780.9890
803.2846	890.5818	1009.7882
1067.3799	1115.8631	1162.8896
1280.0611	1325.9952	1413.7748
1419.6326	1486.2258	1502.2479
1508.5407	1963.7384	3024.8120
3044.8158	3099.4548	3124.2660
3129.8517	3167.5032	3451.5265

i17 – p13

Cartesian coordinates

C	-2.381956	-0.410315	0.120356
C	-0.045744	0.693599	0.017780
C	0.855121	-0.312318	-0.066586
C	2.326041	-0.138140	0.166264
C	-1.462766	0.501440	-0.085443
H	-3.429893	-0.234409	-0.105374
H	-2.132722	-1.387434	0.543294
H	0.314603	1.715312	0.116094
H	0.896508	-0.466256	-2.049841
H	0.485324	-1.333700	-0.126072
H	2.914197	-0.711884	-0.553218
H	2.589790	-0.498827	1.166168
H	2.618017	0.911595	0.094724

Vibrational frequencies

-854.3702	110.3470	157.8803
167.3114	228.3561	351.2350
384.1619	430.0677	505.6650
582.0714	837.0413	899.1416
909.0698	983.5655	1006.6848
1042.7040	1064.9567	1129.0044
1300.5363	1318.2065	1414.2854
1420.8662	1480.7868	1491.4405
1631.7971	1747.4789	3048.1328
3073.3677	3115.9197	3139.4092
3158.6281	3169.3219	3184.9099

i17 – p9
Cartesian coordinates

C	-2.090674	-0.727527	0.000002
C	-0.434433	1.272798	-0.000002
C	1.677506	0.474238	0.000005
C	1.550095	-1.012919	-0.000004
C	-1.311927	0.393998	-0.000002
H	-3.172665	-0.658833	-0.000001
H	-1.642043	-1.715989	0.000010
H	-0.105900	2.289217	-0.000005
H	2.010212	0.954638	0.915756
H	2.010221	0.954648	-0.915738
H	1.011795	-1.362266	-0.885421
H	1.011790	-1.362276	0.885407
H	2.533186	-1.502666	-0.000003

Vibrational frequencies

-568.7997	64.1796	102.9194
179.8727	210.4935	356.9860
373.2945	412.4167	548.4354
577.4835	693.1801	696.2570
813.2355	836.7810	1013.3335
1019.9043	1080.6403	1083.4144
1219.5389	1401.0310	1453.0402

1472.1371 1488.9222 1495.2148
1862.7575 3011.6816 3079.9835
3116.2546 3123.7894 3135.3211
3219.1290 3229.4426 3390.9187

i18 – i19
Cartesian coordinates

C	-2.235754	-0.278659	-0.000006
C	-0.015847	0.955521	0.000015
C	1.434842	0.546561	-0.000022
C	1.426736	-0.979314	0.000005
C	-0.883873	-0.109562	0.000028
H	-2.908497	0.577286	-0.000050
H	-2.686219	-1.264319	-0.000048
H	-0.330628	1.995518	0.000034
H	1.953656	0.953853	0.876099
H	1.953589	0.953821	-0.876199
H	0.093537	-1.090318	0.000052
H	1.784023	-1.466540	0.905020
H	1.783920	-1.466587	-0.905025

Vibrational frequencies

-1875.1739 136.0781 236.8267
272.9801 500.9317 560.3653
582.8253 703.7474 707.3545
771.8113 841.7265 906.1973
970.3745 1027.4148 1060.8225
1063.2681 1192.8569 1228.9602
1274.3820 1284.0732 1317.9333
1415.0317 1464.0221 1483.5209
1493.2945 1705.6560 3034.6411
3063.0157 3119.1451 3121.5611
3171.9758 3202.2008 3231.2131

i18 – i6
Cartesian coordinates

C	-2.418329	-0.325378	0.117942
C	-0.117894	0.836234	0.102416
C	1.035188	0.125422	-0.532571
C	2.158291	-0.383940	0.336751
C	-1.089384	-0.112743	-0.102500
H	-3.026995	0.432254	0.608329
H	-2.905436	-1.243322	-0.186213
H	-0.156272	1.806110	0.587281
H	1.334625	0.495051	-1.517264
H	-0.000399	-0.799521	-0.721413
H	2.814289	-1.057766	-0.218812
H	1.763928	-0.918187	1.205454
H	2.769033	0.447814	0.710408

Vibrational frequencies

-2257.9195 113.4590 199.2449

281.1278 348.0143 375.2015
523.4628 605.4572 722.2113
772.3190 825.8818 900.8521
966.3272 1027.6407 1072.5652
1107.1062 1175.7486 1211.0929
1248.9987 1336.7937 1398.0997
1412.5074 1477.5419 1489.7012
1491.7718 1854.6726 3025.7104
3088.8730 3097.8550 3125.9994
3133.6830 3196.2363 3242.1612

i18 – p10
Cartesian coordinates

C	-2.485506	-0.508505	0.005611
C	-0.229106	0.677915	0.323482
C	0.946706	0.970179	-0.281635
C	-1.292319	-0.045888	-0.292762
H	-2.916066	-0.364400	0.999972
H	-3.094529	-1.047346	-0.714061
H	-0.377691	0.962120	1.368004
H	1.676283	1.601806	0.208977
H	1.079394	0.789945	-1.341457
C	2.411347	-0.901973	0.097595
H	1.780712	-1.664712	-0.339967
H	2.477079	-0.864937	1.177290
H	3.268086	-0.562846	-0.472504

Vibrational frequencies

-372.8175 80.9458 83.4165
182.9367 233.7653 244.9029
442.1684 458.2372 485.0499
529.0485 754.6512 756.7032
876.6915 878.2215 925.0234
961.5606 997.0901 1153.7788
1283.3819 1389.3941 1414.2220
1420.6003 1437.8721 1579.8819
1718.3347 3069.4760 3092.2232
3101.4641 3164.4335 3185.0591
3261.1579 3271.1915 3279.8215

i18 – p11
Cartesian coordinates

C	2.138917	-0.581488	0.000001
C	0.060771	0.974062	-0.000003
C	-1.379100	0.557330	0.000004
C	-1.609423	-0.949788	-0.000003
C	1.118795	0.103134	0.000000
H	3.625817	0.698563	-0.000012
H	2.849551	-1.374173	0.000016
H	0.286785	2.036988	-0.000006
H	-1.869301	1.011701	-0.871576
H	-1.869288	1.011689	0.871599
H	-1.162657	-1.414649	0.882269

H	-1.162671	-1.414638	-0.882289
H	-2.677995	-1.174982	0.000004

Vibrational frequencies

-763.5578 62.6800 138.6938
194.9398 262.0291 289.6345
413.2669 432.1210 481.8826
620.8976 634.8624 786.1043
804.3569 856.7747 995.5762
1075.9501 1098.8182 1157.2615
1283.1630 1365.0501 1393.5021
1431.2146 1477.0056 1502.5159
1507.5142 1963.4051 3013.1713
3036.6199 3051.4850 3127.4731
3132.3360 3166.2691 3451.3560

i18 – p13
Cartesian coordinates

C	-2.414087	-0.324299	-0.043351
C	-0.100564	0.774759	0.140995
C	1.230101	0.551659	0.113399
C	1.869675	-0.801105	0.033639
C	-1.105368	-0.228501	-0.030060
H	-3.048160	0.552910	0.109789
H	-2.923889	-1.269582	-0.205064
H	-0.459536	1.797249	0.275496
H	1.887124	1.391889	0.318826
H	1.545562	1.138528	-1.861359
H	1.158279	-1.555807	-0.306692
H	2.234579	-1.096590	1.023191
H	2.727501	-0.793679	-0.641919

Vibrational frequencies

-653.5770 129.1999 162.8237
167.5467 243.1693 330.6095
366.2823 398.5848 553.2871
622.2140 799.3980 877.1858
891.5132 949.2492 994.4547
1033.4308 1063.8841 1143.9876
1253.2528 1377.3869 1409.9929
1440.2746 1483.5265 1487.7380
1640.6507 1741.0846 3041.9149
3071.2619 3101.7263 3110.2437
3138.2494 3179.2243 3185.2811

i18 – p14
Cartesian coordinates

C	-2.575302	-0.373549	0.000016
C	-0.117879	0.454707	0.000096
C	1.340783	0.604397	0.000050
C	2.066292	-0.744315	-0.000036
C	-1.257518	-0.017135	-0.000114

H	-3.347530	0.387437	0.000011
H	-2.872030	-1.415014	0.000180
H	-0.536204	2.336490	-0.000223
H	1.634828	1.195779	0.873657
H	1.634748	1.195868	-0.873525
H	1.799992	-1.327012	-0.884136
H	1.800019	-1.327115	0.884005
H	3.147919	-0.591063	-0.000042

Vibrational frequencies

-742.5868	102.4066	142.4638
173.1364	270.9375	302.6143
369.2892	433.5872	478.8503
571.8505	664.9867	743.1492
785.9357	990.6287	1019.2329
1091.5844	1100.5306	1248.4274
1288.9093	1357.5614	1418.2054
1457.6446	1476.2296	1499.9516
1508.4750	2066.5991	3047.7128
3054.1820	3079.5916	3134.9020
3139.6641	3152.1458	3250.7488

i19 – i20
Cartesian coordinates

C	-2.280918	0.006191	-0.347188
C	-1.160685	0.440109	0.220829
C	1.159550	-0.587365	-0.245134
C	2.138946	0.546826	-0.165402
C	-0.037844	-0.415783	0.633029
H	-2.447382	-1.050121	-0.534397
H	-3.067462	0.693257	-0.640165
H	-1.046095	1.515678	0.385300
H	1.673859	-1.524860	0.024161
H	0.840111	-0.713302	-1.288718
H	2.939866	0.625666	-0.891774
H	2.150186	1.212964	0.689332
H	0.042625	-0.699151	1.679461

Vibrational frequencies

-218.7028	43.8175	135.3393
241.1323	278.6102	370.1754
475.6167	572.7473	665.6215
827.0487	908.1907	968.3810
987.6353	1018.7597	1058.6235
1068.0912	1144.7648	1191.3839
1308.7767	1320.4350	1375.6622
1452.0936	1456.1125	1461.9844
1714.6908	2962.4180	3025.2594
3077.3038	3144.7628	3146.0913
3161.4249	3235.3898	3256.5030

i19 – i22
Cartesian coordinates

C	-2.508123	0.249630	-0.181238
C	-1.271593	-0.466351	0.093143
C	1.316811	-0.374784	-0.028041
C	2.494427	0.264659	-0.112572
C	0.040135	0.261631	0.184809
H	-2.847063	0.381756	-1.206613
H	-3.088492	0.731028	0.599302
H	-1.192965	-1.536429	-0.083328
H	1.303872	-1.460073	-0.117831
H	3.418940	-0.278218	-0.265018
H	2.560250	1.345370	-0.034691
H	-0.015369	1.345866	0.163334
H	-0.569119	-0.138016	1.208240

Vibrational frequencies

-1912.1032 134.2875 163.6120
198.5917 341.9392 390.8020
470.8166 515.6446 580.8502
696.2218 820.9526 882.0905
928.8967 977.1838 1012.2182
1079.1992 1137.1958 1189.5686
1229.8686 1292.1606 1314.8643
1369.1869 1453.5247 1471.9264
1651.8025 2215.8963 3116.5185
3146.8941 3154.6671 3157.6504
3183.5147 3212.7700 3251.0816

i19 – i28
Cartesian coordinates

C	-1.989401	0.091111	-0.160478
C	-0.726866	-0.028223	0.420608
C	1.532717	-0.282745	0.004458
C	0.856960	1.071404	-0.198558
C	0.246321	-1.045690	0.030098
H	-2.227886	-0.437422	-1.077468
H	-2.724947	0.786962	0.225701
H	-0.623739	0.379790	1.428490
H	2.073784	-0.313284	0.959631
H	2.236237	-0.582704	-0.778851
H	0.640328	1.345865	-1.226822
H	1.104020	1.907845	0.452137
H	0.003823	-1.922196	-0.559589

Vibrational frequencies

-671.3633 152.9561 265.3858
305.5079 442.9051 491.3978
601.1355 686.6401 765.8248
803.0121 874.9583 941.3698
976.0188 987.4566 1025.2512
1062.9800 1158.9324 1218.5500
1224.6465 1278.4863 1287.1549
1429.8776 1452.3150 1487.8079

1508.5669 3019.2877 3072.6631
3085.6794 3112.5965 3148.8158
3199.2222 3217.3041 3248.4125

i19 – p12
Cartesian coordinates

C	2.356195	0.496573	-0.124370
C	1.206709	0.065055	0.399746
C	-0.991383	-1.032098	0.177501
C	-2.516646	0.945205	-0.094068
C	0.176961	-0.627824	-0.353079
H	2.588614	0.345551	-1.174328
H	3.097321	1.009757	0.476708
H	1.003709	0.233311	1.455648
H	-1.187332	-0.933513	1.240042
H	-1.711621	-1.591838	-0.405733
H	-3.572122	0.787484	0.095329
H	-1.977796	1.858772	-0.310780
H	0.368215	-0.790994	-1.411266

Vibrational frequencies

-184.4113 40.5862 67.9008
129.0374 212.3284 294.1977
300.3935 305.0463 523.6157
577.6854 791.5838 907.7600
910.4286 944.9478 990.4112
1010.6056 1052.8131 1114.5417
1233.0581 1307.6507 1324.0136
1410.9697 1474.2006 1627.4161
1694.6550 3114.0272 3146.0252
3153.9905 3158.0204 3164.5122
3243.5766 3252.8026 3329.8787

i19 – p3
Cartesian coordinates

C	2.489679	-0.233634	-0.007918
C	1.281028	0.375277	0.086021
C	-1.214198	0.365984	0.067706
C	-2.420527	-0.300670	0.096995
C	0.041191	-0.288858	-0.032622
H	2.567671	-1.301020	-0.187957
H	3.412837	0.323110	0.093756
H	1.251256	1.448701	0.264584
H	-1.315252	1.100787	-1.715826
H	-1.201173	1.415890	0.351939
H	-3.350746	0.229502	0.254850
H	-2.472212	-1.367133	-0.092570
H	0.044580	-1.358431	-0.229863

Vibrational frequencies

-677.5667 150.2916 200.9297
213.0253 414.2173 459.7682

468.8302 512.5073 564.9527
618.4439 811.9086 840.2243
881.4818 925.0796 1003.8043
1013.5588 1045.1857 1170.2582
1254.2353 1258.6876 1303.4702
1308.7618 1442.5593 1494.4455
1522.1669 1587.5355 3148.0281
3154.1368 3156.0249 3159.8360
3165.2394 3252.0943 3261.2342

i1 – i3
Cartesian coordinates

C	-2.294031	-0.145560	0.194014
C	-0.891461	-0.240434	-0.331501
C	0.960549	0.311237	0.432619
C	2.246252	-0.305651	-0.022080
C	-0.016879	0.817406	-0.495995
H	-2.410746	-0.750565	1.098321
H	-2.996056	-0.541850	-0.548440
H	-2.562286	0.886643	0.420183
H	-0.573322	-1.234521	-0.658229
H	0.768528	0.406486	1.498482
H	2.838011	-0.677979	0.816175
H	2.839498	0.431070	-0.578250
H	2.069796	-1.141263	-0.710584

Vibrational frequencies

-470.1804 68.7003 101.1959
141.5243 256.9429 368.7786
528.8674 607.2621 734.8386
915.2940 937.8879 992.2838
1024.3758 1050.6242 1093.9693
1134.1660 1219.3513 1318.5388
1389.9946 1395.1842 1428.5593
1473.4135 1483.9100 1485.2667
1496.9331 3017.0355 3034.6554
3065.9184 3083.8497 3100.5647
3130.3797 3148.1370 3156.6004

i20 – p12
Cartesian coordinates

C	1.456439	1.081963	0.283121
C	1.445698	-0.137313	-0.258618
C	-0.736090	-1.002387	0.568887
C	-2.191243	0.863191	-0.316996
C	0.285911	-1.026596	-0.303399
H	0.561494	1.517697	0.716815
H	2.356959	1.684870	0.291839
H	2.351735	-0.507595	-0.732910
H	-1.563579	-1.695209	0.478563
H	-0.698163	-0.394501	1.465942
H	-3.136311	1.057619	0.176510
H	-1.692140	1.403445	-1.111257

H	0.255718	-1.739475	-1.123469

Vibrational frequencies

-179.3469	46.9641	85.3741
120.2001	233.3942	280.6894
297.9959	311.2492	509.1746
632.1207	768.9883	897.7331
922.8729	958.2239	1007.9748
1033.1119	1077.3133	1105.4935
1116.2197	1306.9683	1346.9810
1435.9812	1466.9683	1636.1777
1700.8914	3114.4093	3147.3978
3155.4067	3159.7295	3172.4961
3242.3711	3253.5741	3331.5771

i20 – p3
Cartesian coordinates

C	-2.074945	-0.613914	-0.068298
C	-1.390841	0.557145	-0.004058
C	0.976111	-0.328596	-0.066295
C	2.330414	-0.101944	-0.105336
C	0.016013	0.716679	0.033595
H	-1.577496	-1.577175	-0.085427
H	-3.157519	-0.622335	-0.092708
H	-1.971162	1.475449	0.034704
H	0.773873	-1.030398	1.762862
H	0.622261	-1.323446	-0.321840
H	3.031419	-0.912330	-0.258610
H	2.735478	0.890261	0.062035
H	0.402635	1.723753	0.161337

Vibrational frequencies

-653.7949	106.0346	225.6955
237.4660	380.0058	420.7606
431.1469	575.8355	592.9277
615.9665	805.3049	843.5452
872.0496	924.4734	1011.2657
1028.0591	1043.1951	1101.0432
1198.7115	1279.5599	1293.8327
1370.2456	1447.2770	1485.5006
1536.1017	1594.6210	3155.3561
3158.2208	3161.3231	3174.2093
3181.0784	3253.8294	3258.5864

i21 – i18
Cartesian coordinates

C	-2.572347	-0.262752	0.213075
C	-1.399360	0.399562	-0.054298
C	1.126747	-0.494472	-0.323222
C	2.358788	0.129166	0.334463
C	-0.082447	0.377822	-0.253668
H	-2.569293	-1.335124	0.402204

H	-3.522879	0.254145	0.246194
H	-0.732090	1.482080	-0.417241
H	0.887725	-1.456839	0.147246
H	1.339558	-0.703743	-1.378359
H	2.607792	1.081295	-0.139768
H	3.221587	-0.535402	0.246181
H	2.179316	0.317627	1.395447

Vibrational frequencies

-2148.4676 50.3081 133.8331
185.5129 258.4128 301.1733
443.3689 504.5344 621.0989
748.1103 774.4480 809.9802
999.6150 1036.0036 1083.1933
1094.0597 1158.3906 1285.3677
1336.3381 1418.5330 1459.6690
1474.1840 1500.3894 1513.8221
1648.9611 2340.6181 3022.9846
3055.3174 3065.0637 3116.4385
3133.9893 3137.1793 3240.7496

i21 – i20
Cartesian coordinates

C	2.234004	0.388487	-0.000112
C	1.310351	-0.629616	0.000068
C	-0.993522	0.730972	0.000076
C	-2.202833	-0.211689	-0.000121
C	-0.059694	-0.430348	0.000112
H	1.924482	1.428057	-0.000133
H	3.297403	0.181879	-0.000123
H	1.667023	-1.656416	0.000114
H	-0.920519	1.369613	0.886497
H	-0.920313	1.370055	-0.885995
H	-2.778781	-0.291669	0.918590
H	-1.221307	-1.196103	0.000289
H	-2.777820	-0.292258	-0.919385

Vibrational frequencies

-2156.0395 72.4894 184.6884
271.0327 309.3619 480.2638
589.6678 641.0133 770.8999
795.0867 909.3252 953.8881
962.7114 1032.3882 1036.8716
1037.8970 1161.3666 1217.1162
1223.5967 1240.1210 1363.0888
1420.4948 1448.5805 1466.7588
1517.9073 1871.2310 3043.0840
3085.0290 3117.2242 3154.0602
3170.7346 3224.2509 3254.3153

i21 – i7
Cartesian coordinates

C	2.023919	0.753004	0.070036
C	1.468949	-0.469482	-0.232455
C	-1.077697	-0.218188	0.529160
C	-2.130941	0.438459	-0.322573
C	0.130394	-0.764012	-0.051856
H	1.412903	1.559853	0.460246
H	3.083760	0.936191	-0.057786
H	2.115260	-1.253335	-0.619569
H	-0.847393	-1.523230	0.315632
H	-1.056202	0.000066	1.597234
H	-1.874034	1.486884	-0.519115
H	-3.109541	0.414914	0.161584
H	-2.212498	-0.060027	-1.292096

Vibrational frequencies

-2071.7651	60.3168	165.4262
204.3164	229.0453	433.3580
550.8303	615.6564	640.2972
813.6773	830.7391	968.7294
989.6900	1013.9495	1056.7944
1075.7580	1100.8261	1226.1126
1282.4684	1390.8429	1415.9800
1477.9886	1488.4091	1501.2343
1530.2166	2229.0388	3022.2015
3093.6576	3117.8116	3134.7869
3157.7705	3168.3200	3259.5586

i21 – p10
Cartesian coordinates

C	-1.916319	0.933210	0.000006
C	-1.544123	-0.405459	-0.000001
C	1.038920	-1.064714	0.000029
C	2.136871	0.966951	-0.000005
C	-0.268728	-0.849656	-0.000066
H	-1.171500	1.719698	-0.000050
H	-2.961331	1.215158	0.000078
H	-2.333758	-1.156063	0.000044
H	1.547721	-1.337576	0.922003
H	1.547853	-1.337693	-0.921836
H	1.762655	1.393058	-0.922844
H	3.166950	0.627818	0.000642
H	1.761687	1.393613	0.922185

Vibrational frequencies

-463.6879	75.7846	108.0526
146.2675	202.0975	244.8447
500.1841	506.1883	539.3245
542.1669	678.8212	755.4612
791.8911	896.3827	914.2676
936.1182	998.3326	1075.5347
1194.6431	1369.7018	1421.1500
1426.7498	1447.5808	1495.3430
1787.4434	3095.1007	3102.7924

3132.5100 3162.5597 3177.6376
3258.1601 3266.5402 3267.2374

i21 – p14
Cartesian coordinates

C	2.606221	0.333392	-0.034618
C	1.298956	-0.084400	0.014332
C	-1.326236	-0.574856	-0.246747
C	-2.217766	0.587298	0.213832
C	0.093828	-0.259078	-0.194087
H	2.904026	1.066387	-0.774802
H	3.347957	-0.052208	0.650726
H	1.442015	-1.339288	1.509450
H	-1.592732	-0.862913	-1.269684
H	-1.506062	-1.455017	0.381871
H	-1.987541	0.865244	1.244028
H	-3.269789	0.298573	0.159931
H	-2.067899	1.465082	-0.417788

Vibrational frequencies

-694.9632 43.2330 107.4129
152.7939 161.1531 265.1551
368.2678 453.9873 483.3616
530.5735 688.8960 750.8110
790.3691 987.9463 1032.3544
1082.1245 1101.2326 1239.4324
1289.7715 1356.7834 1416.6284
1464.9054 1474.6390 1500.6395
1509.1856 2045.7966 3034.7391
3055.0321 3072.0219 3136.4787
3141.3625 3162.5613 3268.3005

i21 – p4
Cartesian coordinates

C	2.416691	-0.481146	0.077487
C	1.397152	0.399156	-0.259198
C	-1.165058	0.286728	0.446920
C	-2.215084	-0.530417	-0.274015
C	0.110823	0.294326	0.131777
H	2.226527	-1.343458	0.704336
H	3.423883	-0.320151	-0.283615
H	1.638913	1.253542	-0.891552
H	-1.463290	0.725370	1.400162
H	-1.642273	2.095529	-0.321317
H	-1.868273	-0.830285	-1.263379
H	-3.139305	0.039973	-0.384090
H	-2.443321	-1.432398	0.301627

Vibrational frequencies

-622.4389 102.5885 136.0623
179.4065 223.6144 363.4372
384.2535 455.7693 546.1524

580.5306 758.7398 815.0798
828.5967 945.1727 1004.6966
1057.2363 1075.9243 1109.2833
1200.1750 1316.4731 1405.5156
1410.2714 1490.3291 1497.2018
1499.3651 1866.8865 3049.1369
3108.8693 3121.0702 3128.4832
3150.4498 3165.6948 3270.9937

i22 – i20
Cartesian coordinates

C	2.065622	-0.689006	-0.055367
C	1.374884	0.597420	-0.065183
C	-0.990648	-0.351375	0.082567
C	-2.348285	-0.218506	-0.129018
C	0.001896	0.745830	0.035465
H	2.358155	-1.180265	-0.979561
H	2.361370	-1.170947	0.874162
H	1.971567	1.507920	-0.079601
H	-0.561030	-1.346353	0.174185
H	-3.000578	-1.077016	-0.047410
H	-2.800643	0.749754	-0.310451
H	-0.527716	0.266092	1.194024
H	-0.421940	1.744639	-0.036132

Vibrational frequencies

-1889.3236 169.8434 174.2051
198.3602 324.3892 377.6036
452.7055 556.7501 640.0422
665.9148 711.3653 864.3339
887.8627 983.1546 1011.2198
1033.0717 1125.0535 1190.6262
1249.9653 1276.4509 1360.1117
1422.6030 1456.4926 1510.5689
1594.2444 1725.5476 3115.5345
3130.3206 3160.4212 3165.2969
3172.9032 3207.1269 3267.6297

i22 – p15
Cartesian coordinates

C	1.907462	-0.791910	0.059675
C	1.586891	0.440911	-0.349723
C	-1.293924	0.339382	-0.277701
C	-1.778268	-0.882519	0.037232
C	-0.327363	1.046362	0.495670
H	1.411505	-1.671304	-0.355706
H	2.554946	-0.958713	0.917162
H	1.349904	0.872769	-1.312780
H	-1.617797	0.800779	-1.208457
H	-2.488695	-1.393235	-0.601533
H	-1.476399	-1.385864	0.950634
H	-0.135212	0.720103	1.511030
H	-0.167037	2.102113	0.308731

Vibrational frequencies

-756.8681 79.4527 118.3984
218.1510 271.3881 429.0318
476.6447 630.8551 677.3523
716.7123 759.1867 831.2786
878.6767 928.7868 950.4282
1011.4416 1021.9886 1028.1395
1212.2595 1308.6052 1350.6518
1428.1354 1485.8541 1504.7666
1595.2219 3081.7769 3145.9845
3149.7589 3156.8599 3176.5320
3226.4169 3244.7165 3247.8542

i22 – p3
Cartesian coordinates

C	2.473781	-0.222184	-0.042631
C	1.192414	0.469320	-0.100902
C	-1.286529	0.412731	0.043481
C	-2.444671	-0.234166	-0.070890
C	0.022892	-0.242903	0.006469
H	2.520940	-1.291179	-0.210039
H	3.398010	0.317609	0.113613
H	1.175091	1.549053	0.008176
H	-1.281476	1.490391	0.189053
H	-3.392305	0.289829	-0.036291
H	-2.479010	-1.311665	-0.200813
H	0.026361	-1.282615	-0.326928
H	0.285069	-0.858209	1.450070

Vibrational frequencies

-1952.6379 113.2863 155.7316
202.1458 218.8660 420.9903
465.2368 524.3639 528.5118
635.1400 688.6846 850.9723
915.7957 954.0383 994.6316
1023.8263 1135.6539 1154.8220
1200.4258 1283.9051 1296.1349
1335.3714 1448.6941 1476.3000
1611.8002 1711.2063 3101.4624
3149.4528 3164.9659 3167.1871
3184.8069 3244.8736 3279.1805

i23 – i24
Cartesian coordinates

C	1.355819	0.043677	0.656103
C	0.811677	0.748024	-0.523063
C	-0.969659	-0.794102	-0.023080
C	-1.578176	0.546702	0.151379
C	0.460083	-0.701334	-0.354709
H	2.412264	-0.207650	0.652254
H	0.944427	0.250220	1.639800

H	1.372735	1.215661	-1.321527
H	-1.489301	-1.728813	0.147814
H	-1.865976	0.854138	1.161073
H	-2.333009	0.841593	-0.583036
H	-0.454603	1.196460	-0.193652
H	0.934996	-1.479412	-0.942511

Vibrational frequencies

-1884.9186 207.5044 314.4090
421.8445 560.3012 577.4704
687.6711 777.1102 817.2719
826.9188 888.3097 953.4820
975.2409 1028.9314 1037.4620
1044.4276 1072.3879 1113.6493
1131.9471 1204.6178 1332.6003
1350.3685 1357.0406 1439.6171
1470.3892 1662.4772 3053.7484
3116.5709 3117.7854 3176.7175
3200.7695 3212.8402 3214.9481

i23 – i6
Cartesian coordinates

C	-1.766098	-0.706149	-0.270105
C	-1.563230	0.661809	0.173769
C	0.913982	0.431524	-0.233895
C	2.212623	-0.267599	-0.011614
C	-0.255361	0.134612	0.481084
H	-2.197088	-1.458083	0.383322
H	-1.649838	-0.959314	-1.318578
H	-1.781253	1.585517	-0.348727
H	0.845194	1.124146	-1.068983
H	3.048736	0.439122	-0.007708
H	2.420115	-0.996654	-0.806532
H	2.216600	-0.808212	0.938628
H	-0.153964	-0.451698	1.393150

Vibrational frequencies

-601.3977 140.7670 165.9867
253.9002 284.5012 464.6880
572.6723 650.4795 697.0817
754.8883 882.6460 908.7281
980.1536 1018.6690 1066.9500
1120.5146 1170.1078 1241.8740
1249.5451 1320.6271 1411.5270
1438.4067 1463.0888 1481.5145
1507.5629 3013.1643 3076.7900
3120.4333 3129.2108 3136.4340
3170.4693 3201.4323 3233.4667

i23 – p24
Cartesian coordinates

C	1.343494	0.892032	-0.053527

C	1.695428	-0.552957	-0.109862
C	-0.935445	-0.634846	-0.101939
C	-2.064581	0.335000	-0.035176
C	0.381418	-0.271205	0.072124
H	1.587980	1.473315	0.833908
H	1.347643	1.468056	-0.980121
H	2.471487	-1.278472	-0.275398
H	-1.164188	-1.693329	-0.186055
H	-2.650224	0.191313	0.881898
H	-2.754394	0.198070	-0.874253
H	-1.701746	1.364558	-0.045511
H	0.341560	-0.331659	2.015808

Vibrational frequencies

-635.9739	112.1046	169.6761
202.8938	299.8474	383.2252
479.3165	524.1682	552.2063
696.7011	728.6917	927.6521
946.5317	993.7706	1016.8324
1032.4152	1070.4299	1111.6692
1144.1051	1204.0471	1366.7368
1415.1469	1479.1173	1480.8421
1497.4243	1613.6388	3019.0372
3068.4191	3078.5446	3130.1887
3145.3946	3172.9532	3297.1477

i24 – i19
Cartesian coordinates

C	2.317854	-0.213805	0.084174
C	1.003660	0.244869	-0.362860
C	-1.485172	0.639536	-0.042997
C	-1.633687	-0.831457	-0.096091
C	-0.121655	0.263633	0.431851
H	3.051113	0.477615	0.489358
H	2.636630	-1.241607	-0.069888
H	0.891791	0.531659	-1.411292
H	-1.497870	1.147103	-1.006268
H	-2.104399	1.157643	0.686436
H	-2.029666	-1.382130	0.746166
H	-1.416503	-1.364255	-1.010722
H	-0.017091	0.057316	1.491753

Vibrational frequencies

-639.1558	169.0307	242.6155
259.2857	343.7392	438.6474
525.6972	574.7195	646.0263
697.0730	821.2396	902.8269
960.6480	991.7249	1057.5728
1112.9443	1171.6350	1212.4344
1220.9181	1285.1375	1304.5941
1447.8339	1455.4994	1495.2902
1519.7994	3098.6663	3105.8022
3119.2328	3173.3086	3179.1129

3196.6546 3212.3309 3295.5249

i24 – i20
Cartesian coordinates

C	-1.854375	-0.594029	0.015998
C	-1.092607	0.637616	-0.183848
C	1.105836	-0.255395	0.746809
C	1.512755	-0.433237	-0.664029
C	0.240625	0.793876	0.131494
H	-1.965913	-1.325835	-0.780388
H	-2.396724	-0.782296	0.938456
H	-1.594748	1.472507	-0.672619
H	0.555497	-1.088195	1.181261
H	1.873164	0.116316	1.422693
H	2.362806	0.096647	-1.071179
H	0.999146	-1.151026	-1.287561
H	0.693369	1.768892	-0.009208

Vibrational frequencies

-638.0841 144.5322 236.0818
273.4425 375.9973 450.4335
548.7813 627.0858 671.8637
676.9554 820.5435 898.0547
933.5979 990.8140 1050.8166
1083.1963 1145.3896 1215.8895
1225.9341 1246.1630 1397.6953
1450.9448 1456.9181 1490.6630
1497.0413 3103.1052 3117.1975
3118.0326 3171.6069 3181.9036
3195.3141 3210.0947 3297.7480

i25 – i27
Cartesian coordinates

C	1.600922	-0.120608	-0.355027
C	0.446045	-0.238293	0.611502
C	-1.335505	0.334388	-0.431011
C	-0.777770	-0.993508	0.027784
C	-0.159234	1.115338	0.116989
H	2.520538	0.287081	0.060235
H	0.936860	0.964125	-0.806513
H	1.732223	-0.890175	-1.115135
H	0.676028	-0.403915	1.662599
H	-2.377076	0.631892	-0.339363
H	-0.533371	-1.731706	-0.744340
H	-1.399963	-1.489564	0.781067
H	-0.201995	2.048360	0.680029

Vibrational frequencies

-2027.2590 89.2615 380.8499
443.8112 532.7670 614.3027
720.2367 786.6127 847.5288
887.9804 915.1211 977.2208

985.9501 1042.9052 1055.3049
1078.4308 1116.3161 1157.6583
1204.7154 1257.6950 1277.1967
1319.7165 1336.7034 1428.1649
1474.9041 1817.1279 3035.7594
3076.1112 3089.6597 3120.4938
3140.2307 3166.8667 3199.6434

i25 – i28
Cartesian coordinates

C	1.475763	-0.011456	-0.400261
C	0.467481	0.103714	0.729572
C	-0.921949	0.009399	-0.806304
C	-0.598421	-0.970270	0.334722
C	-0.537267	1.103922	0.172992
H	2.070747	0.871846	-0.621750
H	0.405501	-0.053297	-1.260956
H	2.016884	-0.953980	-0.487086
H	0.846182	0.169778	1.749176
H	-1.755250	-0.028026	-1.501949
H	-0.218326	-1.962777	0.067982
H	-1.409620	-1.056578	1.062283
H	-1.269753	1.601179	0.807972

Vibrational frequencies

-1930.9017 389.6878 423.2817
564.5355 586.4881 756.4284
799.3889 838.2899 880.7520
885.5064 895.6722 958.7118
974.4471 1024.5906 1066.6908
1081.0032 1109.3538 1149.9989
1185.6503 1234.4452 1256.6571
1282.6000 1356.3496 1453.2469
1489.4978 1753.7021 3042.6407
3099.4611 3112.8824 3130.0662
3149.8878 3183.5169 3195.5439

i25 – i29
Cartesian coordinates

C	1.857488	0.031453	0.196694
C	0.447843	0.001516	-0.287927
C	-1.578631	-0.081077	0.220507
C	-0.635819	1.072516	-0.120268
C	-0.577648	-1.125890	-0.147770
H	2.381224	-0.892295	-0.062083
H	1.886188	0.132517	1.290690
H	2.409097	0.872104	-0.232723
H	0.030839	-0.678387	-1.258011
H	-2.069059	-0.117230	1.192818
H	-0.449720	1.768422	0.705450
H	-0.868244	1.656473	-1.016019
H	-0.399719	-2.132710	0.212461

Vibrational frequencies

-1790.9603 178.3707 188.7768
303.5913 356.4418 572.0884
681.5588 708.0197 836.1401
906.8631 936.2299 978.2506
990.8586 1045.8822 1109.5584
1130.4464 1187.3693 1190.0273
1235.7316 1276.5634 1350.1308
1412.5212 1479.0026 1490.3420
1490.7687 2236.3599 3007.6841
3037.7312 3075.2862 3088.3658
3127.2482 3132.0226 3197.9688

i25 – i30
Cartesian coordinates

C	-1.808707	-0.015031	0.258472
C	-0.488431	-0.027343	-0.497059
C	1.613939	0.114493	0.157269
C	0.578240	-0.998420	0.026386
C	0.510814	1.077863	-0.132374
H	-2.415228	0.842570	-0.046456
H	-2.384429	-0.923553	0.058824
H	-1.641581	0.053114	1.337535
H	-0.679923	-0.127553	-1.571126
H	1.542003	-0.846610	-0.764190
H	2.465504	0.152152	0.824914
H	0.449922	-1.871724	0.659644
H	0.228597	1.812231	0.624697

Vibrational frequencies

-1794.1198 183.8326 234.0245
325.3579 441.3332 596.1679
703.2703 745.4783 778.8973
870.0851 887.6404 932.3083
1027.7005 1070.1910 1095.7994
1110.0385 1162.1234 1184.4499
1233.8669 1253.6070 1293.4435
1373.7244 1411.9564 1497.8521
1500.7310 2248.4516 3035.3374
3036.6686 3102.3714 3114.0864
3115.8961 3160.0820 3205.2183

i25 – p18
Cartesian coordinates

C	1.957394	-0.045493	-0.391423
C	0.174272	0.146336	0.753731
C	-1.355002	0.032192	-0.647990
C	-0.642100	-1.032078	0.187400
C	-0.596190	1.085751	0.109298
H	2.481645	0.880295	-0.182143
H	1.594356	-0.159772	-1.406782
H	2.371952	-0.939257	0.065264

H	0.734503	0.212560	1.680692
H	-2.410113	0.036907	-0.911358
H	-0.086824	-1.805192	-0.347591
H	-1.298022	-1.512501	0.922359
H	-0.617730	2.166720	0.113463

Vibrational frequencies

-847.3845	128.3258	167.7928
224.3033	339.0358	565.3413
602.1802	605.0487	696.5890
844.1840	872.1230	879.7934
923.2804	970.6605	995.9945
1008.9934	1099.7822	1128.9348
1208.1905	1231.5809	1312.6264
1425.4127	1434.7453	1464.6412
1489.8519	3044.8815	3084.2405
3104.1215	3154.5235	3172.6411
3232.9743	3241.2435	3251.8211

i25 – p21
Cartesian coordinates

C	-1.903711	0.030245	-0.088656
C	-0.424416	-0.054018	0.084670
C	1.633570	-0.130092	0.043142
C	0.657525	1.037507	-0.057404
C	0.492354	-1.065320	-0.075083
H	-2.375873	-0.935454	0.103416
H	-2.140783	0.332475	-1.114414
H	-2.337636	0.771412	0.586790
H	-0.296242	-0.041207	1.754130
H	2.661864	-0.209704	-0.290460
H	0.651589	1.498563	-1.052927
H	0.698860	1.816612	0.703965
H	0.406290	-2.142630	-0.130512

Vibrational frequencies

-1564.2067	167.8623	201.8631
309.1496	436.4679	548.4598
585.8715	641.1679	678.7648
835.1376	888.7423	924.8101
964.5215	985.1616	1025.6845
1040.4930	1110.2269	1201.5084
1217.8505	1250.4478	1307.7962
1408.8604	1477.3169	1482.2275
1486.6742	1596.9360	3037.4161
3039.1768	3108.1974	3125.9982
3134.6124	3198.0563	3225.9941

i26 – i20
Cartesian coordinates

C	1.258663	-0.658626	-0.318497
C	1.133507	0.600639	0.217811

C	-1.280431	0.222082	-0.131715
C	-0.749203	-1.125862	0.284196
C	-0.160418	1.230864	-0.073161
H	0.904103	-0.855150	-1.327629
H	2.020168	-1.344519	0.040199
H	1.694539	0.872767	1.110698
H	-2.110819	0.531211	0.520404
H	-1.708447	0.181676	-1.143851
H	-1.057771	-2.003829	-0.275188
H	-0.622049	-1.294167	1.348647
H	-0.332435	2.297423	-0.145079

Vibrational frequencies

-782.8820	158.0345	301.7629
356.7884	487.8841	611.6764
617.5880	689.5139	798.9917
834.9623	908.5932	948.0358
963.6518	998.4375	1018.2673
1046.8775	1078.3571	1200.4775
1257.1666	1292.4401	1337.5551
1416.6823	1452.7234	1481.4524
1553.9324	2997.0871	3020.2284
3123.2784	3130.3735	3135.7542
3214.9659	3219.9916	3230.3172

i26 – p16
Cartesian coordinates

C	1.065652	-0.576502	-0.004887
C	1.011856	0.778585	-0.140683
C	-1.277059	0.034293	0.028407
C	-0.326318	-1.181411	-0.109619
C	-0.375394	1.226964	0.055839
H	1.960149	-1.165713	-0.172326
H	1.112912	-0.663339	1.643929
H	1.866490	1.436864	-0.216972
H	-1.893920	-0.030026	0.932015
H	-1.983812	0.084280	-0.811786
H	-0.437453	-1.662871	-1.086554
H	-0.509542	-1.945579	0.648811
H	-0.707241	2.254801	0.088534

Vibrational frequencies

-1642.1715	126.3549	274.5281
307.3977	541.4239	643.1697
726.0555	786.2087	794.0699
816.6858	909.1841	928.7215
970.3294	1012.2675	1033.8152
1062.3997	1113.9118	1151.9484
1229.7533	1285.4201	1299.2363
1345.9663	1392.9357	1460.8683
1495.6195	1579.3914	3003.3650
3045.5921	3058.1703	3105.1649
3199.2768	3231.3664	3245.3330

i27 – i22
Cartesian coordinates

C	-1.876167	0.163028	-0.234145
C	-0.713199	-0.075744	0.451306
C	1.481900	-0.187040	-0.129436
C	0.878172	1.152055	-0.047035
C	0.326006	-1.110208	0.013332
H	-2.634578	0.830185	0.158456
H	-2.026696	-0.232260	-1.233842
H	-0.687907	0.185310	1.506756
H	2.510492	-0.435546	-0.368832
H	0.655626	1.688441	-0.971756
H	1.117955	1.814710	0.785531
H	0.030642	-1.578019	-0.938098
H	0.454190	-1.925372	0.737661

Vibrational frequencies

-739.3203	128.4029	266.0759
348.3079	421.0057	491.8990
650.2786	670.3241	789.0538
828.2405	862.2646	921.7242
957.8736	989.7865	1004.3332
1047.5472	1077.5180	1188.3928
1271.3986	1296.7047	1330.0574
1426.8294	1442.0449	1469.8423
1549.2295	2992.0836	3035.5307
3071.0642	3145.3632	3148.2908
3154.7780	3180.3969	3243.8865

i27 – i28
Cartesian coordinates

C	-1.862370	-0.064011	-0.269314
C	-0.567677	-0.021228	0.438786
C	1.499961	-0.019684	-0.245776
C	0.494955	1.086094	0.015667
C	0.489328	-1.072490	0.119464
H	-1.914649	-0.456600	-1.279282
H	-2.747192	0.403094	0.147812
H	-0.730401	0.052998	1.520160
H	2.580406	-0.036430	-0.179905
H	0.211448	1.711465	-0.835161
H	0.760700	1.736627	0.852935
H	0.884679	-0.787781	-1.083654
H	0.629827	-2.075466	0.504133

Vibrational frequencies

-1897.5749	149.0470	166.7986
311.9307	439.6805	537.1243
600.1701	633.4108	766.0293
851.8783	879.7150	935.7671
967.2381	989.8540	1059.9699

1117.1912 1169.2896 1191.2545
1215.6967 1231.1767 1269.4538
1296.0690 1363.7601 1465.5830
1484.7237 2244.3668 3040.3358
3057.0097 3106.7179 3147.5283
3196.3697 3214.0925 3256.9370

i27 – i29
Cartesian coordinates

C	-1.922906	0.000000	-0.122107
C	-0.483682	0.000000	0.213007
C	1.554101	0.000000	-0.136496
C	0.545561	1.106206	0.015125
C	0.545561	-1.106206	0.015125
H	-2.401092	0.935327	-0.386580
H	-2.401092	-0.935327	-0.386581
H	-1.432677	0.000000	1.093086
H	2.635995	0.000000	-0.168204
H	0.378537	1.719253	-0.885515
H	0.704992	1.795156	0.855691
H	0.378537	-1.719253	-0.885515
H	0.704992	-1.795156	0.855691

Vibrational frequencies

-1940.9708 124.0567 205.9410
275.3178 333.2373 340.5816
665.5520 719.2357 784.4137
856.4105 910.3425 956.0522
965.4042 1010.1848 1019.5213
1086.8791 1160.9469 1215.2735
1226.1577 1257.6504 1304.9488
1360.2863 1428.3833 1445.5473
1469.7486 2246.7041 2965.0582
2972.1903 3019.3748 3021.1675
3150.8534 3223.5592 3271.1700

i28 – i30
Cartesian coordinates

C	1.625295	0.022989	-0.427644
C	0.528709	0.261213	0.615604
C	-1.415637	-0.181064	-0.323745
C	-0.233528	-1.016267	0.187841
C	-0.645436	1.039249	0.099869
H	1.770422	0.755327	-1.219957
H	2.532274	-0.449613	-0.053954
H	0.867556	0.436714	1.639204
H	-2.346224	-0.344695	0.239961
H	-1.662994	-0.282654	-1.387837
H	0.769935	-1.022726	-0.782733
H	-0.301879	-1.944615	0.750871
H	-0.785506	2.095539	-0.097106

Vibrational frequencies

-2171.3199 187.2854 291.3407
 414.3389 451.9477 622.2981
 732.6432 825.7070 849.5567
 893.8700 924.3696 953.9024
 966.4982 1016.4344 1030.4679
1063.8348 1092.8746 1166.9078
1198.6197 1240.8484 1283.2988
1314.3505 1346.3954 1422.1608
1461.0811 1805.6980 2992.4311
3039.1495 3088.3263 3099.3141
3161.0256 3205.9110 3209.3171

i28 – i37
Cartesian coordinates

C	-1.873074	0.008269	0.265132
C	-0.532153	0.037373	-0.389641
C	1.470104	0.073999	0.352057
C	0.530557	-1.048468	-0.185859
C	0.463587	1.109000	-0.106094
H	-2.271481	0.931440	0.670663
H	-2.258805	-0.937570	0.631237
H	-1.704586	0.044565	-1.006633
H	2.451512	0.136136	-0.128354
H	1.622549	0.036612	1.435970
H	0.262539	-1.839822	0.518834
H	0.898233	-1.495911	-1.110975
H	0.645918	2.043513	-0.624317

Vibrational frequencies

-1931.2420 138.4369 270.6428
 300.8551 350.5742 513.0358
 699.8577 769.0611 796.3226
 865.6208 928.2775 931.8474
 976.7004 1000.6125 1077.4362
1136.3776 1195.0542 1207.6885
1226.4651 1239.1247 1270.8115
1296.9119 1416.9475 1470.5123
1497.9523 2220.1924 3039.8632
3070.4769 3085.2444 3124.5558
3127.8294 3197.9089 3247.1424

i28 – p19
Cartesian coordinates

C	1.941394	-0.010208	-0.125385
C	0.565233	0.034859	0.063027
C	-1.563620	0.114329	-0.040009
C	-0.518878	-1.045016	-0.050605
C	-0.395258	1.060773	-0.052444
H	2.522356	0.903284	-0.169542
H	2.467941	-0.956275	-0.146722
H	0.620444	0.011060	1.912437
H	-2.175631	0.155812	0.868049

H	-2.230045	0.158784	-0.906724
H	-0.478165	-1.582783	-1.000168
H	-0.583021	-1.758480	0.770659
H	-0.317107	2.140177	-0.095496

Vibrational frequencies

-760.7928 173.3419 326.7455
467.6352 482.4581 504.3873
556.6896 663.1717 705.7281
766.8993 797.6007 890.1964
925.7660 960.0279 1006.3124
1022.8582 1093.2231 1192.6959
1223.3307 1227.2637 1275.0635
1326.3460 1420.2935 1462.8054
1488.3155 1510.7536 3039.2380
3081.2624 3087.6203 3145.6160
3158.1441 3212.3810 3261.2287

i28 – p23
Cartesian coordinates

C	2.178974	-0.046823	0.385993
C	0.177576	-0.057279	-0.837003
C	-1.331212	-0.087121	0.628537
C	-0.576074	1.056329	-0.124575
C	-0.554475	-1.036401	-0.253287
H	2.157037	-0.569696	1.334908
H	2.945943	0.624032	0.013552
H	0.824070	-0.046791	-1.705594
H	-2.417652	-0.091977	0.499696
H	-1.105803	-0.149113	1.698046
H	0.018740	1.727062	0.498302
H	-1.221621	1.648756	-0.778403
H	-0.569452	-2.114502	-0.358495

Vibrational frequencies

-359.0144 48.8174 122.3989
162.1397 316.3542 371.5721
375.9401 675.9174 851.2943
857.1075 898.3596 911.1358
920.4362 1003.8330 1029.6127
1095.3215 1130.0070 1149.6324
1180.8254 1229.6650 1242.6316
1325.6652 1468.1332 1490.2114
1545.2598 3046.0950 3065.4942
3092.2112 3103.9781 3121.8069
3195.7854 3221.9594 3309.5932

i29 – p21
Cartesian coordinates

C	-1.932463	-0.002387	-0.017860
C	-0.454396	0.005016	-0.072362
C	1.588011	0.049241	-0.092387

C	0.544434	0.986728	-0.176049
C	0.595838	-1.093010	0.088761
H	-2.339786	0.988593	-0.229683
H	-2.354844	-0.710522	-0.739752
H	-2.288834	-0.309955	0.973701
H	2.666270	0.105789	-0.110411
H	0.513554	2.044249	-0.410103
H	0.539449	1.650721	1.761833
H	0.602000	-1.858437	-0.694713
H	0.613644	-1.583965	1.068515

Vibrational frequencies

-439.3381 101.0892 182.4978
263.2235 309.1037 363.6596
459.0974 517.4879 657.4061
887.9871 897.3997 939.8926
948.3569 987.7389 1020.7944
1056.6653 1091.2770 1189.0059
1207.3307 1276.4545 1375.4069
1406.9832 1454.3637 1473.4281
1478.3348 1525.0753 3013.8849
3039.7263 3067.7662 3086.1204
3123.3519 3207.5492 3252.2544

i2 – i5
Cartesian coordinates

C	1.711413	0.812872	-0.014977
C	1.153019	-0.571327	0.123220
C	-0.927579	-0.486451	0.278055
C	-1.903850	0.605496	-0.045308
C	-0.014698	-1.036167	-0.596321
H	1.870307	1.295645	0.956696
H	1.056966	1.448925	-0.615507
H	2.685984	0.781575	-0.518738
H	1.698942	-1.272381	0.755946
H	-0.975716	-0.882728	1.295660
H	-1.561539	1.549805	0.393956
H	-2.885634	0.390045	0.387020
H	-1.999141	0.742573	-1.123048

Vibrational frequencies

-596.9651 116.1237 155.2683
192.8910 277.2245 390.2596
473.8275 583.3857 736.9361
919.3692 933.7100 1006.8766
1033.0617 1039.5625 1094.2256
1152.6459 1231.9085 1320.0215
1389.6243 1411.2928 1426.7125
1483.3783 1486.4439 1495.1346
1505.5789 3011.6268 3034.7111
3061.1657 3088.0025 3098.6538
3113.7093 3123.9913 3147.9881

i30 – i37
Cartesian coordinates

C	-1.962465	0.025331	0.086574
C	-0.521232	0.029033	-0.280809
C	1.662820	0.031990	0.033120
C	0.542369	-1.009082	0.073868
C	0.542003	1.064573	-0.087068
H	-2.521686	0.774799	-0.479042
H	-2.412927	-0.951210	-0.112718
H	-2.097662	0.237100	1.158373
H	0.012486	-0.901568	-1.068888
H	2.348853	-0.049453	-0.815203
H	2.254759	0.104915	0.949529
H	0.426849	-1.877439	0.716442
H	0.408357	1.811791	0.697396

Vibrational frequencies

-1814.9762	178.3878	184.9549
297.6038	359.5647	607.0054
661.8097	704.9395	881.7669
900.1922	911.0811	949.5447
1029.6166	1050.2212	1090.9030
1138.4958	1176.2536	1225.5378
1238.7926	1265.3559	1379.9970
1425.9996	1477.6244	1492.4930
1498.3269	2222.2595	2982.4272
3045.4691	3077.2833	3085.6047
3108.8191	3117.6044	3160.3399

i30 – p18
Cartesian coordinates

C	2.063869	-0.000006	0.427024
C	0.189209	0.000017	-0.789930
C	-1.449085	-0.000011	0.549694
C	-0.611459	1.017838	-0.212874
C	-0.611434	-1.017834	-0.212871
H	2.531075	-0.921585	0.096602
H	2.531303	0.921354	0.096311
H	1.672032	0.000203	1.437593
H	0.831493	0.000022	-1.661697
H	-2.520465	-0.000022	0.319812
H	-1.326838	-0.000003	1.640269
H	-0.602584	2.098274	-0.247527
H	-0.602626	-2.098268	-0.247624

Vibrational frequencies

-454.6411	120.0417	147.0740
182.7175	385.2035	477.5521
491.5475	557.6196	568.9392
834.9109	898.0112	904.5456
933.9491	949.3752	970.8966
996.1292	1073.9132	1177.6834

1199.5092 1225.3093 1336.1736
1388.8797 1423.2249 1425.9966
1477.2658 3023.2922 3067.6212
3087.9576 3200.3278 3233.3000
3242.1257 3247.7890 3253.4146

i30 – p20
Cartesian coordinates

C	1.938329	-0.000009	-0.114603
C	0.450057	0.000005	0.042950
C	-1.658683	-0.000001	-0.053788
C	-0.525335	-1.016247	-0.043969
C	-0.525325	1.016241	-0.044040
H	2.382514	0.885647	0.342469
H	2.382540	-0.885469	0.342822
H	2.194641	-0.000220	-1.178316
H	0.535948	0.000113	1.976285
H	-2.302434	0.000031	0.832790
H	-2.286912	-0.000033	-0.950687
H	-0.490279	-2.097038	-0.042367
H	-0.490272	2.097031	-0.042303

Vibrational frequencies

-626.1257 167.1211 232.4348
314.2634 438.9120 465.8822
477.0446 560.3928 617.0469
692.1910 907.9435 936.2005
951.8215 958.2905 1029.0151
1052.8095 1085.3090 1195.3981
1202.8208 1249.8597 1299.8267
1409.5492 1469.8817 1490.8399
1494.3755 1552.1947 3040.3009
3051.0444 3084.4076 3123.0427
3145.6778 3231.0232 3236.1417

i30 – p22
Cartesian coordinates

C	-1.767382	-0.000004	0.349491
C	-0.517363	0.000004	-0.521914
C	1.477851	0.000001	0.152782
C	0.570460	-1.018614	-0.183104
C	0.570455	1.018620	-0.183081
H	-2.379934	0.884269	0.151764
H	-2.379957	-0.884251	0.151718
H	-1.495022	-0.000035	1.408365
H	-0.790543	0.000018	-1.584394
H	2.536718	0.000000	0.378984
H	1.304599	-0.000041	2.147913
H	0.600002	-2.099293	-0.169701
H	0.600008	2.099298	-0.169696

Vibrational frequencies

-543.2745 179.4521 245.4357
315.5768 367.5401 382.2546
484.1569 561.2619 631.6853
804.8295 877.4316 916.7919
963.4661 965.3733 1034.0527
1058.4955 1100.9260 1199.9590
1201.5644 1220.5173 1344.4079
1352.3931 1406.1696 1429.6213
1498.8454 1498.9493 3037.3853
3040.2402 3113.6811 3121.5156
3210.2138 3234.2611 3247.0791

i31 – i22
Cartesian coordinates

C	0.969813	-1.118041	-0.128970
C	1.250627	0.317492	-0.016660
C	-1.117654	0.465708	-0.284229
C	-1.230146	-0.795018	0.226200
C	0.076514	1.252279	0.174072
H	1.064902	-1.591594	-1.106820
H	1.236107	-1.780417	0.695578
H	2.261877	0.707364	-0.087484
H	-1.598439	0.727956	-1.221022
H	-1.899700	-1.523459	-0.219999
H	-0.947682	-0.995509	1.255358
H	-0.020852	1.532048	1.237124
H	0.208863	2.189097	-0.375211

Vibrational frequencies

-618.6088 115.9800 299.0048
340.4790 464.8412 592.6201
646.9141 709.8893 772.9379
862.0597 913.1328 918.9420
943.1658 953.3916 982.7721
1056.3375 1096.6873 1182.8304
1265.1901 1283.6793 1343.0479
1421.7298 1448.7922 1471.7257
1570.5449 2957.9496 3078.9980
3084.4493 3139.1222 3152.0565
3175.6148 3191.2752 3226.3824

i31 – i26
Cartesian coordinates

C	1.159534	0.463021	0.220457
C	-0.048528	1.279430	-0.139485
C	-0.756856	-0.993098	0.005656
C	0.743213	-0.983506	-0.167742
C	-1.245098	0.439576	0.109533
H	2.069804	0.787304	-0.284769
H	1.345510	0.507468	1.302122
H	-0.021746	1.912391	-1.026019
H	-1.090605	-0.437577	1.097344
H	-1.391882	-1.800650	-0.340889

H	0.990148	-1.150977	-1.223137
H	1.255351	-1.755332	0.413581
H	-2.270169	0.704825	-0.108742

Vibrational frequencies

-1866.2167 240.0277 301.3454
530.9245 600.0460 652.0997
693.6520 797.4037 857.9373
899.1081 925.6985 951.8665
1010.3042 1043.9346 1083.6012
1155.6480 1203.4333 1224.9118
1255.0026 1277.5872 1292.9960
1334.0742 1347.4728 1490.6192
1504.3496 2218.5114 3022.8596
3036.2198 3089.9397 3116.9818
3135.5953 3191.8399 3229.2322

i31 – i28
Cartesian coordinates

C	-1.472302	0.223611	0.427799
C	-0.656094	-0.732294	-0.338640
C	1.173616	0.553264	0.311988
C	0.771347	-0.945038	0.087336
C	0.045629	1.022116	-0.540805
H	-2.362511	0.617631	-0.043279
H	-1.457729	0.224618	1.518290
H	-1.078742	-1.323443	-1.148278
H	1.041244	0.826902	1.360133
H	2.173395	0.831244	-0.023751
H	0.899307	-1.551226	0.993556
H	1.354386	-1.396190	-0.719906
H	0.257471	1.040507	-1.622830

Vibrational frequencies

-1899.8820 237.0440 330.4599
467.2093 515.1320 585.5955
637.6752 704.2845 811.1091
893.0825 894.1511 927.5875
968.5891 999.3900 1089.9542
1125.3556 1151.2530 1177.6730
1207.2639 1253.6589 1293.4882
1380.5310 1452.4768 1472.7624
1498.3476 2945.1732 3017.3128
3081.2333 3089.8751 3095.1535
3138.2548 3147.3638 3241.8908

i31 – p16
Cartesian coordinates

C	1.013161	-0.776480	0.039556
C	-0.433729	-1.148010	-0.108144
C	-0.433179	1.148270	-0.107667
C	1.013613	0.775997	0.039062

C	-1.231704	0.000312	-0.111915
H	1.435991	-1.182335	0.966291
H	1.618156	-1.186913	-0.776738
H	-0.799047	-2.165079	-0.146308
H	-0.798053	2.165517	-0.145318
H	1.437712	1.182352	0.964977
H	1.617929	1.185434	-0.778263
H	-2.295170	0.000595	-0.316170
H	-1.786488	-0.000104	1.726177

Vibrational frequencies

-611.7959 98.9375 281.8718
456.3358 511.6810 608.7790
633.4572 728.9813 803.7843
815.7271 921.8182 922.1021
987.9435 1003.1610 1042.2775
1076.3936 1095.2975 1149.5386
1231.4639 1293.9667 1304.5138
1338.8138 1414.7279 1465.1367
1469.7550 1493.3273 3025.7982
3037.9587 3050.5418 3070.6971
3210.6015 3229.7509 3239.8363

i31 – p17
Cartesian coordinates

C	-0.988856	0.807865	-0.093614
C	0.455761	1.162533	0.062201
C	0.310743	-1.167806	-0.114426
C	-0.951256	-0.705967	-0.113210
C	1.317945	-0.059371	0.034538
H	-1.619367	1.203235	0.713008
H	-1.419583	1.196781	-1.030052
H	0.829722	2.172006	0.163640
H	0.586843	-2.213096	-0.178501
H	-1.379702	-1.037156	1.823868
H	-1.829333	-1.311903	-0.298957
H	2.043544	-0.055116	-0.794377
H	1.921858	-0.178279	0.948436

Vibrational frequencies

-668.7398 197.0658 256.0454
325.3344 395.7090 444.5725
722.8611 747.5342 795.4969
890.3247 924.4917 936.3924
943.6749 972.6904 989.9331
1044.8746 1124.1676 1134.3134
1142.0867 1296.8518 1306.3231
1337.8306 1397.2495 1455.8253
1467.0043 1626.0138 2974.7690
2982.1696 2986.7708 3031.4992
3205.4104 3226.5603 3231.3713

i32 – i34

Cartesian coordinates

C	1.399211	-0.945753	0.159919
C	0.638056	0.209136	-0.475554
C	-1.813788	-0.556351	0.137663
C	0.303841	1.381981	0.375537
C	-0.825219	0.111985	-0.492066
H	2.450558	-0.677316	0.290857
H	1.338393	-1.838954	-0.465744
H	0.984449	-1.187630	1.141785
H	1.053276	0.487500	-1.446645
H	-1.611506	-1.170004	1.016323
H	-2.849999	-0.448523	-0.162588
H	0.241522	1.263824	1.449440
H	0.180700	2.365121	-0.056418

Vibrational frequencies

-693.1901	186.4854	227.3244
293.1470	350.6025	448.4066
514.1002	635.6706	660.3469
701.2981	832.4567	884.7009
922.2129	986.8042	1059.8397
1158.8680	1174.9711	1222.5928
1343.1410	1401.5774	1406.9065
1461.2399	1491.3593	1498.9919
1521.4659	3052.6702	3087.5562
3098.3403	3134.0468	3136.4822
3168.0719	3214.7686	3286.8605

i32 – p10
Cartesian coordinates

C	0.978581	1.607929	-0.097063
C	0.425523	-0.440736	0.471266
C	-2.066712	0.062749	-0.171799
C	1.279920	-1.246837	-0.305116
C	-0.950494	-0.444771	0.265593
H	2.038779	1.626723	0.131198
H	0.340188	2.195451	0.554979
H	0.723457	1.622041	-1.150665
H	0.744899	-0.212415	1.485868
H	-2.083257	1.030579	-0.678394
H	-3.021136	-0.444038	-0.055452
H	2.314644	-1.385208	-0.019255
H	0.941516	-1.663143	-1.245565

Vibrational frequencies

-494.3926	119.4369	130.1848
178.5830	249.3335	337.6941
420.4497	475.2744	585.1716
590.5587	614.6911	706.7612
860.3010	903.9638	924.5580
982.7307	993.6583	1087.4967
1197.4400	1372.3826	1425.7583

1429.5246 1442.1352 1490.1964
1852.9616 3074.2738 3086.4657
3147.6783 3163.4071 3172.5935
3244.7918 3250.8607 3271.0657

i32 – p26
Cartesian coordinates

C	1.222921	1.263835	-0.257110
C	0.301414	0.345934	0.514756
C	-2.172127	-0.128237	-0.207024
C	1.209826	-1.655892	-0.096482
C	-0.976375	0.187315	0.192625
H	2.260725	0.942453	-0.156796
H	1.147732	2.285198	0.127335
H	0.961501	1.275574	-1.316212
H	0.586592	0.109033	1.536862
H	-3.027769	0.514948	-0.021968
H	-2.351704	-1.057581	-0.744168
H	2.116446	-1.614810	-0.691628
H	0.792524	-2.532551	0.385986

Vibrational frequencies

-441.6685 46.0710 113.2881
157.3221 208.9445 231.6642
356.1214 395.7477 408.5870
494.9322 580.3637 861.7357
892.0654 903.3569 1000.6276
1046.7024 1097.3781 1135.1677
1163.5250 1356.6649 1414.2890
1462.5450 1492.6361 1506.1787
1990.2698 3050.7638 3102.5243
3114.1337 3122.5731 3144.4481
3160.2998 3194.5585 3302.1459

i32 – p8
Cartesian coordinates

C	-1.263419	-1.182823	-0.057812
C	-0.440481	0.094745	0.024403
C	2.194095	-0.079403	0.010881
C	-1.087017	1.338100	-0.069264
C	0.914785	-0.000470	-0.197089
H	-2.205202	-1.060328	0.479295
H	-0.723375	-2.026315	0.372231
H	-1.488227	-1.411610	-1.102721
H	-0.313413	0.049242	1.897055
H	2.910737	-0.156373	-0.803041
H	2.595857	-0.069033	1.025541
H	-2.166043	1.397500	0.001224
H	-0.518112	2.256026	-0.136296

Vibrational frequencies

-715.5688 153.5031 171.1002

177.8408 373.4408 448.9307
479.5267 495.8283 513.5921
584.4740 622.0530 742.2047
789.8287 905.4774 952.8531
976.7908 1016.1609 1059.9946
1275.8824 1315.0525 1414.1867
1439.5004 1484.7367 1496.4667
1501.4664 1890.5999 3057.3958
3085.3531 3133.5668 3155.6355
3163.9746 3173.5054 3272.9134

i33 – i28
Cartesian coordinates

C	-1.912112	-0.238650	-0.104317
C	-0.543174	0.022320	0.400540
C	1.729117	-0.230631	0.027205
C	0.195637	1.230467	-0.198226
C	0.546661	-0.945226	-0.050976
H	-2.121808	-0.146799	-1.164825
H	-2.693388	-0.616294	0.543935
H	-0.560919	0.105913	1.494254
H	1.974601	0.326363	0.927072
H	2.592311	-0.481453	-0.587526
H	0.062659	1.366566	-1.267968
H	0.287335	2.147605	0.383193
H	0.362432	-1.731580	-0.773484

Vibrational frequencies

-878.9936 134.9237 190.7730
322.0174 429.7503 512.6525
541.9394 587.2194 643.6554
821.5419 859.7406 903.3990
914.4265 948.6068 969.7572
1040.9317 1111.2362 1154.6569
1227.8688 1241.2359 1331.1164
1373.4933 1445.9524 1467.2915
1538.4365 3036.6875 3099.7963
3115.3336 3150.6733 3186.9768
3209.6276 3216.7209 3261.9217

i33 – i32
Cartesian coordinates

C	-1.119622	-1.182630	-0.257274
C	-0.581116	0.106739	0.438485
C	1.978142	0.094961	-0.089328
C	-0.915687	1.415453	-0.163912
C	0.806335	-0.422646	0.227903
H	0.193490	-1.594594	-0.155085
H	-1.367834	-1.089549	-1.311019
H	-1.749958	-1.844814	0.330864
H	-0.856295	0.079912	1.497254
H	2.134911	1.172464	-0.029910
H	2.819789	-0.519065	-0.388309

H	-1.733289	2.014160	0.218444
H	-0.449121	1.710222	-1.097486

Vibrational frequencies

-2130.0672 99.3459 140.4564
222.7414 318.8520 386.6478
511.5865 545.2642 626.1634
677.7730 818.7613 895.2551
916.7166 952.1125 967.4580
1033.0708 1087.4765 1168.2207
1223.2735 1243.7590 1339.3745
1404.0743 1425.8574 1457.7516
1724.1089 1901.5168 3066.4366
3109.1653 3115.8786 3156.4102
3219.2967 3232.2988 3267.8158

i33 – i36
Cartesian coordinates

C	-1.340228	1.054678	0.083340
C	-0.694025	-0.161921	-0.440338
C	1.673399	0.605899	0.189470
C	-0.469569	-1.283188	0.523127
C	0.815633	-0.220772	-0.482087
H	-2.172740	1.507922	-0.437260
H	-1.027816	1.483961	1.027644
H	-1.135662	-0.491107	-1.380017
H	1.317611	1.416726	0.813953
H	2.743005	0.448720	0.132699
H	-0.386944	-1.066588	1.579131
H	-0.471208	-2.312648	0.191629
H	1.222490	-0.955167	-1.168852

Vibrational frequencies

-597.4385 77.4578 223.2194
295.0405 374.3467 459.4765
507.5920 527.3261 609.6213
665.6175 765.3267 848.3024
894.7457 940.7548 955.1849
1048.1023 1121.8327 1197.6387
1218.3076 1297.9592 1384.0025
1407.7738 1447.4574 1480.5533
1539.9123 3122.3988 3165.1822
3169.6928 3170.9596 3186.9646
3262.1663 3278.0442 3293.4179

i33 – p12
Cartesian coordinates

C	-1.015893	-1.725821	-0.107096
C	-0.385541	0.404807	0.395721
C	2.039993	-0.008716	0.120836
C	-1.459708	1.135856	0.004882
C	0.865664	0.371655	-0.374528

H	-0.516096	-2.476207	0.495901
H	-1.470772	-1.855766	-1.081916
H	-0.322811	0.076498	1.429950
H	2.136370	-0.348045	1.147951
H	2.940442	0.005203	-0.481476
H	-2.328004	1.245197	0.642437
H	-1.504412	1.580504	-0.984052
H	0.798194	0.705933	-1.407678

Vibrational frequencies

-433.6156	76.8543	115.3007
158.4385	237.3647	304.0379
403.3468	410.1579	510.9557
545.0913	717.5916	866.7942
890.2401	949.1522	981.9873
1004.3390	1046.1635	1155.5466
1223.6960	1288.3479	1322.9816
1401.6621	1470.5073	1583.4778
1728.2137	3107.7335	3146.5979
3151.9243	3159.4975	3167.1514
3242.4247	3252.1915	3313.0366

i33 – p15
Cartesian coordinates

C	0.830564	1.378581	0.034346
C	0.923411	0.032718	0.424332
C	-2.072253	0.120355	-0.284387
C	1.546612	-0.935665	-0.382673
C	-1.177324	-0.636147	0.303323
H	0.478928	2.137654	0.721323
H	1.038585	1.672422	-0.988553
H	0.854154	-0.176507	1.488485
H	-1.817502	1.104928	-0.670346
H	-3.105374	-0.203775	-0.408389
H	1.743899	-1.933363	-0.011591
H	1.760221	-0.728854	-1.425167
H	-1.258974	-1.631564	0.724596

Vibrational frequencies

-402.3690	51.8738	179.0794
211.2558	314.2604	400.1574
442.5990	459.4232	475.4672
707.2257	726.2504	838.9560
919.3686	932.6098	955.5858
966.7075	1016.0349	1124.7321
1204.3439	1242.9528	1397.4238
1412.5868	1499.9711	1510.2994
1669.1470	3097.8937	3153.8368
3155.4220	3160.9699	3180.4778
3210.6053	3259.0864	3261.4305

i33 – p7
Cartesian coordinates

C	1.564541	0.866083	-0.252750
C	0.513203	-0.000466	0.094035
C	-1.976726	-0.016512	-0.202011
C	0.688487	-1.393934	0.010738
C	-0.856310	0.587501	0.173702
H	1.416503	1.938437	-0.281500
H	2.561637	0.482384	-0.430249
H	0.686333	0.136799	1.899231
H	-1.982990	-1.023736	-0.604980
H	-2.932477	0.488396	-0.125863
H	1.667953	-1.809552	-0.190498
H	-0.117015	-2.076783	0.247201
H	-0.899121	1.608026	0.544376

Vibrational frequencies

-871.1731	112.2658	288.7641
399.3027	444.2435	474.4533
490.5435	508.9690	549.9869
596.0339	716.9936	750.7991
790.5845	830.1173	961.5910
980.7835	1020.9331	1038.8258
1077.5228	1304.3735	1350.9046
1369.7557	1456.9548	1489.7059
1512.8700	1727.2137	3154.9465
3160.0956	3166.4065	3174.2485
3245.4869	3265.3365	3270.3391

i34 – i40
Cartesian coordinates

C	1.583237	-0.813189	0.133984
C	0.850884	0.343706	-0.457532
C	-1.750520	-0.774725	0.035576
C	-0.040387	1.216857	0.349359
C	-1.033969	0.330664	-0.260146
H	2.587239	-0.518158	0.467116
H	1.700578	-1.626029	-0.587108
H	1.055683	-1.213600	1.004521
H	1.093360	0.667313	-1.462321
H	-1.547381	-1.355211	0.936272
H	-2.495841	-1.164376	-0.648657
H	0.048763	1.127597	1.436936
H	-0.097872	2.262592	0.045796

Vibrational frequencies

-696.6251	62.4786	174.2742
272.2150	367.4673	399.8702
485.1116	681.2235	688.0267
852.3332	895.2070	913.9136
959.9322	1023.1720	1097.0319
1168.7518	1191.3004	1196.7117
1381.3801	1400.3809	1422.2149
1459.6698	1483.8990	1492.5594

1524.4603 3018.3959 3042.7079
3087.2938 3096.8365 3122.0501
3123.3711 3207.7399 3210.9383

i35 – i13
Cartesian coordinates

C	-1.608417	-0.803891	0.020149
C	-0.598154	0.219512	-0.337326
C	1.643036	-0.779072	0.246797
C	-0.182058	1.437311	0.330743
C	0.839543	0.086007	-0.497305
H	-1.385206	-1.259972	0.997497
H	-1.626144	-1.609787	-0.717714
H	-2.605587	-0.362491	0.090202
H	1.221362	-1.399720	1.029748
H	2.718951	-0.786201	0.122150
H	-0.022758	1.441773	1.405487
H	-0.161733	2.395361	-0.179920
H	1.297416	0.621834	-1.325791

Vibrational frequencies

-593.8899 145.2819 162.2017
287.5073 303.0502 446.8414
491.0923 680.6783 707.8605
766.0128 803.3882 905.4846
919.1982 959.0755 1037.0875
1067.9397 1159.0608 1229.5466
1353.8840 1399.1127 1425.4398
1471.7003 1483.1297 1485.7912
1495.8516 2985.9376 3084.1840
3121.5115 3133.0864 3144.6473
3158.1771 3220.4243 3258.2053

i35 – i38
Cartesian coordinates

C	-1.755525	-0.654002	0.031330
C	-0.849913	0.436764	-0.360381
C	1.552215	-0.914600	0.187215
C	0.168063	1.219659	0.328055
C	1.007060	0.208926	-0.395701
H	-1.202580	-1.435814	0.574047
H	-2.200127	-1.129096	-0.847841
H	-2.572128	-0.294584	0.668919
H	1.411716	-1.125498	1.242184
H	2.102537	-1.636301	-0.402640
H	0.170905	1.123079	1.417650
H	0.287957	2.259236	0.022740
H	1.270318	0.458501	-1.418168

Vibrational frequencies

-628.1814 132.5464 174.0196
269.5725 383.2749 428.0561

519.1012 718.2780 824.7821
861.7759 906.6833 954.0722
966.4807 1030.0964 1129.2433
1157.4783 1194.8657 1269.8761
1355.8089 1399.4641 1414.5157
1458.8727 1464.5623 1475.2847
1532.5621 2986.2648 3059.0352
3059.8769 3103.4896 3133.5332
3157.3719 3183.1384 3258.3414

i35 – p28
Cartesian coordinates

C	-1.940178	-0.584680	0.028216
C	-0.618520	0.058611	0.038631
C	1.888100	-0.738083	0.139803
C	0.109137	1.354338	0.081947
C	0.732523	-0.018766	-0.068863
H	-2.545746	-0.239659	0.872327
H	-1.854692	-1.671756	0.073697
H	-2.485897	-0.318592	-0.885217
H	1.865059	-1.821077	0.161489
H	2.846825	-0.238426	0.191278
H	0.205935	1.871244	1.038531
H	0.089043	2.018223	-0.782451
H	0.853098	-0.028474	-1.988063

Vibrational frequencies

-639.9945 80.3608 140.5090
218.8798 333.7395 427.3651
454.7726 505.5312 561.5286
695.7514 754.4521 799.6271
946.7168 952.6466 1013.4886
1041.7368 1055.2067 1105.4863
1187.1536 1323.3821 1407.4199
1467.6359 1475.3872 1480.5121
1490.1256 1690.1451 3023.3920
3057.8735 3083.6387 3130.7303
3132.9234 3157.9852 3262.0503

i36 – i22
Cartesian coordinates

C	1.610020	-0.873227	0.049751
C	0.936933	0.337310	-0.393415
C	-1.601047	-0.810892	0.120310
C	0.017915	1.116312	0.483135
C	-0.976816	0.335421	-0.311272
H	1.150432	-1.851278	-0.057612
H	2.589640	-0.818539	0.516675
H	1.230642	0.801218	-1.331954
H	-1.382878	-1.239433	1.092532
H	-2.289525	-1.344876	-0.522288
H	0.055204	0.856740	1.539650
H	0.003375	2.193432	0.328355

H	-1.278924	0.773193	-1.256415

Vibrational frequencies

-607.6173	186.8839	273.7116
329.7435	396.0127	429.7692
500.9630	530.0258	691.1295
745.7389	884.7359	919.1955
928.5540	988.1061	1001.7237
1099.1907	1164.8695	1187.1752
1212.3206	1275.1892	1356.2753
1418.3091	1452.9419	1492.9582
1533.9708	3100.3424	3120.9982
3152.2801	3160.2232	3174.7898
3197.9327	3217.1821	3259.7211

i37 – p19
Cartesian coordinates

C	-1.887756	0.014995	-0.066925
C	-0.541698	-0.005995	-0.183643
C	1.588343	-0.102060	0.110870
C	0.540683	1.048909	-0.035126
C	0.464199	-1.082631	-0.067330
H	-2.427107	0.955433	-0.106512
H	-2.073404	-0.245456	1.608909
H	-2.461704	-0.887888	-0.247836
H	2.098749	-0.143481	1.079302
H	2.356559	-0.126781	-0.671204
H	0.422607	1.686140	0.845703
H	0.683522	1.683560	-0.912808
H	0.418157	-2.160838	-0.142628

Vibrational frequencies

-1476.7202	95.3377	226.9769
262.0740	296.1453	366.7807
606.2835	698.6220	735.5436
861.5864	884.0409	925.6330
952.9090	968.0524	1000.4700
1027.8220	1075.7558	1201.9670
1213.1498	1221.0644	1277.0771
1301.8990	1437.1868	1452.4047
1477.0863	1686.7862	3027.2329
3062.8330	3065.3602	3117.1911
3144.0959	3229.3189	3235.8377

i37 – p20
Cartesian coordinates

C	-1.967349	-0.032739	-0.051252
C	-0.488764	-0.010836	-0.068918
C	1.627788	-0.023262	-0.147183
C	0.464034	0.968687	-0.023612
C	0.544422	-1.080969	0.041802
H	-2.381475	0.962696	-0.221548

H	-2.327419	-0.393551	0.920409
H	-2.359543	-0.714160	-0.812111
H	2.418014	0.022692	0.602995
H	2.071898	-0.035664	-1.147791
H	0.526673	1.176162	1.712242
H	0.412546	2.037638	-0.205649
H	0.558525	-1.981103	0.646432

Vibrational frequencies

-1408.9388 130.9674 208.5917
278.4191 309.4130 321.7443
537.0997 629.9962 673.4518
883.1042 902.3226 922.9346
969.9395 974.6229 1020.6341
1045.3023 1107.8306 1181.5439
1208.4837 1240.1575 1329.0857
1410.9106 1475.5522 1477.3147
1484.7420 1620.2276 3023.4543
3056.9607 3088.5981 3125.3712
3134.1510 3186.0057 3199.3210

i37 – p21
Cartesian coordinates

C	-1.924803	-0.040658	0.157411
C	-0.518065	-0.019453	-0.304657
C	1.504369	-0.105529	0.122684
C	0.550109	1.066140	-0.143936
C	0.566575	-1.044067	-0.193433
H	-2.452285	0.864282	-0.157751
H	-1.998279	-0.094465	1.255163
H	-2.459064	-0.907623	-0.242632
H	1.483107	-0.118792	1.872987
H	2.588289	-0.146017	0.147393
H	0.402802	1.792366	0.657837
H	0.775906	1.594104	-1.076371
H	0.590414	-2.122458	-0.285041

Vibrational frequencies

-1496.9880 123.2003 137.0923
264.1958 314.7668 492.8116
518.7944 672.7228 761.5737
870.6151 905.1261 917.4311
961.3489 977.6110 1025.1230
1058.6153 1111.6066 1168.9734
1213.9054 1275.2176 1367.0191
1410.1512 1471.6399 1478.3919
1482.6574 1530.8440 2974.6711
3054.3585 3066.3504 3112.8352
3116.1685 3186.2081 3225.1112

i38 – i29
Cartesian coordinates

C	-2.062585	-0.247631	-0.052840
C	-0.607336	-0.037078	-0.225781
C	1.541549	0.275730	-0.127691
C	0.305989	1.082387	0.177736
C	1.199830	-1.046249	0.123129
H	-2.634997	0.601008	-0.452571
H	-2.399785	-1.150661	-0.567374
H	-2.331094	-0.350312	1.010239
H	2.257282	0.566391	-0.886566
H	0.211759	2.012245	-0.399412
H	0.191155	1.353716	1.241616
H	1.701371	-1.871140	-0.381540
H	0.739628	-1.324209	1.068289

Vibrational frequencies

-806.7575 98.7415 159.3659
269.5046 282.7540 549.7538
606.2003 793.4773 853.8565
878.2967 955.7869 967.6479
990.9119 1046.5441 1049.4259
1134.7689 1202.2780 1267.9664
1302.6712 1382.0851 1386.5766
1461.5191 1465.9666 1471.0293
1536.0006 2950.7962 2977.3775
3022.3243 3034.5659 3111.1983
3113.3315 3183.5394 3221.3724

i38 – i40
Cartesian coordinates

C	1.184775	-1.032821	0.133231
C	1.214490	0.301629	-0.264580
C	-1.540854	-0.696199	-0.047364
C	0.130602	1.218126	0.261351
C	-1.125404	0.602033	-0.236971
H	1.052855	-1.246800	1.196653
H	1.813649	-1.748596	-0.387417
H	-0.190025	-1.226433	-0.145707
H	1.685976	0.585529	-1.200002
H	-1.745915	-1.030671	0.977652
H	-2.185833	-1.164564	-0.790230
H	0.131133	1.231083	1.365293
H	0.256509	2.243835	-0.090246

Vibrational frequencies

-2139.9890 274.8493 285.9709
436.0006 465.3485 526.0931
578.0805 686.8603 845.0652
872.2839 880.8548 923.6944
961.3894 994.7586 1061.9995
1112.6501 1205.2287 1237.5606
1271.3030 1345.9265 1392.5957
1403.9412 1432.7541 1454.0846
1508.5481 1538.2438 2953.2045

3025.8994 3085.9023 3116.0449
3148.8942 3189.2797 3210.6816

i38 – i6
Cartesian coordinates

C	-2.515385	-0.047860	-0.300075
C	-1.214972	-0.161685	0.394255
C	2.542035	0.091960	-0.212099
C	0.118716	0.378967	0.196085
C	1.325444	-0.413827	0.034493
H	-2.811750	1.006028	-0.402772
H	-3.311473	-0.559849	0.244879
H	-2.456847	-0.472713	-1.311837
H	2.699450	1.159502	-0.332212
H	3.408483	-0.550868	-0.307094
H	-0.445826	0.383684	1.355298
H	0.173720	1.437604	-0.072750
H	1.209210	-1.488716	0.150533

Vibrational frequencies

-2057.9412 85.5506 126.1300
135.2325 268.6760 342.8620
473.9175 540.4778 741.6116
851.9818 896.4202 981.3086
1004.7365 1017.0490 1048.1704
1100.8704 1180.4956 1264.1255
1320.6160 1380.9353 1395.1545
1462.6611 1472.2364 1481.2816
1659.4710 2185.8454 2987.4153
3040.6729 3084.7794 3113.4782
3153.6633 3167.2196 3250.4840

i39 – i28
Cartesian coordinates

C	0.503884	1.057073	0.069170
C	-0.597948	0.010826	0.251027
C	1.554781	-0.073374	-0.132705
C	-1.987841	0.041273	-0.129657
C	0.440949	-1.094068	0.006233
H	0.664571	1.750132	0.898544
H	0.347501	1.640525	-0.843742
H	2.358599	-0.127384	0.606088
H	2.007282	-0.058002	-1.127565
H	-2.268783	0.373758	-1.128241
H	-2.773932	-0.348844	0.506679
H	-0.114056	-0.806467	1.136966
H	0.295869	-2.074097	-0.433136

Vibrational frequencies

-1882.4343 175.8850 270.4710
308.3159 384.6473 509.7332
603.1906 690.9433 790.2540

868.9029 929.3200 959.2488
976.7063 1007.2945 1047.2519
1103.1933 1193.3069 1202.2375
1223.4101 1258.1998 1273.9711
1354.0001 1454.6934 1476.4684
1507.6659 2223.7226 3052.4791
3066.0111 3098.1035 3110.9525
3116.1065 3192.9883 3224.0940

i39 – i41
Cartesian coordinates

C	0.771741	-1.175738	0.088121
C	-0.778577	0.163369	-0.334027
C	1.523747	0.124933	-0.067735
C	-2.034096	-0.136639	0.033891
C	0.328109	1.072372	0.094880
H	0.829071	-1.946115	-0.672913
H	0.576433	-1.531531	1.095918
H	1.951633	0.209790	-1.068598
H	2.324699	0.281742	0.660005
H	-2.332327	-0.116419	1.084985
H	-2.760120	-0.533855	-0.669913
H	0.363968	2.008117	-0.473287
H	0.181087	1.338494	1.153032

Vibrational frequencies

-814.3587 149.9213 250.0425
292.2069 441.1481 556.1737
628.4776 762.2210 786.1245
803.7122 845.4571 917.5201
961.1184 987.7384 1038.2614
1110.6031 1222.9073 1230.7785
1300.9286 1318.0018 1406.9296
1455.8777 1465.3644 1507.6421
1549.4829 2992.4318 3063.2357
3069.1267 3071.2443 3119.1752
3138.2718 3178.3987 3239.8642

i39 – p19
Cartesian coordinates

C	-0.501560	-1.073324	0.118033
C	0.553393	-0.007033	-0.085035
C	-1.551164	0.064854	-0.072524
C	1.996570	-0.040834	-0.026502
C	-0.362075	1.005745	-0.146457
H	-0.501024	-1.530076	1.114003
H	-0.521813	-1.867016	-0.635031
H	-2.234248	0.219758	0.765529
H	-2.128695	-0.011273	-0.997178
H	2.550707	-0.905544	-0.369691
H	2.543511	0.806298	0.369762
H	-0.236605	1.554695	1.502404
H	-0.282816	2.036716	-0.474885

Vibrational frequencies

-1365.1686 162.0614 214.8695
287.7909 319.6213 466.5853
521.9131 604.5843 686.7517
786.4572 892.9867 926.1943
956.1154 981.3785 999.1853
1043.1912 1097.6421 1176.6978
1215.1753 1228.7745 1252.3668
1307.4037 1449.2322 1462.7143
1487.9822 1616.0781 3040.4518
3066.6575 3091.7442 3119.6645
3157.9625 3186.6007 3266.1639

i3 – i21
Cartesian coordinates

C	-1.471451	0.894117	-0.007804
C	-1.427774	-0.586395	-0.232370
C	0.810156	-0.040125	0.555591
C	1.995161	0.214549	-0.336510
C	-0.220234	-1.023541	0.079250
H	-1.528192	1.522539	-0.897345
H	-0.188555	0.945293	0.411986
H	-2.088278	1.249004	0.818356
H	-2.257649	-1.185008	-0.589050
H	1.033157	-0.099190	1.621243
H	2.627285	-0.680216	-0.407581
H	2.612409	1.031118	0.044985
H	1.674671	0.464830	-1.351535

Vibrational frequencies

-1833.9723 111.0444 175.6977
248.2899 411.3775 506.1500
551.6562 721.5565 751.8093
805.4785 885.8512 948.2161
1041.2478 1043.4494 1079.5381
1095.3058 1119.3282 1238.0895
1323.0513 1368.6917 1406.6237
1430.8561 1483.0725 1492.5439
1612.7555 1694.0980 3020.2650
3084.3145 3092.8608 3122.2420
3137.6468 3169.9616 3206.2327

i3 – i4
Cartesian coordinates

C	-1.727781	0.817520	0.153553
C	-1.284484	-0.566667	-0.266552
C	1.176272	-0.470368	0.492531
C	1.921000	0.550885	-0.291659
C	-0.079724	-1.060681	-0.105216
H	-2.034580	1.402886	-0.718345
H	-0.929462	1.356784	0.667185

H	-2.586604	0.755020	0.827972
H	-2.042655	-1.194483	-0.735413
H	1.225369	-0.431705	1.578568
H	2.863255	0.812486	0.196205
H	1.344102	1.483293	-0.407211
H	2.128879	0.191586	-1.304900

Vibrational frequencies

-258.7127	132.4868	158.8106
191.2193	251.9449	377.1206
492.5772	604.8674	708.5852
848.1760	943.2920	979.7158
1049.1056	1051.4804	1087.4532
1130.9619	1273.4307	1332.5151
1395.3996	1400.4056	1469.1198
1480.5304	1489.2521	1491.3397
1747.9575	2973.6306	3041.9057
3065.6422	3109.1686	3124.3139
3125.6124	3139.8532	3158.4709

i3 – i5
Cartesian coordinates

C	-2.276949	0.525416	-0.075035
C	-1.384532	-0.661274	0.014709
C	1.058043	0.070893	0.335604
C	2.486414	0.177892	-0.123947
C	0.074960	-0.485966	-0.328797
H	-3.320801	0.250206	0.095050
H	-2.187892	1.009788	-1.053164
H	-2.014580	1.289693	0.674107
H	-1.621560	-1.439646	0.736374
H	0.830351	0.500008	1.320456
H	3.158115	-0.314473	0.585437
H	2.791746	1.226462	-0.190078
H	2.617005	-0.283808	-1.103386

Vibrational frequencies

-350.7610	128.1261	173.6900
183.1718	233.5525	344.4806
484.8404	512.6561	740.1063
861.8858	971.5278	989.7399
1061.6498	1085.0032	1096.4039
1143.7337	1251.5426	1328.0311
1402.5165	1408.1048	1473.6351
1484.8968	1488.8666	1493.4910
1762.6275	2977.5297	3031.8551
3046.0741	3061.8219	3109.2259
3121.6156	3141.4572	3162.0968

i3 – i6
Cartesian coordinates

C	2.229085	0.376140	-0.000002

C	1.161130	-0.675569	0.000003
C	-1.043208	0.674735	0.000003
C	-2.326606	-0.090036	-0.000003
C	-0.176922	-0.389077	0.000002
H	2.874020	0.277315	0.880380
H	1.805836	1.382317	-0.000002
H	2.874011	0.277312	-0.880391
H	1.476139	-1.714152	0.000001
H	-0.871025	1.744699	0.000007
H	-2.917832	-0.106866	-0.917403
H	-2.917839	-0.106868	0.917393
H	-1.384186	-1.130924	-0.000002

Vibrational frequencies

-2246.8317 96.5329 136.9777
184.8292 334.5427 457.8846
515.2174 672.8433 677.9175
738.2470 911.4086 962.0403
1013.3289 1020.3946 1039.2323
1075.8939 1150.9749 1187.5733
1258.2091 1376.9213 1408.1021
1420.6242 1450.9584 1479.6392
1505.4417 1860.3796 3025.8668
3064.3608 3081.8785 3128.9489
3155.8065 3181.3085 3200.7803

i3 – i8
Cartesian coordinates

C	-2.574899	-0.265264	0.019300
C	-1.283322	0.472811	-0.024813
C	1.161011	-0.456190	-0.017978
C	2.565479	0.046686	0.020559
C	0.040367	0.346426	-0.032087
H	-3.076188	-0.108540	0.979087
H	-2.407268	-1.340204	-0.111798
H	-3.253165	0.079586	-0.765424
H	-0.543902	1.527818	0.049145
H	1.010344	-1.537095	-0.034471
H	3.140847	-0.324462	-0.835597
H	3.084647	-0.301460	0.921455
H	2.592874	1.137546	0.007722

Vibrational frequencies

-2143.3553 63.0370 100.8342
126.4450 151.2005 319.4952
332.5031 448.1497 519.9516
705.1133 795.8036 957.2446
1013.1576 1025.7413 1042.7048
1101.6709 1185.9224 1388.4737
1397.3155 1410.9793 1474.4709
1476.3598 1483.1610 1496.1846
1668.4390 2349.0814 3025.1856
3026.1899 3075.8892 3101.4998

3109.2443 3114.1879 3139.3771

i3 – p1
Cartesian coordinates

C	-2.769180	-0.515008	0.000064
C	-1.007778	0.918724	-0.000094
C	1.175341	-0.490795	-0.000084
C	2.595457	-0.022453	0.000064
C	0.092290	0.348167	-0.000063
H	-3.243312	-0.218002	0.928521
H	-2.276259	-1.478965	-0.006962
H	-3.251610	-0.208873	-0.921141
H	-1.653438	1.768188	0.000073
H	0.990704	-1.563050	-0.000141
H	3.130734	-0.398894	-0.879429
H	3.130443	-0.398588	0.879869
H	2.655961	1.066374	-0.000106

Vibrational frequencies

-563.8175 46.5129 88.1733
89.4860 118.8156 240.6672
393.2474 497.3365 502.2364
521.9149 548.0103 645.7802
734.4697 858.2515 874.9542
1010.5433 1091.6121 1155.0271
1387.9242 1408.6116 1417.7388
1424.3830 1479.9677 1497.7334
1882.4736 3022.4801 3074.7581
3095.7875 3136.2010 3149.8580
3258.9444 3266.1126 3409.1505

i3 – p2
Cartesian coordinates

C	-2.609198	0.082524	-0.000002
C	-1.148244	0.007961	0.000011
C	1.367936	-0.630009	-0.000001
C	2.388264	0.465027	0.000003
C	0.018937	-0.388015	0.000003
H	-2.972223	0.616579	0.881895
H	-3.034917	-0.923583	0.000220
H	-2.972219	0.616181	-0.882143
H	1.709974	-1.660442	-0.000033
H	3.037268	0.393760	-0.880325
H	3.037539	0.393493	0.880106
H	1.913200	1.446788	0.000216
H	-0.824793	1.892298	-0.000023

Vibrational frequencies

-765.7710 76.8254 117.5617
129.4557 148.9095 275.3678
362.9802 422.9433 478.0521
610.3231 618.4521 740.3273

980.7235 1009.0596 1044.4064
1050.1206 1111.4942 1228.3449
1402.4220 1407.1515 1420.6943
1475.4553 1480.7345 1482.8318
1500.5698 2078.1841 3023.5261
3044.3627 3077.0317 3115.0809
3127.6099 3138.3919 3175.0364

i3 – p4
Cartesian coordinates

C	2.371624	-0.073554	-0.174462
C	1.062563	-0.357282	-0.090722
C	-1.296090	0.671002	0.003676
C	-2.221127	-0.521356	0.051838
C	0.016562	0.619919	-0.056278
H	3.110613	-0.862885	-0.236750
H	2.717509	0.948433	-0.278090
H	0.753602	-1.403364	-0.024454
H	-1.779503	1.647740	0.019453
H	-2.903769	-0.508242	-0.803169
H	-2.832698	-0.491767	0.958602
H	-1.673477	-1.465019	0.038190
H	3.006528	0.102738	1.921909

Vibrational frequencies

-521.5007 75.5374 142.3554
160.0547 196.1309 276.6365
352.5626 377.5510 607.4450
724.4357 778.3755 857.4922
964.7453 978.1969 1003.4801
1051.1357 1063.4758 1137.6958
1304.2428 1321.0292 1404.8497
1436.7490 1483.6875 1493.7433
1640.3021 1767.0617 3040.3600
3094.1476 3104.3395 3122.1789
3141.9955 3162.9932 3259.0812

i40 – i22
Cartesian coordinates

C	1.481863	-0.975227	0.000035
C	1.428506	0.502017	-0.000212
C	-2.153920	-0.364907	-0.000105
C	0.031849	1.057196	0.000130
C	-0.857266	-0.150131	0.000141
H	1.863496	-1.462246	0.902546
H	1.863211	-1.462551	-0.902428
H	0.139732	-1.096533	0.000253
H	2.306614	1.137031	-0.000469
H	-2.872085	0.455828	-0.000359
H	-2.564591	-1.370021	-0.000067
H	-0.161109	1.692236	0.877731
H	-0.161460	1.692568	-0.877145

Vibrational frequencies

-1888.2589 58.4224 199.9790
284.8604 384.0835 507.5341
553.1088 609.6756 686.0462
877.6663 888.4531 919.2558
923.7627 979.3112 1007.6307
1101.1850 1110.2983 1132.9759
1281.1335 1284.2716 1334.0039
1427.3825 1437.9661 1448.4932
1692.1058 1755.0472 2989.0258
3010.8068 3051.0089 3107.8550
3113.0399 3199.8431 3202.5378

i40 – p13
Cartesian coordinates

C	-1.688472	-0.937286	0.053630
C	-1.311887	0.493820	-0.106421
C	2.178844	-0.536915	0.036287
C	0.010532	0.967616	-0.100511
C	1.120240	0.173648	-0.208893
H	-2.506571	-1.207726	-0.620530
H	-2.040201	-1.134516	1.074922
H	-0.842969	-1.601319	-0.138796
H	-2.104336	1.233659	-0.131858
H	2.750518	-1.015911	-0.755310
H	2.537500	-0.675741	1.057305
H	0.164546	2.028395	-0.284474
H	0.185977	1.407859	1.754191

Vibrational frequencies

-613.3501 78.6544 149.7658
156.2159 223.1945 353.6738
447.4882 483.8769 544.3918
653.8374 678.8145 897.8826
907.6278 964.4172 980.7620
984.6650 1021.4650 1109.0045
1212.0368 1376.8634 1411.6067
1441.8915 1452.4316 1482.5643
1506.7482 1900.5667 3016.9058
3081.6784 3086.4715 3127.7976
3156.9672 3169.6524 3195.5451

i41 – i22
Cartesian coordinates

C	2.272271	-0.363690	-0.221249
C	-1.046945	-0.185180	-0.138132
C	1.020298	-0.095768	0.491419
C	-2.354767	-0.311003	-0.035426
C	-0.015108	0.891841	-0.113619
H	3.108381	0.325518	-0.135257
H	2.349668	-1.161043	-0.951245
H	1.076426	-0.033953	1.579997

H	0.016990	-1.015088	0.226235
H	-3.007210	0.561997	-0.058587
H	-2.829279	-1.281381	0.059246
H	0.274841	1.218613	-1.115552
H	-0.244312	1.768133	0.497208

Vibrational frequencies

-2172.7067 66.8408 163.6427
283.3126 308.1038 394.1927
519.4041 573.6377 602.6685
770.1982 862.1427 904.5757
920.3359 974.4007 1028.6756
1106.9054 1130.9777 1138.7528
1226.5968 1236.7700 1305.1959
1426.1971 1450.1587 1465.0645
1743.7615 1867.3516 3067.0891
3104.5404 3105.9452 3124.1423
3132.8914 3212.9903 3238.2858

i41 – i40
Cartesian coordinates

C	1.724767	-0.929489	0.070030
C	1.263689	0.442158	-0.265813
C	-2.115815	-0.587286	-0.025160
C	-0.033101	0.948238	0.309979
C	-1.208853	0.307295	-0.321063
H	2.217289	0.175929	0.565095
H	2.405841	-1.442834	-0.595440
H	1.152552	-1.509374	0.783683
H	1.630934	0.877681	-1.188019
H	-2.155143	-1.046207	0.967134
H	-2.868747	-0.910465	-0.738706
H	-0.069461	0.734488	1.392605
H	-0.097390	2.035285	0.205813

Vibrational frequencies

-1915.4271 87.8824 120.7241
274.6465 334.2532 368.8078
425.8030 581.7511 734.5765
760.6132 862.4705 894.9100
902.8001 930.1195 1016.7746
1112.2675 1190.0987 1229.7132
1279.2719 1315.7209 1380.2670
1418.2407 1434.2971 1459.6748
1753.8001 2246.2201 2956.5142
3067.0663 3083.0060 3160.9184
3182.4964 3193.0910 3279.9071

i41 – p27
Cartesian coordinates

C	1.745872	-0.956786	0.280584
C	-1.306871	0.271593	0.075566

C	1.619166	0.326895	-0.398041
C	-2.076934	-0.747305	-0.167399
C	-0.354154	1.184486	0.249562
H	2.621155	-1.584850	0.135443
H	0.958271	-1.336936	0.924225
H	1.460970	0.320455	-1.477261
H	2.255654	1.150324	-0.068202
H	-1.672314	-1.666101	-0.589436
H	-3.144248	-0.722992	0.035693
H	-0.273279	2.008692	-0.451340
H	0.031308	1.358102	1.249241

Vibrational frequencies

-547.6611	64.1064	105.6200
214.6611	279.1474	361.1200
374.1871	402.3901	422.3448
676.9354	756.4533	865.9033
874.6756	890.9284	971.8657
1000.5937	1005.8010	1051.8933
1063.4273	1133.5575	1423.0396
1429.7778	1455.1534	1470.0128
1966.9466	3068.1086	3105.3897
3118.5117	3137.1175	3141.4353
3185.6164	3213.0228	3222.3138

i42 – i27
Cartesian coordinates

C	1.495785	0.000010	-0.211205
C	0.305471	0.000003	0.713007
C	-0.637584	-1.096129	0.117175
C	-0.637609	1.096119	0.117174
C	-0.819419	-0.000006	-0.920725
H	2.083227	-0.915027	-0.265341
H	2.083268	0.915025	-0.265285
H	0.525306	0.000040	-1.241436
H	0.485231	0.000004	1.793132
H	-1.529301	-1.269191	0.725630
H	-0.179119	-2.039143	-0.182435
H	-1.529324	1.269173	0.725633
H	-0.179147	2.039130	-0.182450

Vibrational frequencies

-1966.0865	405.2158	459.8416
555.9445	587.7844	805.4232
822.0437	836.6250	905.2074
935.1473	983.1586	983.2354
1000.2082	1056.3314	1080.7120
1094.5037	1140.2586	1141.9803
1212.6074	1219.1117	1264.8239
1383.5260	1456.0806	1486.0870
1516.2340	1740.9345	3060.9503
3073.2336	3080.0466	3106.2595
3145.5524	3145.6127	3197.1499

i42 – i40
Cartesian coordinates

C	1.735385	-0.390732	-0.270381
C	0.580362	0.051257	0.571158
C	-1.267962	-0.968988	0.078624
C	-0.300941	1.181176	0.018976
C	-1.317313	0.253720	-0.553481
H	2.174134	-1.320267	0.098824
H	2.528374	0.371071	-0.282673
H	1.420998	-0.545765	-1.307880
H	0.719610	0.023809	1.651350
H	-1.483035	-1.041681	1.147666
H	-1.433383	-1.905594	-0.457799
H	-0.697692	1.838165	0.802780
H	0.193810	1.821659	-0.721646

Vibrational frequencies

-869.6287	161.6578	252.1338
261.9279	369.9960	609.7725
670.2182	772.4602	844.8517
869.9566	927.4111	966.6166
1002.6521	1031.0754	1091.4526
1122.1429	1195.6198	1250.6989
1325.2991	1341.0794	1413.0948
1466.7302	1490.7040	1493.5663
1500.7658	3003.1008	3025.1009
3060.2348	3062.8798	3075.2563
3121.0330	3135.9243	3140.4658

i43 – i26
Cartesian coordinates

C	-0.666410	0.959186	0.215303
C	-0.062347	-1.293522	0.042321
C	0.833635	0.895311	-0.152407
C	-1.251835	-0.419689	-0.189044
C	1.225626	-0.556148	0.051121
H	-1.180058	1.790794	-0.270833
H	-0.773664	1.085418	1.296919
H	1.431561	1.603023	0.426800
H	0.962262	1.144483	-1.214315
H	-2.132902	-0.687992	0.396237
H	-1.535958	-0.419937	-1.249977
H	0.601242	-1.044561	1.119062
H	2.155492	-0.982060	-0.307656

Vibrational frequencies

-2002.7650	242.3913	271.5926
548.7845	624.4037	740.5350
838.6422	876.9845	891.1210
932.9069	952.1873	1028.9299
1040.2604	1116.6683	1161.3392

1181.5577 1213.4065 1229.0824
1286.2590 1301.7548 1329.2485
1344.5219 1485.9927 1492.4113
1510.8331 2207.8987 3008.7959
3022.1057 3061.9997 3099.2110
3108.0455 3121.5173 3182.1809

i43 – i31
Cartesian coordinates

C	-0.611054	0.925796	0.290145
C	-0.215004	-1.117372	0.366801
C	0.836664	0.880389	-0.161680
C	-1.284575	-0.316097	-0.329298
C	1.151888	-0.654739	-0.047117
H	-1.124578	1.878353	0.419685
H	1.493662	1.505198	0.446461
H	0.933228	1.201744	-1.206562
H	-2.281122	-0.487165	0.076781
H	-1.304500	-0.372749	-1.425020
H	1.925023	-0.865661	0.693878
H	1.466846	-1.088224	-1.001842
H	-0.376078	-0.079348	1.283508

Vibrational frequencies

-2199.5101 263.9544 396.0272
664.1263 765.8025 804.0000
827.3426 848.3356 921.0728
957.6831 974.9475 997.0241
1021.3461 1112.9615 1166.7102
1182.3223 1203.7321 1214.4152
1233.9559 1304.6096 1308.3659
1410.8519 1478.3144 1491.7628
1507.5322 1811.9096 3032.2300
3039.1042 3058.4852 3104.0192
3121.9247 3133.6269 3142.6598

i43 – i41
Cartesian coordinates

C	-1.273740	0.111241	-0.185957
C	0.894201	-0.859359	-0.281250
C	-0.438864	1.332927	0.086824
C	-0.464227	-1.164806	0.201853
C	1.583386	0.266988	0.012731
H	-1.516666	0.055162	-1.249860
H	-2.220450	0.138772	0.364108
H	-0.380051	1.685978	1.112573
H	-0.374201	2.107325	-0.668716
H	-0.462255	-1.283249	1.296517
H	-0.897580	-2.073323	-0.222291
H	1.741644	0.565417	1.051714
H	2.305023	0.681972	-0.689250

Vibrational frequencies

-584.1804 169.5248 311.4180
478.7064 497.2573 581.8231
631.2864 783.2214 819.0482
871.6829 889.9917 908.1596
958.8285 989.5304 1050.3142
1124.2941 1195.0292 1223.3909
1307.0187 1339.3080 1402.3348
1463.4514 1476.0758 1497.9026
1537.0963 2993.2770 3056.6412
3069.2096 3102.6440 3112.4240
3139.6957 3155.3559 3240.2518

i45 – i20
Cartesian coordinates

C	-2.066183	-0.664506	0.034020
C	0.017357	0.863015	-0.124892
C	1.113221	0.092248	0.572277
C	2.100677	-0.509365	-0.371855
C	-1.259716	0.504272	-0.087000
H	-2.246839	0.277566	-0.894724
H	-2.998653	-0.601840	0.585028
H	-1.691481	-1.655624	-0.224745
H	0.313841	1.766992	-0.651463
H	0.660747	-0.694101	1.196984
H	1.638748	0.751405	1.277925
H	3.008983	-0.965494	0.005426
H	1.882521	-0.592886	-1.429724

Vibrational frequencies

-1944.9260 58.8831 150.9381
206.8888 282.9258 333.6925
457.8925 497.0758 569.6549
789.0934 835.1684 844.7218
951.0681 1017.3681 1032.6407
1091.8095 1107.6331 1138.3454
1188.3226 1318.3578 1365.8193
1446.2452 1458.2641 1459.8974
1705.5348 2232.6704 2984.4577
3020.9216 3088.0596 3152.7876
3160.1944 3218.8792 3263.6921

i45 – i37
Cartesian coordinates

C	-2.113965	-0.149684	-0.031148
C	0.281244	1.015589	0.143851
C	1.583284	0.312584	-0.233959
C	1.051670	-1.050725	0.181428
C	-0.676854	0.095888	-0.212995
H	-2.354410	-1.201665	-0.199805
H	-2.694007	0.453719	-0.736469
H	-2.437035	0.112878	0.987180
H	0.245092	1.449507	1.148721

H	2.454458	0.680790	0.312091
H	1.798304	0.353467	-1.304281
H	1.099909	-1.879106	-0.523604
H	1.135414	-1.311505	1.233110

Vibrational frequencies

-1146.9168 149.1290 185.1919
232.1594 303.4409 527.0658
609.2501 746.3880 778.4330
797.9717 863.1526 968.5525
981.7706 1027.9899 1047.0496
1086.5181 1196.6601 1241.4770
1251.7471 1384.6439 1428.4756
1456.6599 1461.8702 1474.5994
1497.8280 2993.7477 3061.4166
3073.6192 3084.2159 3105.4499
3123.0664 3126.3675 3220.6635

i45 – i6
Cartesian coordinates

C	-2.364924	-0.288625	0.064476
C	0.034127	0.771807	0.272260
C	1.202898	0.189712	-0.503097
C	2.262784	-0.492720	0.250256
C	-0.912162	-0.055225	-0.131632
H	-2.547841	-1.288377	0.467262
H	-2.902524	-0.211109	-0.884182
H	-2.782572	0.447228	0.761310
H	0.023870	1.607769	0.964087
H	1.511040	0.767077	-1.378842
H	0.130447	-0.630176	-0.892024
H	3.103514	0.068474	0.650111
H	2.127732	-1.510579	0.598698

Vibrational frequencies

-2206.3432 135.8287 152.2617
246.3288 288.6170 310.7081
390.9216 524.4217 589.1557
800.9342 840.4047 949.3108
971.1869 1009.3566 1045.2372
1086.9561 1109.4125 1173.9973
1218.9477 1271.9374 1399.7526
1445.6865 1473.5989 1481.4462
1755.7979 1862.3766 3026.8051
3082.7496 3104.8478 3119.6617
3133.4528 3197.1414 3238.5300

i45 – i8
Cartesian coordinates

C	2.625825	0.087288	-0.017128
C	0.015780	0.239927	0.026776
C	-1.253368	-0.449808	0.024667

C	-2.562552	0.246664	-0.083451
C	1.215781	-0.325754	-0.037896
H	2.705300	1.179956	0.081838
H	3.146995	-0.203833	-0.934451
H	3.162381	-0.361405	0.825154
H	-0.026900	1.334368	0.098870
H	-1.944983	-0.222352	1.043470
H	-1.251553	-1.517863	-0.162646
H	-3.447978	-0.326491	-0.315436
H	-2.592062	1.327724	-0.114604

Vibrational frequencies

-1915.4010 121.4573 158.5096
168.5833 213.4684 375.1230
407.2899 460.1093 607.4604
789.8144 841.9184 874.9984
975.7804 1035.5301 1042.8352
1129.1143 1206.4206 1233.7521
1272.6184 1394.4731 1413.1366
1439.1482 1459.7702 1483.0571
1684.4267 2235.5596 2993.2952
3037.9412 3073.4556 3097.4977
3172.4481 3196.0914 3295.9936

i45 – i9
Cartesian coordinates

C	-2.411571	-0.291933	-0.007011
C	-0.016488	0.764280	0.016478
C	1.413149	0.551189	0.014166
C	2.027097	-0.794173	0.037016
C	-0.947071	-0.185582	0.044773
H	-2.866948	0.707027	-0.075706
H	-2.812876	-0.780547	0.886251
H	-2.744074	-0.867790	-0.876873
H	-0.346589	1.806399	-0.042137
H	2.053983	1.385236	0.277604
H	1.860563	0.052154	-1.037455
H	3.074451	-0.900285	0.280034
H	1.390792	-1.664882	-0.044254

Vibrational frequencies

-1885.2566 124.1724 159.3523
200.4956 263.2931 326.7676
474.7097 583.7178 629.0711
727.7475 859.0435 883.2618
954.6873 1019.1311 1041.0144
1104.0805 1203.3415 1254.9617
1298.7747 1400.6649 1408.9444
1450.9985 1458.4355 1484.0876
1665.8835 2246.5621 2994.4827
3068.8135 3072.8836 3098.2946
3177.9484 3193.8192 3301.9367

i45 – p29
Cartesian coordinates

C	-2.080902	-0.656201	0.108399
C	-0.258353	1.267179	-0.164523
C	1.743342	0.342257	0.233600
C	1.672091	-1.056740	-0.166558
C	-1.183437	0.475442	-0.072283
H	-2.465621	-1.004291	-0.853554
H	-2.934741	-0.383503	0.734459
H	-1.561393	-1.490718	0.591452
H	0.152521	2.238591	-0.334390
H	1.767898	0.573563	1.298389
H	2.365894	1.012296	-0.363709
H	2.514513	-1.727675	-0.017633
H	0.804483	-1.449886	-0.686825

Vibrational frequencies

-565.9891	48.0886	81.2256
103.5581	218.3237	293.1207
358.8283	378.9269	423.0137
639.6080	697.6551	714.1415
810.9451	940.1095	972.6925
997.6109	1037.1837	1059.9802
1133.1010	1412.1178	1426.3702
1451.7199	1477.9983	1481.8558
2085.0787	3032.5627	3066.1627
3100.1162	3117.9901	3119.9335
3145.7664	3215.3961	3396.6417

i4 – i9
Cartesian coordinates

C	1.881324	0.847375	-0.000021
C	1.400469	-0.572966	0.000076
C	-1.212968	-0.534245	-0.000182
C	-2.147585	0.624320	0.000060
C	0.063026	-0.911255	-0.000119
H	1.048198	1.552467	-0.000234
H	2.502145	1.051840	-0.880136
H	2.501859	1.052041	0.880251
H	2.146535	-1.360809	0.000322
H	-0.921670	-1.789879	0.000419
H	-2.795858	0.601518	-0.880402
H	-1.593803	1.570114	-0.001790
H	-2.793001	0.603333	0.882683

Vibrational frequencies

-2149.1875	53.3875	70.2326
130.9923	132.1369	328.6972
358.1721	446.5855	591.0541
692.1714	774.2002	935.5470
1009.3728	1021.7168	1034.3416
1108.5747	1184.6517	1387.3741

1391.4674 1403.2354 1469.2737
1476.0504 1478.6672 1497.4179
1662.4501 2355.4290 3019.5444
3020.9956 3073.7581 3098.3392
3106.9014 3129.1748 3182.1572

i4 – p1
Cartesian coordinates

C	-2.186810	0.934826	-0.000114
H	-3.225230	0.621914	0.020900
H	-1.823346	1.345500	-0.934189
H	-1.792409	1.365073	0.912334
C	-1.105679	-1.062317	0.000310
C	1.437339	-0.538570	-0.000159
C	1.849406	0.901248	0.000042
C	0.128555	-0.943197	0.000045
H	-2.017677	-1.615952	-0.000095
H	2.217144	-1.294806	-0.000141
H	2.463482	1.131104	-0.878333
H	2.458637	1.132274	0.881525
H	0.982532	1.562957	-0.002751

Vibrational frequencies

-568.7837 48.1876 79.7412
82.9427 155.0266 255.4306
403.9568 492.1907 505.9651
534.3397 541.0507 644.1069
728.9333 861.3852 884.8183
1007.9336 1096.9488 1146.1914
1384.4267 1405.4489 1421.2509
1424.4672 1480.7783 1496.3921
1874.9355 3022.4084 3075.6963
3094.5189 3138.7959 3168.4984
3254.7022 3266.6860 3408.6930

i4 – p4
Cartesian coordinates

C	1.732232	0.721764	-0.043010
C	1.285000	-0.532019	-0.266057
C	-1.273547	-0.612624	0.180678
C	-1.788674	0.774189	-0.125199
C	-0.023743	-1.004084	0.079856
H	2.718724	1.024547	-0.373626
H	1.082040	1.496371	0.347255
H	2.448371	0.611884	1.845391
H	1.971580	-1.264290	-0.683569
H	-2.019734	-1.338725	0.504011
H	-2.010318	1.316598	0.799729
H	-2.716523	0.715753	-0.700307
H	-1.061747	1.354509	-0.696490

Vibrational frequencies

-807.8234 96.4896 128.7810
193.3116 217.4910 342.3805
370.9253 434.8803 643.1734
727.1648 770.1780 839.9503
974.4805 982.8568 1016.6826
1051.2093 1086.7349 1104.9143
1311.1292 1314.7248 1400.5236
1438.1544 1490.0458 1492.2674
1614.1589 1767.7711 3038.8919
3105.6117 3117.1975 3138.4462
3155.9719 3163.4863 3253.5144

i5 – i6
Cartesian coordinates

C	2.178791	-0.606205	0.000000
C	1.404257	0.671041	-0.000003
C	-1.176002	0.510747	0.000005
C	-2.326995	-0.439750	-0.000003
C	0.139777	0.140538	0.000004
H	2.692214	-0.899747	-0.917449
H	2.692213	-0.899742	0.917452
H	1.750683	1.697818	-0.000016
H	-1.401162	1.578344	0.000007
H	-2.963756	-0.287851	-0.879096
H	-2.963745	-0.287886	0.879103
H	-1.981605	-1.474959	-0.000025
H	0.856189	-1.084202	0.000005

Vibrational frequencies

-2255.8660 121.6778 185.2070
215.2403 223.7665 496.5594
545.7269 593.7749 661.9946
760.1154 906.5426 948.4388
1012.3137 1027.0241 1048.4359
1113.5297 1185.0780 1186.4572
1223.5071 1354.5061 1412.7223
1419.9070 1464.1284 1480.8051
1512.8224 1851.7012 3023.5625
3063.1986 3075.8902 3111.5066
3135.0263 3154.5097 3202.0149

i5 – p2
Cartesian coordinates

C	2.564675	0.381866	-0.000003
C	1.195935	-0.134871	-0.000009
C	-1.369583	-0.538761	0.000031
C	-2.450968	0.493752	0.000005
C	-0.031549	-0.243250	0.000003
H	3.110998	0.038298	0.882192
H	2.552396	1.474298	-0.000422
H	3.111276	0.037614	-0.881754
H	-1.653735	-1.587843	-0.000091
H	-3.096457	0.383851	0.879125

H	-3.095020	0.385341	-0.880371
H	-2.039433	1.503813	0.001157
H	1.658916	-1.987790	0.000001

Vibrational frequencies

-776.6676 73.8711 115.1621
122.4775 193.9787 224.5481
384.9807 423.0902 449.9265
580.3885 621.6857 753.1670
987.3005 1010.4385 1044.6676
1050.5579 1110.3862 1223.9736
1405.4424 1408.9746 1424.4587
1475.7679 1480.1258 1483.0488
1503.4538 2079.5957 3022.7797
3044.0186 3075.0383 3114.6603
3127.2250 3136.4971 3162.9669

i5 – p4
Cartesian coordinates

C	-2.419909	0.305053	0.211849
C	-1.319548	-0.440727	0.029259
C	1.240133	-0.426778	-0.068491
C	2.513358	0.363953	0.011939
C	0.023485	0.053471	0.062461
H	-3.404813	-0.145264	0.212798
H	-2.348606	1.358154	0.458151
H	-1.428230	-1.507892	-0.180823
H	1.347528	-1.502272	-0.252801
H	3.080903	0.274669	-0.919579
H	3.151464	-0.014244	0.816704
H	2.311352	1.419710	0.195677
H	-2.934713	0.987310	-1.812226

Vibrational frequencies

-519.3861 109.8263 139.3605
161.8598 191.2241 262.5041
294.6167 426.5777 471.9102
695.2896 796.3498 868.0737
962.2514 997.4176 1011.1658
1061.1148 1098.1681 1161.1572
1272.4231 1312.1388 1410.3229
1439.2635 1486.7980 1490.7630
1646.1809 1772.0889 3037.9720
3049.5599 3092.5812 3099.5995
3143.3321 3163.5859 3259.5279

i6 – i19
Cartesian coordinates

C	2.479697	-0.108539	-0.198313
C	1.198810	0.385062	-0.079009
C	-1.240512	0.219908	0.502184
C	-2.294796	-0.099279	-0.515689

C	0.107101	-0.349975	0.362036
H	2.703161	-1.143147	0.040297
H	3.297935	0.519422	-0.527250
H	1.028118	1.431186	-0.327994
H	-1.380669	1.137560	1.064327
H	-3.117921	0.589478	-0.656722
H	-2.231864	-0.600718	0.676368
H	-2.061051	-0.814483	-1.293758
H	0.260495	-1.402362	0.597475

Vibrational frequencies

-1905.9355 89.6023 151.8934
243.4536 370.9890 412.7580
517.5101 565.7993 716.0647
752.4198 760.6266 808.6733
892.9607 995.8961 1006.4560
1100.3777 1184.0726 1198.3473
1228.1122 1297.9618 1307.1763
1371.2307 1419.1222 1492.5328
1523.2912 2245.3767 3137.9795
3151.8931 3156.3820 3156.6676
3182.5091 3256.7964 3280.0676

i6 – i22
Cartesian coordinates

C	-2.148285	0.292554	-0.402486
C	-1.297805	-0.522856	0.490356
C	1.172898	-0.335193	-0.216970
C	2.401669	0.176904	-0.083189
C	-0.037882	0.251117	0.352904
H	-2.523009	-0.144111	-1.329531
H	-2.800956	1.049650	0.037547
H	-1.407298	-1.566601	0.759756
H	1.036994	-1.237992	-0.809078
H	3.261317	-0.287431	-0.551669
H	2.579600	1.075225	0.500377
H	-0.819774	0.911397	-0.560922
H	0.129555	1.024706	1.109832

Vibrational frequencies

-2178.1715 97.4591 124.9002
229.7430 340.4721 443.0681
485.4260 605.7603 697.9349
885.6033 901.1958 922.7090
937.0405 966.3710 1020.4397
1066.8251 1106.9411 1170.8457
1252.3137 1288.7298 1314.5424
1337.8040 1416.3946 1460.5980
1662.8204 1757.0567 3063.7350
3067.7601 3151.8295 3157.6398
3165.9022 3212.5172 3246.8192

i6 – i7

Cartesian coordinates

C	-2.370806	0.479549	-0.225470
C	-1.401225	-0.453270	0.325397
C	1.004779	0.191746	0.347251
C	2.410815	0.161049	-0.168445
C	-0.010181	-0.493553	-0.172714
H	-2.923733	0.255723	-1.135926
H	-2.500828	1.473119	0.197423
H	-1.723395	-1.218975	1.031012
H	0.817005	0.826919	1.211436
H	3.106075	-0.178345	0.606009
H	2.736962	1.160892	-0.472842
H	2.505066	-0.505929	-1.028647
H	0.182554	-1.126526	-1.044582

Vibrational frequencies

-231.4307	154.8118	172.5249
205.3005	339.2716	352.3668
459.5398	551.1996	594.7171
795.3403	910.3025	935.0438
975.6788	1035.1315	1069.4611
1116.4011	1152.6564	1288.0501
1326.1395	1332.2079	1415.0873
1441.1510	1478.0450	1496.0758
1743.8626	3040.3412	3078.2511
3100.2081	3102.6023	3124.6358
3126.7873	3155.9462	3191.7520

i6 – i8
Cartesian coordinates

C	-2.672201	-0.118008	-0.000236
C	-1.270045	0.220967	0.000469
C	1.171598	0.434897	-0.000040
C	2.537079	-0.166152	-0.000140
C	0.005130	-0.296422	0.000332
H	-3.169141	-0.376080	0.932267
H	-3.167616	-0.378487	-0.932886
H	-2.188251	1.127893	-0.001494
H	1.095363	1.519151	-0.000237
H	3.110905	0.151579	0.878217
H	3.110567	0.151130	-0.878876
H	2.494858	-1.258081	0.000137
H	0.083946	-1.388794	0.000568

Vibrational frequencies

-2069.8932	56.5579	113.3856
172.4640	225.6024	238.9672
409.8340	482.0695	746.8730
774.1241	879.9070	922.8733
976.5078	1002.9763	1027.1570
1051.3610	1131.2654	1254.3031
1276.5956	1405.1846	1410.7661

1468.3048 1474.0733 1513.0699
1531.8987 2249.3843 3022.1703
3072.7914 3073.0046 3099.2043
3122.0342 3173.0065 3205.6398

i6 – i9
Cartesian coordinates

C	1.981407	-0.751068	0.003860
C	1.352903	0.601630	0.009248
C	-1.002588	-0.109344	-0.031116
C	-2.433070	-0.294765	0.010476
C	-0.005289	0.839165	-0.010169
H	1.231967	-1.537843	0.109298
H	2.709130	-0.850595	0.816187
H	2.526632	-0.925593	-0.931355
H	2.017841	1.459994	0.015138
H	-3.004922	-0.311064	-0.914303
H	-2.971281	-0.149041	0.944425
H	-1.531607	-1.280090	0.081568
H	-0.337932	1.880526	-0.014749

Vibrational frequencies

-2061.6966 84.5961 128.5213
178.0240 204.2899 353.4687
387.4889 626.9357 686.4790
777.1191 892.2982 919.2675
955.2736 977.8510 1031.5941
1056.0664 1114.9356 1215.3752
1334.8098 1404.2781 1412.4464
1459.2332 1483.2444 1508.2406
1531.2822 2250.2900 3030.1097
3084.4781 3088.9911 3097.8044
3130.4512 3183.5215 3205.2309

i6 – p13
Cartesian coordinates

C	-2.635639	-0.053895	-0.000067
C	-1.321059	-0.052422	0.000052
C	1.104785	0.413375	-0.000009
C	2.502618	-0.103991	-0.000025
C	-0.016514	-0.407702	0.000070
H	-3.203361	-0.004842	0.927228
H	-3.203198	-0.004998	-0.927471
H	-1.144889	1.932355	0.000260
H	0.954429	1.489034	-0.000167
H	3.056047	0.249830	0.877765
H	3.055527	0.248426	-0.878723
H	2.531079	-1.196363	0.000822
H	0.149213	-1.485635	0.000162

Vibrational frequencies

-807.3116 104.1772 136.8557

159.2720 211.8315 310.2644
426.5588 531.0285 532.7168
547.2604 734.2060 883.7322
914.7695 927.5196 991.5853
1023.4309 1034.1525 1130.2755
1225.0829 1302.1408 1416.5759
1438.1317 1476.7881 1477.7645
1515.9960 1829.4827 3019.6593
3070.7372 3099.9722 3116.5760
3127.7216 3170.6552 3177.0294

i6 – p3
Cartesian coordinates

C	-2.536593	-0.246576	0.031587
C	-1.305200	0.390537	0.034644
C	1.193593	0.447496	-0.079583
C	2.384462	-0.191165	-0.096986
C	-0.090579	-0.248173	-0.091919
H	-2.606054	-1.323819	-0.073148
H	-3.458878	0.310334	0.134111
H	-1.294502	1.473717	0.144420
H	1.168257	1.527752	0.039030
H	2.633021	-0.684009	1.628448
H	3.314389	0.363822	-0.127891
H	2.439959	-1.250448	-0.329461
H	-0.070290	-1.330060	-0.201970

Vibrational frequencies

-1269.9039 100.9122 182.1222
211.0296 299.6168 459.8347
470.7241 500.4578 522.9391
724.9157 781.2374 838.4121
914.6896 990.3848 1007.0168
1015.6258 1032.8219 1165.6416
1206.1466 1295.3442 1302.1287
1318.2252 1433.7349 1505.1568
1520.8108 1669.8640 3146.1783
3147.8262 3157.5656 3161.3700
3169.4692 3244.0172 3261.3166

i6 – p4
Cartesian coordinates

C	2.442219	0.348039	0.107744
C	1.329745	-0.479789	0.148891
C	-1.220561	-0.235170	-0.511304
C	-2.310582	0.211760	0.422962
C	0.064958	-0.190557	-0.236988
H	2.368733	1.360196	-0.271030
H	3.402184	-0.010593	0.455229
H	1.464556	-1.489963	0.534121
H	-1.525323	-0.517135	-1.520435
H	-3.087632	-0.554907	0.494286
H	-2.784503	1.123975	0.045617

H	-1.919032	0.412476	1.420636
H	0.246353	1.750248	-0.746257

Vibrational frequencies

-731.0239 91.0903 168.7481
182.1506 241.9689 334.1802
454.1376 526.2729 535.3505
569.4765 753.6294 771.3030
828.3284 942.7730 1004.0627
1055.8715 1079.9141 1116.7550
1203.5191 1316.4419 1406.8137
1415.3397 1486.3749 1487.2727
1497.2105 1849.3667 3042.9932
3106.2884 3113.1300 3141.8109
3151.6499 3163.3240 3271.2854

i7 – i20
Cartesian coordinates

C	1.839434	-0.609060	-0.362611
C	1.045515	0.329012	0.491333
C	-1.378514	0.387691	-0.182907
C	-1.632040	-0.928507	0.127839
C	-0.143954	1.015600	-0.043907
H	2.185020	0.606811	-0.054116
H	1.558371	-0.730889	-1.400378
H	2.462623	-1.355123	0.112960
H	1.141235	0.194584	1.565797
H	-2.199312	0.988548	-0.568590
H	-2.618229	-1.355989	-0.003347
H	-0.847170	-1.577068	0.501191
H	-0.065185	2.060705	-0.332002

Vibrational frequencies

-1912.7773 63.0389 216.2712
254.9610 383.5326 426.6513
553.3184 612.3971 708.1341
726.0207 750.5425 828.9931
894.2886 999.2168 1026.9266
1055.5280 1130.7411 1207.0126
1224.5507 1264.6840 1340.9904
1420.0169 1428.5088 1443.6778
1530.7205 2248.7269 3151.2341
3153.8858 3159.1935 3163.0472
3174.8985 3258.9780 3285.0479

i7 – i22
Cartesian coordinates

C	-1.922278	-0.302768	-0.470774
C	-1.018946	-0.234628	0.694432
C	1.299706	0.511467	-0.147436
C	1.867270	-0.699267	-0.083029
C	-0.094406	0.803939	0.176350

H	-1.899491	-1.188683	-1.108381
H	-2.892077	0.197001	-0.421754
H	-0.885602	-0.924608	1.518088
H	1.889973	1.353646	-0.501103
H	2.902490	-0.850809	-0.364523
H	1.311406	-1.567714	0.256015
H	-0.294084	1.826451	0.510821
H	-0.920692	0.682256	-0.906423

Vibrational frequencies

-2182.6417 103.8364 187.4368
224.2847 292.8840 452.4428
590.2077 599.9341 698.5058
875.9555 904.6337 917.7906
930.3781 967.5589 1023.6360
1031.7887 1065.1736 1138.8381
1264.5121 1290.8813 1324.2187
1360.7239 1420.0044 1444.8647
1657.6595 1778.3623 3062.3723
3080.3264 3151.6658 3154.8374
3168.6575 3219.0884 3250.4450

i7 – i25
Cartesian coordinates

C	1.938828	0.164176	0.265381
C	0.593232	0.085804	-0.401516
C	-1.547348	-0.415395	0.093229
C	-1.169072	0.976476	0.079540
C	-0.264172	-1.058431	-0.228007
H	2.635822	-0.529028	-0.222886
H	1.876565	-0.112632	1.319887
H	2.365222	1.166526	0.190953
H	0.556446	0.596067	-1.362745
H	-2.212422	-0.834178	0.843088
H	-1.434355	1.612000	0.928810
H	-1.164997	1.531589	-0.856359
H	0.068911	-1.946128	0.307493

Vibrational frequencies

-934.6601 57.1410 128.7985
271.8980 374.2322 546.6492
571.2804 674.2847 755.6402
845.6182 924.0822 959.8704
995.8236 1025.1176 1047.1499
1130.9557 1154.5309 1216.5226
1291.5072 1361.8532 1395.7913
1441.1078 1481.6794 1490.0798
1495.3682 3029.2877 3071.6657
3105.3445 3112.8166 3136.9732
3142.1523 3152.9504 3170.4501

i7 – i8
Cartesian coordinates

C	-2.355057	-0.490800	-0.009863
C	-1.324533	0.521051	0.022416
C	0.944430	-0.348295	0.021505
C	2.426735	-0.178857	-0.010981
C	0.042988	0.695078	0.005014
H	-2.739072	-0.906781	0.918578
H	-2.554059	-1.029810	-0.933843
H	-2.567810	0.823903	-0.124233
H	0.552827	-1.362411	0.056429
H	2.864588	-0.668759	-0.888496
H	2.897218	-0.633862	0.868284
H	2.708512	0.876664	-0.037778
H	0.430424	1.711990	-0.027495

Vibrational frequencies

-2080.9921 81.1262 152.0068
154.1286 205.2194 342.9862
369.0492 620.2190 755.4667
775.1796 904.3481 911.2514
967.0053 981.1252 1031.9995
1048.6271 1130.6879 1238.8188
1314.8018 1399.9805 1418.3427
1472.6896 1478.2365 1487.8571
1525.2093 2253.1926 3025.7363
3078.6898 3094.3477 3117.0418
3151.1572 3168.3239 3200.8417

i7 – i9
Cartesian coordinates

C	1.600856	-0.908003	0.000003
C	1.459874	0.574177	-0.000012
C	-0.736294	-0.119510	0.000004
C	-2.206912	-0.261420	-0.000005
C	0.127886	0.958117	0.000003
H	0.239365	-1.079437	-0.000014
H	2.001450	-1.366764	0.905842
H	2.001503	-1.366814	-0.905786
H	2.298490	1.260186	-0.000026
H	-2.557573	-0.810252	-0.881105
H	-2.695226	0.720350	0.000492
H	-2.557484	-0.811096	0.880604
H	-0.202986	1.993659	0.000033

Vibrational frequencies

-1949.4411 52.8935 194.4611
265.8043 373.4985 516.1397
531.9904 653.4409 730.6789
916.5346 929.4911 953.2654
1013.7714 1026.2899 1037.9446
1100.0381 1105.2927 1191.1438
1285.9406 1398.1013 1404.7529
1453.6000 1461.1287 1466.2279

1501.7977 1725.2431 3015.9397
3081.1495 3082.3734 3088.3860
3155.2961 3168.4353 3213.7097

i7 – p13
Cartesian coordinates

C	1.711620	-0.880311	0.000005
C	1.307272	0.553663	-0.000052
C	-1.108357	0.242643	0.000005
C	-1.952218	-0.766252	-0.000012
C	-0.005520	1.026973	-0.000012
H	2.325117	-1.113322	-0.877912
H	0.847991	-1.547711	-0.001440
H	2.322559	-1.113975	0.879555
H	2.097474	1.297315	0.000066
H	-2.445543	1.652839	0.000141
H	-2.355037	-1.168509	0.927682
H	-2.355053	-1.168464	-0.927721
H	-0.154294	2.101538	0.000029

Vibrational frequencies

-871.4812 69.5221 160.8413
187.6423 232.3674 345.1908
407.8410 517.6602 559.4704
647.3839 690.1210 887.6925
904.2821 937.1583 973.8325
992.4966 1022.5782 1111.0431
1213.3564 1379.4686 1413.1388
1438.4143 1456.3069 1482.9812
1510.3061 1830.4422 3024.1677
3075.1442 3099.4397 3131.6154
3177.0905 3178.0635 3194.8058

i7 – p3
Cartesian coordinates

C	-2.258958	-0.166978	-0.114815
C	-0.925587	-0.379590	-0.090572
C	1.418250	0.556774	0.012129
C	2.118158	-0.639238	0.041812
C	0.046003	0.709388	-0.055332
H	-2.956453	-0.993369	-0.180498
H	-2.659050	0.826224	-0.295905
H	-2.679902	0.140728	1.660004
H	-0.559218	-1.398166	-0.014823
H	2.004865	1.471332	0.042846
H	3.199233	-0.643181	0.095782
H	1.623009	-1.602126	0.012651
H	-0.359678	1.716420	-0.079391

Vibrational frequencies

-1178.5246 72.4033 211.7258
239.1013 326.1547 408.0123

456.2691 524.9660 610.2167
697.5115 785.6389 805.8945
916.6776 998.7141 1005.3577
1018.9564 1035.7466 1110.1179
1197.7146 1246.4546 1321.5246
1387.9400 1446.5556 1501.0703
1529.9281 1668.1770 3146.6342
3161.6672 3166.8112 3184.7111
3190.3894 3244.6564 3264.6420

i7 – p4
Cartesian coordinates

C	2.207425	-0.415306	-0.349737
C	1.126947	0.126273	0.544541
C	-1.398457	0.450480	-0.179479
C	-2.237762	-0.641407	0.008517
C	-0.083575	0.448697	0.144770
H	3.006994	0.322932	-0.471307
H	1.816549	-0.667991	-1.335756
H	2.654112	-1.309734	0.094327
H	1.410481	0.353958	1.573327
H	-1.813379	1.358253	-0.606788
H	-3.282423	-0.584930	-0.268481
H	-1.866086	-1.565378	0.433987
H	0.386287	2.280473	-0.430986

Vibrational frequencies

-764.4010 111.0644 139.6209
212.5636 258.6021 290.4043
464.9084 487.9645 539.8665
589.6113 755.7629 783.2877
827.1158 962.0277 1002.6257
1052.3891 1083.3334 1124.1148
1200.2335 1325.0233 1404.8281
1408.8579 1485.1615 1493.3214
1494.4181 1855.4578 3038.0720
3101.9593 3107.8137 3147.7333
3163.8231 3175.7176 3270.4319

i8 – i9
Cartesian coordinates

C	-2.306029	0.533484	0.044991
C	-1.316729	-0.544869	-0.233471
C	1.103131	0.035827	-0.289369
C	2.531271	0.257206	-0.019677
C	0.051239	-0.469109	0.308763
H	-1.933366	1.504962	-0.304962
H	-2.487702	0.648551	1.123892
H	-3.266334	0.339987	-0.436871
H	-1.627028	-1.449544	-0.745759
H	3.157285	-0.271347	-0.744059
H	2.795495	-0.104104	0.984847
H	2.783444	1.319880	-0.074734

H	0.200910	-0.863622	1.330219

Vibrational frequencies

-315.0077	88.5693	124.3519
168.9862	201.9702	299.6786
369.0202	518.9876	751.7441
871.8705	978.4655	982.8860
1048.2437	1049.7133	1107.8279
1149.0919	1256.5629	1354.8678
1397.8319	1412.3301	1456.6402
1477.0587	1479.0628	1491.3787
1770.6505	2935.5281	2994.6132
3002.7259	3042.6950	3089.3524
3116.9015	3125.2402	3186.8981

i8 – p13
Cartesian coordinates

C	2.537953	0.028525	0.000100
C	1.268933	-0.295009	-0.000148
C	-1.060682	0.400898	-0.000161
C	-2.514242	0.068544	0.000122
C	-0.051950	-0.558549	-0.000069
H	3.105894	0.098178	-0.925897
H	3.105465	0.098241	0.926358
H	2.543097	2.132484	0.000194
H	-0.775530	1.448505	-0.000410
H	-3.018232	0.487987	-0.878554
H	-3.018070	0.488996	0.878401
H	-2.680591	-1.011464	0.000755
H	-0.342106	-1.609381	0.000088

Vibrational frequencies

-508.4131	121.9120	132.9309
133.0632	205.4509	271.9170
289.0330	403.1544	562.3524
605.5443	726.4657	914.4736
918.1510	922.8046	991.8450
1018.8118	1023.4071	1128.2575
1226.1374	1303.8143	1416.3044
1437.5319	1475.8916	1477.0778
1515.5001	1870.8235	3019.5389
3070.4364	3098.4482	3117.1660
3129.2365	3173.0632	3181.0871

i8 – p2
Cartesian coordinates

C	-2.660033	0.144058	-0.065459
C	-1.236829	-0.148726	-0.077306
C	1.315254	-0.566254	0.097273
C	2.455362	0.365407	-0.145685
C	-0.013920	-0.188613	0.088127
H	-3.043405	0.292313	-1.079094

H	-2.852492	1.059005	0.506040
H	-3.224135	-0.671174	0.394511
H	1.534696	-1.599529	0.349065
H	3.166012	-0.067467	-0.857288
H	3.009487	0.557624	0.781853
H	2.109612	1.324563	-0.533178
H	0.141218	1.469429	1.056387

Vibrational frequencies

-653.2708 51.5998 76.1598
97.8733 143.5384 180.9725
339.6756 440.2630 524.8065
556.1334 578.0908 761.7421
992.1297 1009.6489 1026.8046
1051.2478 1114.8694 1229.6839
1402.6247 1409.9350 1425.8564
1472.4894 1478.2596 1478.6912
1500.2193 2083.4548 3020.1698
3028.8959 3078.5428 3096.3859
3115.7707 3138.0443 3173.2796

i9 – p13
Cartesian coordinates

C	1.672436	0.941332	-0.000010
C	1.373161	-0.518815	0.000016
C	-1.064496	-0.373086	-0.000011
C	-2.170281	0.327733	-0.000006
C	0.091629	-1.065779	0.000002
H	0.760451	1.542284	0.000071
H	2.264512	1.220646	-0.879132
H	2.264684	1.220651	0.878994
H	2.210215	-1.209169	0.000033
H	-1.543764	2.361062	0.000098
H	-2.686326	0.573382	0.926433
H	-2.686315	0.573424	-0.926440
H	0.001853	-2.150584	-0.000003

Vibrational frequencies

-441.9677 61.0212 154.5061
166.9075 193.5160 292.9125
360.1980 402.9330 594.3558
667.3422 672.2401 899.0411
911.5059 923.8662 967.0257
993.5268 1020.1824 1104.2743
1207.2016 1372.6942 1411.9366
1438.1378 1457.8409 1482.7780
1505.7801 1870.2547 3021.9470
3074.3673 3104.7437 3124.2124
3151.0420 3179.7750 3196.2047

i9 – p2
Cartesian coordinates

C	-2.302043	-0.616515	-0.000018
C	-1.378068	0.559390	0.000023
C	1.145591	-0.019075	0.000013
C	2.564346	-0.328597	-0.000002
C	-0.006960	0.420716	0.000008
H	-1.749918	-1.557086	-0.000214
H	-2.955960	-0.599353	-0.879695
H	-2.955729	-0.599594	0.879839
H	-1.803992	1.555748	0.000090
H	2.842989	-0.908345	0.884895
H	3.151444	0.595181	-0.000329
H	2.842852	-0.908887	-0.884585
H	0.491115	2.326827	-0.000147

Vibrational frequencies

-662.0690 42.2471 72.4987
98.3220 137.0889 178.8458
308.9341 416.6385 480.8633
589.9356 603.4914 735.4588
984.7842 1006.8477 1037.0692
1040.8820 1116.8952 1238.7915
1403.1188 1408.1018 1422.6537
1472.4483 1478.3674 1480.2172
1500.4778 2060.3162 3021.1954
3031.3630 3072.9708 3103.4125
3104.7834 3138.8527 3196.9347

Products

p10
Cartesian coordinates

C	-1.747103	-0.389169	0.000035
C	-0.681655	0.504127	0.000016
C	1.874118	-0.177454	0.000074
C	0.620395	0.156887	-0.000200
H	-1.578562	-1.458747	-0.000127
H	-2.767036	-0.028281	0.000171
H	-0.898444	1.570668	0.000020
H	2.424921	-0.325106	-0.927157
H	2.424592	-0.324878	0.927541

Vibrational frequencies

209.0211 213.8649 505.0050
530.0106 579.4298 748.2557
899.1667 913.7865 947.7007
984.0837 1090.8450 1196.3940
1378.3399 1453.0183 1498.6362
1930.1390 3100.4277 3149.6628
3167.5102 3172.9718 3272.9783

p11
Cartesian coordinates

C	-2.202863	-0.504601	-0.000002
C	-0.106095	1.019827	0.000001
C	1.303492	0.508372	0.000000
C	1.436144	-1.010363	0.000001
C	-1.219188	0.214970	-0.000001
H	-3.064853	-1.126733	0.000001
H	-0.258243	2.094726	0.000002
H	1.823650	0.928717	0.871549
H	1.823649	0.928716	-0.871550
H	0.959304	-1.445526	-0.881510
H	0.959305	-1.445524	0.881514
H	2.488247	-1.303609	0.000001

Vibrational frequencies

60.3804	156.1602	253.8724
362.8701	389.1295	484.3600
585.1426	628.4224	677.5132
786.1714	859.2530	996.3693
1074.5459	1101.7148	1159.8397
1283.1720	1365.4321	1396.6775
1432.1584	1478.1352	1501.2419
1507.2860	2027.3656	3011.5488
3034.2103	3052.1639	3129.1699
3131.6292	3177.2384	3476.8076

p12
Cartesian coordinates

C	-1.838653	0.110858	-0.000008
C	-0.609548	-0.401480	0.000009
C	1.838645	-0.110858	-0.000004
C	0.609566	0.401478	0.000012
H	-2.002296	1.184459	-0.000006
H	-2.718148	-0.522053	-0.000018
H	-0.477316	-1.481597	0.000009
H	2.002239	-1.184459	-0.000015
H	2.718125	0.522066	-0.000030
H	0.477335	1.481592	0.000004

Vibrational frequencies

162.9880	302.2604	524.5115
541.3506	789.3805	904.6972
956.9402	957.4035	1009.4093
1015.6683	1065.0182	1233.7199
1323.3513	1325.1547	1421.9497
1476.6660	1683.0870	1749.8620
3144.9270	3148.1787	3157.3437
3161.7194	3242.4849	3242.7456

p13
Cartesian coordinates

C	1.689969	-0.907174	0.000015
C	1.302425	0.532219	0.000009

C	-1.121349	0.234292	-0.000009
C	-2.193253	-0.498728	-0.000015
C	-0.012113	0.998923	-0.000003
H	0.814677	-1.559989	0.000029
H	2.297734	-1.151447	0.878943
H	2.297715	-1.151460	-0.878923
H	2.096713	1.271090	0.000012
H	-2.665756	-0.820447	-0.926883
H	-2.665771	-0.820442	0.926846
H	-0.169388	2.075502	-0.000007

Vibrational frequencies

71.8475	154.8857	181.5267
308.8985	379.4322	519.6382
647.0516	676.1402	898.2040
903.3770	926.7364	981.0990
987.7493	1022.1436	1108.4888
1206.3386	1376.6725	1413.2354
1440.8621	1458.8287	1482.4723
1510.2871	1926.2971	3022.7538
3073.9716	3095.0270	3126.5141
3151.5004	3165.5666	3191.2873

p14
Cartesian coordinates

C	-2.656412	0.246374	0.003629
C	-1.321667	-0.058816	0.000085
C	1.294562	-0.638855	-0.018117
C	2.174532	0.616272	0.017082
C	-0.131827	-0.335097	-0.003258
H	-3.401842	-0.527824	0.137489
H	-2.990593	1.267839	-0.130729
H	1.531203	-1.285553	0.834300
H	1.521638	-1.226153	-0.915783
H	1.963710	1.259077	-0.839890
H	3.231657	0.341843	-0.008294
H	1.989092	1.191505	0.926382

Vibrational frequencies

69.9059	131.2549	138.7818
255.1923	319.5944	421.0983
513.0661	670.1329	744.8342
778.4634	991.8172	1032.6406
1092.3697	1093.7701	1248.2997
1288.5665	1365.9234	1417.6361
1467.0508	1470.5753	1497.2957
1503.9087	2160.5804	3036.4247
3056.5137	3069.4076	3135.5883
3143.0672	3159.3901	3256.7635

p15
Cartesian coordinates

C	-0.000170	-0.444518	-0.000062
C	-1.222690	0.196580	-0.000093
C	1.222823	0.196457	0.000034
H	-0.000317	-1.532379	-0.000161
H	-2.151852	-0.359027	0.000633
H	-1.283714	1.279825	0.000051
H	1.284086	1.279725	-0.000066
H	2.152018	-0.359253	0.000269

Vibrational frequencies

436.6270	535.9585	558.4950
793.5155	816.8455	941.8769
1020.2912	1044.9793	1199.2086
1280.5116	1422.0844	1515.6846
1524.2355	3150.5281	3152.6205
3160.1593	3254.5426	3257.3500

p16
Cartesian coordinates

C	-0.489608	-1.141875	-0.000084
C	-1.271527	0.000021	0.000002
C	0.969049	0.776055	-0.000100
C	0.969021	-0.776087	0.000102
C	-0.489569	1.141892	0.000081
H	-0.856395	-2.159684	-0.000153
H	-2.354960	0.000040	0.000004
H	1.485700	1.184129	-0.876414
H	1.486080	1.184420	0.875846
H	1.485662	-1.184184	0.876412
H	1.486037	-1.184463	-0.875847
H	-0.856321	2.159714	0.000150

Vibrational frequencies

116.4844	448.9270	606.3629
655.3756	729.5717	810.2367
817.8343	921.7886	922.6947
958.9741	994.8594	1044.7579
1070.9008	1112.8034	1152.3538
1229.6070	1294.3993	1305.7154
1329.7358	1404.1177	1472.0336
1493.3270	1500.3939	3027.3179
3040.5256	3050.9496	3071.7965
3204.6701	3223.4450	3236.7560

p17
Cartesian coordinates

C	-1.233153	-0.368472	0.000091
C	0.000361	-1.215101	0.000118
C	0.664014	1.030757	-0.000053
C	-0.664629	1.030409	-0.000164
C	1.233393	-0.367809	0.000074
H	-1.875474	-0.549789	-0.875734

H	-1.875169	-0.549397	0.876245
H	0.000641	-2.296665	-0.001081
H	1.286606	1.917548	-0.000007
H	-1.287829	1.916746	-0.000017
H	1.875652	-0.548473	0.876090
H	1.875656	-0.548674	-0.875893

Vibrational frequencies

201.9393	327.6304	391.0987
689.4807	745.8296	796.4700
896.1874	926.6435	936.9874
946.5199	975.4256	987.1284
1042.1797	1134.9736	1137.4872
1140.5454	1295.5132	1306.3693
1338.0042	1398.3661	1461.9748
1468.5418	1709.4988	2978.9350
2982.8655	2993.8054	2994.0427
3197.6219	3222.9117	3228.0010

p18
Cartesian coordinates

C	0.088603	-1.015217	0.000021
C	0.088875	1.015168	-0.000081
C	-1.052873	0.000139	0.000001
C	1.042682	-0.000106	-0.000006
H	0.122075	-2.095670	0.000077
H	0.122436	2.095614	0.000328
H	-1.687021	0.000098	-0.891951
H	-1.687057	0.000208	0.891929
H	2.125845	-0.000151	0.000010

Vibrational frequencies

384.7473	549.7229	561.8496
885.5934	912.5635	914.0652
943.3166	956.6048	1008.3377
1087.5342	1187.6607	1205.1930
1227.8636	1333.8354	1456.1363
1492.2393	3051.5792	3098.3157
3207.8324	3235.0205	3250.2218

p19
Cartesian coordinates

C	-1.948767	-0.011621	0.000016
C	-0.579668	0.036879	-0.000053
C	1.545720	0.117370	0.000015
C	0.499245	-1.042711	-0.000001
C	0.369196	1.058303	-0.000004
H	-2.536902	0.899037	0.000032
H	-2.477355	-0.957416	0.000035
H	2.186574	0.160203	-0.886907
H	2.186554	0.160203	0.886951
H	0.517329	-1.675298	0.890239

H	0.517396	-1.675353	-0.890199
H	0.292046	2.139300	0.000017

Vibrational frequencies

180.6409 344.5974 420.6217
543.7633 662.6934 706.0833
785.2689 806.9079 888.8901
925.4346 958.5936 1015.5109
1029.0692 1092.2054 1188.3009
1222.3171 1224.5413 1271.3644
1351.8202 1400.1488 1465.5954
1492.0125 1518.4284 3039.8848
3071.2582 3080.5811 3127.1420
3154.3355 3204.9573 3252.1036

p1
Cartesian coordinates

C	-1.965185	-0.230220	0.000487
C	0.500513	0.569778	-0.003717
C	1.664539	-0.367476	-0.000378
C	-0.807920	0.150444	-0.000818
H	-2.976699	-0.557405	0.003466
H	0.692655	1.637965	0.011080
H	2.233072	-0.278402	0.933280
H	2.357419	-0.133430	-0.815816
H	1.341869	-1.403881	-0.105450

Vibrational frequencies

94.1383 207.4407 379.1494
473.0995 554.9791 574.7342
659.8551 872.5174 1004.8772
1101.3952 1158.0976 1395.0353
1408.5305 1480.7411 1497.4440
2031.6863 3028.2598 3082.4272
3146.5900 3186.5458 3475.0851

p20
Cartesian coordinates

C	1.948636	-0.000084	-0.000858
C	0.456408	0.000874	0.002477
C	-1.647490	0.002352	-0.002069
C	-0.501945	1.011178	0.001165
C	-0.508137	-1.012922	0.001145
H	2.342764	1.009355	0.131247
H	2.334658	-0.395211	-0.944781
H	2.339562	-0.629508	0.802758
H	-2.279534	0.004403	-0.895992
H	-2.285190	0.004370	0.887827
H	-0.461643	2.092605	0.003761
H	-0.475452	-2.094402	0.004019

Vibrational frequencies

49.1895 233.8297 332.3987
445.8700 527.2514 588.6780
686.1524 903.0499 935.9686
936.7835 972.5330 1034.4681
1056.6398 1092.2452 1186.8927
1199.2164 1246.6273 1279.7546
1409.3172 1473.9747 1490.0255
1494.7117 1605.6121 3045.6800
3050.8779 3090.1901 3117.4581
3138.2269 3229.1864 3236.4949

p21
Cartesian coordinates

C	-1.917813	0.003095	0.000003
C	-0.437679	0.047917	-0.000009
C	1.597149	0.134144	0.000004
C	0.539415	1.042047	-0.000002
C	0.630958	-1.048094	-0.000001
H	-2.342956	1.009385	-0.000076
H	-2.300149	-0.528707	-0.879759
H	-2.300142	-0.528560	0.879856
H	2.674564	0.213484	0.000011
H	0.487484	2.124989	-0.000001
H	0.654515	-1.682623	-0.892336
H	0.654506	-1.682622	0.892335

Vibrational frequencies

114.9632 206.6723 316.6672
401.6225 523.0925 657.3034
881.1378 893.4783 936.0397
946.3417 984.2909 1027.8576
1060.8160 1094.2664 1181.6413
1207.9132 1275.4112 1377.0031
1408.9050 1464.2081 1473.7197
1483.0835 1547.2702 3015.0409
3043.5622 3064.9514 3089.9436
3119.9122 3201.7161 3247.7402

p22
Cartesian coordinates

C	-1.756898	0.000014	-0.303879
C	-0.456651	-0.000001	0.487051
C	1.505948	-0.000003	-0.258588
C	0.614023	1.015132	0.077048
C	0.614000	-1.015147	0.077026
H	-2.356876	-0.884123	-0.068769
H	-2.356892	0.884130	-0.068723
H	-1.553232	0.000045	-1.378283
H	-0.661369	-0.000012	1.564157
H	2.521264	0.000014	-0.636565
H	0.642324	2.096326	0.058105
H	0.642249	-2.096344	0.058128

Vibrational frequencies

220.0295 228.5734 320.3748
485.2480 560.0548 615.7559
803.7980 872.1339 918.4370
923.5117 949.7137 1038.9307
1056.8876 1109.4600 1186.4227
1209.8835 1214.2977 1328.5409
1367.1845 1413.9391 1467.6513
1494.5413 1496.3254 3037.3393
3053.1781 3110.0460 3121.9156
3210.1317 3233.9297 3250.4568

p23
Cartesian coordinates

C	-0.812054	0.666765	-0.000004
C	0.698495	-0.782464	0.000000
C	0.698355	0.782572	0.000001
C	-0.811957	-0.666891	0.000000
H	-1.598534	1.412621	0.000008
H	1.140056	-1.240759	0.889324
H	1.140057	-1.240761	-0.889323
H	1.139871	1.240919	-0.889320
H	1.139864	1.240919	0.889325
H	-1.598356	-1.412832	0.000003

Vibrational frequencies

319.9760 655.4275 868.1155
876.8549 911.0973 911.2540
954.8167 1009.8197 1045.8899
1108.4307 1145.8902 1178.4441
1231.5335 1242.3630 1331.6685
1471.7694 1496.8349 1667.5614
3054.7028 3061.1089 3099.8861
3114.2921 3189.7878 3222.9979

p24
Cartesian coordinates

C	-1.350791	0.884093	0.000031
C	-1.700067	-0.568412	-0.000194
C	0.922919	-0.644015	0.000292
C	2.054495	0.328862	-0.000049
C	-0.389491	-0.279095	0.000210
H	-1.481481	1.465070	-0.914249
H	-1.482143	1.464951	0.914287
H	-2.495179	-1.292362	-0.000384
H	1.158293	-1.704961	-0.000303
H	2.690785	0.194999	-0.882505
H	2.699024	0.186425	0.874960
H	1.688307	1.357274	0.006457

Vibrational frequencies

47.4465 192.1989 197.7188
331.7694 475.6747 526.0740
697.6990 723.2032 927.4766
946.6138 992.4511 1013.7444
1038.3652 1064.9110 1101.5192
1138.6945 1230.8510 1374.7336
1408.3859 1476.5974 1477.8199
1498.6212 1603.2416 3029.2843
3063.3629 3081.2093 3132.5949
3133.7834 3169.3162 3302.7246

p25
Cartesian coordinates

C	1.275556	0.088141	-0.000039
C	-0.000002	-0.367065	0.000141
C	-1.275556	0.088137	-0.000019
H	1.488605	1.158528	0.000047
H	2.125016	-0.586178	-0.000251
H	-1.488592	1.158513	-0.000019
H	-2.125022	-0.586141	-0.000275

Vibrational frequencies

306.0051 451.1905 750.1272
768.4342 768.9432 901.7609
1022.0413 1158.0630 1370.6993
1459.4272 1464.5126 3088.3705
3097.0719 3211.8160 3212.5712

p26
Cartesian coordinates

C	-1.739300	-0.366606	0.000005
C	-0.554257	0.561280	0.000010
C	1.932196	-0.214933	-0.000005
C	0.689771	0.175575	0.000016
H	-2.363256	-0.194496	-0.882028
H	-2.364043	-0.193548	0.881296
H	-1.422673	-1.410454	0.000702
H	-0.755898	1.630618	-0.000086
H	2.467753	-0.381962	0.929147
H	2.467662	-0.382056	-0.929193

Vibrational frequencies

118.1172 209.7121 343.1086
545.3436 576.7370 885.7515
895.6732 897.6275 1028.2666
1057.8732 1097.0247 1160.2803
1369.6025 1406.8708 1476.4313
1484.7119 1508.6952 2091.5245
3046.1259 3109.8452 3138.7261
3145.1929 3158.1722 3227.1204

p27
Cartesian coordinates

C	-0.000001	-0.000041	-0.000003
C	1.300986	0.000005	-0.000005
C	-1.300989	0.000013	-0.000003
H	1.859560	0.640889	-0.673839
H	1.859611	-0.640819	0.673843
H	-1.859639	-0.673842	-0.640791
H	-1.859510	0.673909	0.640851

Vibrational frequencies

374.9389 374.9525 890.4041
890.4386 896.8536 1020.9806
1020.9898 1116.9465 1422.2995
1484.9125 2081.0765 3151.2468
3153.5377 3236.4136 3236.4674

p28
Cartesian coordinates

C	1.920707	-0.579642	-0.000033
C	0.591424	0.052038	0.000133
C	-1.909612	-0.737843	-0.000036
C	-0.137942	1.353066	-0.000030
C	-0.752164	-0.026053	0.000079
H	2.494913	-0.270091	-0.880460
H	1.843789	-1.668394	0.001273
H	2.496148	-0.268017	0.878835
H	-1.892821	-1.821736	0.000031
H	-2.870887	-0.239689	-0.000182
H	-0.172785	1.949174	-0.914520
H	-0.172837	1.949351	0.914343

Vibrational frequencies

52.6714 155.2396 214.1857
389.6725 408.5001 527.0558
693.9449 766.3007 797.1834
944.2279 953.0852 1016.5380
1044.7207 1048.7455 1107.2070
1182.4358 1338.3751 1405.9575
1469.3241 1471.4382 1479.8739
1504.9111 1678.1841 3026.0369
3045.3704 3080.8840 3112.8752
3134.5816 3163.1690 3262.2961

p2
Cartesian coordinates

C	2.629793	0.210949	0.001239
C	1.202162	-0.071064	-0.004475
C	-1.342528	-0.575974	0.001299
C	-2.389278	0.492137	0.000319
C	0.006538	-0.313786	-0.001025

H	3.038424	0.146679	1.014734
H	2.831468	1.215820	-0.378783
H	3.172176	-0.504350	-0.623227
H	-1.664280	-1.612911	0.003185
H	-3.040086	0.406397	0.878537
H	-3.036664	0.408187	-0.880663
H	-1.941157	1.486608	0.002076

Vibrational frequencies

25.0016 67.3385 134.2057
181.6293 309.8925 401.3617
542.3313 587.5461 738.5151
988.0727 1008.7420 1036.7202
1053.8955 1114.5790 1233.6792
1406.2765 1410.8077 1428.9303
1479.1984 1480.4435 1481.4504
1503.4221 2173.6917 3019.8440
3035.2783 3070.3452 3100.9629
3115.1581 3135.6297 3174.4757

p3
Cartesian coordinates

C	-2.451855	-0.228497	0.000004
C	-1.245906	0.393886	0.000003
C	1.245900	0.393887	-0.000007
C	2.451860	-0.228496	0.000007
C	0.000001	-0.271964	-0.000009
H	-2.524284	-1.311379	-0.000016
H	-3.378031	0.332600	0.000008
H	-1.223124	1.482402	0.000019
H	1.223116	1.482402	-0.000018
H	3.378035	0.332603	0.000004
H	2.524291	-1.311378	0.000024
H	0.000001	-1.360147	-0.000011

Vibrational frequencies

153.9843 208.7314 248.8273
462.2849 496.9225 594.1087
633.6012 835.0821 871.8874
882.4372 929.0858 993.9172
1015.9494 1034.1591 1148.4042
1260.0161 1297.2197 1305.6405
1312.8301 1446.0148 1484.6350
1530.9418 1608.2888 3145.5878
3145.9573 3154.1483 3155.9862
3158.9126 3251.3980 3251.5066

p4
Cartesian coordinates

C	2.342305	-0.489943	0.143201
C	1.367202	0.387084	-0.319859
C	-1.173183	0.369340	0.425938

C	-2.272397	-0.412700	-0.250285
C	0.073371	0.377979	0.059918
H	3.361668	-0.417094	-0.212877
H	2.102185	-1.258304	0.867481
H	1.658690	1.144229	-1.045801
H	-1.466649	0.969470	1.289582
H	-3.060540	0.260461	-0.600406
H	-2.729484	-1.115794	0.452309
H	-1.889656	-0.973532	-1.103770

Vibrational frequencies

112.9723	142.9820	194.2992
280.5136	456.1719	542.0041
568.4205	749.5419	761.7857
826.0672	958.1365	1004.3659
1058.4305	1078.6453	1121.6850
1194.8139	1321.4747	1405.8853
1417.5192	1488.3949	1494.4979
1497.4302	1946.3181	3045.1041
3095.9106	3108.9247	3149.3637
3151.3562	3170.7846	3276.1738

p5
Cartesian coordinates

C	-1.968072	-0.000167	0.000566
C	-0.513473	0.002800	-0.002937
C	2.076691	-0.000879	0.000895
C	0.707263	0.000617	-0.000695
H	-2.362716	1.000571	-0.191578
H	-2.353876	-0.336583	0.967874
H	-2.358727	-0.675234	-0.766212
H	2.631470	0.929311	0.001553
H	2.629396	-0.932294	0.001395

Vibrational frequencies

17.3065	186.9843	207.5406
394.9424	423.7264	666.8616
777.9574	1033.8977	1034.5066
1056.5970	1259.9055	1417.8850
1468.5783	1478.9087	1479.9726
2166.3513	3036.8655	3102.9894
3117.4865	3157.1937	3254.3069

p6
Cartesian coordinates

C	1.103712	-1.285163	0.000017
C	0.334096	0.000000	-0.000109
C	-2.262065	0.000000	0.000021
C	1.103714	1.285162	0.000014
C	-1.044143	0.000001	-0.000034
H	1.756654	-1.344560	-0.879825
H	0.444013	-2.152854	-0.000347

H	1.755928	-1.344802	0.880389
H	-3.325086	0.000000	0.000097
H	1.756831	1.344455	-0.879704
H	1.755755	1.344904	0.880510
H	0.444015	2.152853	-0.000573

Vibrational frequencies

43.8497 46.3019 184.2468
259.9227 345.6798 436.6828
454.1709 588.6374 662.9817
734.6881 961.8370 970.8522
1013.4789 1052.5385 1256.5518
1347.3834 1401.7779 1413.2281
1471.1582 1474.2053 1490.0392
1502.5178 2040.7091 3013.8730
3017.6479 3065.2432 3065.2715
3145.8542 3147.1825 3473.9588

p7
Cartesian coordinates

C	0.701639	1.381394	-0.068743
C	0.524125	0.003121	-0.033321
C	-1.978003	0.007897	0.126786
C	1.603676	-0.855108	0.100290
C	-0.827475	-0.596542	-0.150985
H	-0.123370	2.060797	-0.240812
H	1.689345	1.810774	0.049457
H	-2.021397	1.031558	0.484617
H	-2.922646	-0.511628	0.016668
H	1.469977	-1.930334	0.115739
H	2.611576	-0.470341	0.202549
H	-0.847254	-1.635400	-0.472383

Vibrational frequencies

52.0524 305.4528 408.4536
438.3310 520.9583 547.1918
557.6751 737.3508 770.2858
810.2861 828.2382 956.6255
986.1990 1027.3359 1043.9385
1076.6776 1294.4776 1348.4201
1378.3109 1464.9125 1494.7621
1539.4170 1723.8776 3154.9501
3159.6247 3164.9019 3169.6388
3247.7087 3260.4735 3267.1894

p8
Cartesian coordinates

C	-1.268216	-1.180280	-0.000128
C	-0.449536	0.098254	0.004216
C	2.191613	-0.079779	-0.000171
C	-1.096876	1.334829	-0.001267
C	0.896287	0.008269	0.000343

H	-2.028993	-1.146497	0.783271
H	-0.639913	-2.055527	0.165786
H	-1.777090	-1.300505	-0.960151
H	2.759683	-0.124796	-0.927906
H	2.762028	-0.108361	0.926777
H	-2.179148	1.387525	0.006455
H	-0.536201	2.260398	-0.012191

Vibrational frequencies

108.5003 170.3744 184.3320
374.4977 473.8834 495.9449
520.4394 605.4976 714.4258
783.2024 897.5692 964.8258
986.1904 1002.2934 1064.6634
1276.8269 1302.0085 1413.4175
1451.8486 1485.8944 1495.8517
1506.2368 1931.3198 3057.6667
3100.6443 3127.2493 3155.6989
3165.6448 3172.7509 3270.5180

p9
Cartesian coordinates

C	1.251980	-0.000026	-0.000043
C	-1.335917	0.000079	0.000100
C	-0.117028	0.000029	0.000061
H	1.802487	-0.932357	-0.000063
H	1.802572	0.932258	-0.000064
H	-2.399262	-0.000394	-0.000581

Vibrational frequencies

355.7936 404.5840 494.4671
653.2853 674.3839 1036.3006
1088.1528 1459.5704 2025.6777
3166.2038 3267.3059 3471.4444

Fragments

c2h3
Cartesian coordinates

C	0.586147	0.030189	0.000001
C	-0.705696	-0.145205	0.000019
H	1.031493	1.027972	0.000013
H	1.281814	-0.806373	-0.000053
H	-1.596012	0.468493	-0.000083

Vibrational frequencies

714.1762 840.5379 933.8798
1052.8803 1393.8191 1668.5151
3080.5621 3173.9127 3244.1245

c2h4

Cartesian coordinates

C	-0.662222	-0.000001	0.000010
C	0.662223	0.000001	0.000001
H	-1.231151	-0.924081	-0.000015
H	-1.231144	0.924097	-0.000029
H	1.231133	-0.924093	-0.000015
H	1.231156	0.924080	-0.000001

Vibrational frequencies

840.4410 983.4893 992.0774
1072.8263 1241.9404 1388.2063
1471.2187 1715.5325 3140.8644
3160.9323 3222.6122 3249.0323

triplet c2h4
Cartesian coordinates

C	-0.723342	-0.000022	0.000015
C	0.723350	0.000005	0.000001
H	-1.293845	-0.615243	-0.692407
H	-1.293767	0.615342	0.692372
H	1.293750	0.692404	-0.615314
H	1.293816	-0.692397	0.615251

Vibrational frequencies

430.7607 430.9237 729.2745
928.3534 928.3907 1146.2211
1426.9022 1451.5171 3108.0850
3112.0578 3196.7826 3196.9298

c2h5
Cartesian coordinates

C	-0.792813	0.000002	-0.021364
C	0.692585	0.000016	-0.001422
H	-1.347849	-0.927752	0.046402
H	-1.347964	0.927688	0.046394
H	1.086616	-0.001010	1.027311
H	1.105276	0.886831	-0.490836
H	1.105287	-0.885862	-0.492556

Vibrational frequencies

95.3957 460.2571 819.5850
979.9623 1078.0755 1194.6183
1403.1776 1469.4774 1485.9505
1491.7366 2983.3893 3072.2970
3119.3360 3159.0279 3264.8008

triplet ch2
Cartesian coordinates

C	0.000000	0.105329	0.000000

H	0.996152	-0.316086	0.000000
H	-0.996152	-0.315889	0.000000

Vibrational frequencies

1070.0552 3125.6743 3359.5031

ch3
Cartesian coordinates

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

Vibrational frequencies

470.9451 1399.8856 1409.5749
3117.6199 3301.0861 3304.8947

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(2) Kondo, S.; Hirota, E.; Morino, Y. Microwave spectrum and rotational isomerism in butene-1. *J. Mol. Spectrosc*. **1968**, *28* (4), 471–489. https://doi.org/10.1016/0022-2852(68)90180-X.