

Electronic Supporting Information

The Hidden Path to the Resonance-Stabilized Fulvenallenyl Radical (C₇H₅) via the Bimolecular Reaction of Tricarbon (C₃, X¹Σ_g⁺) with 1,3- Butadiene (C₄H₆; X¹A_g)

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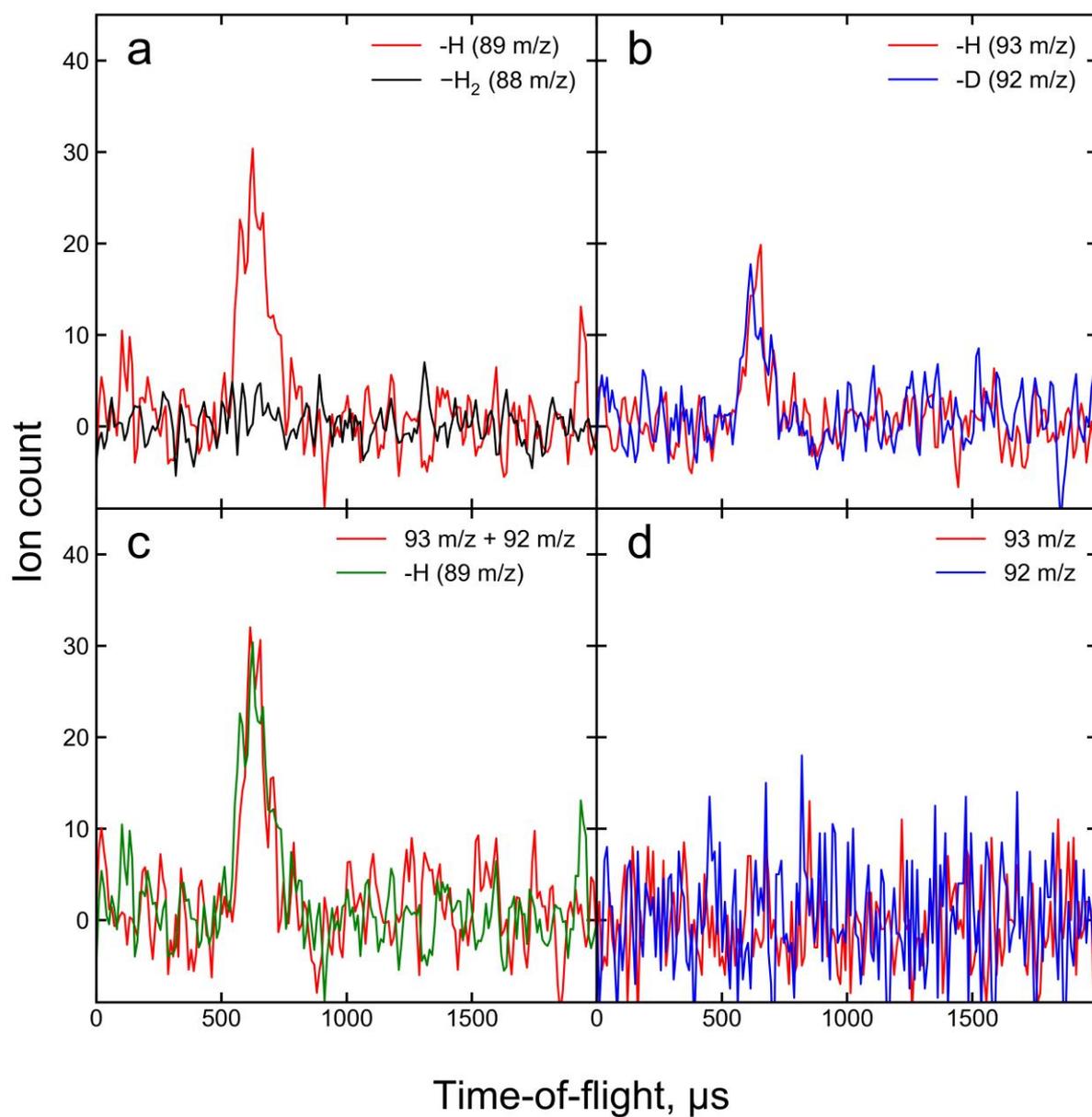


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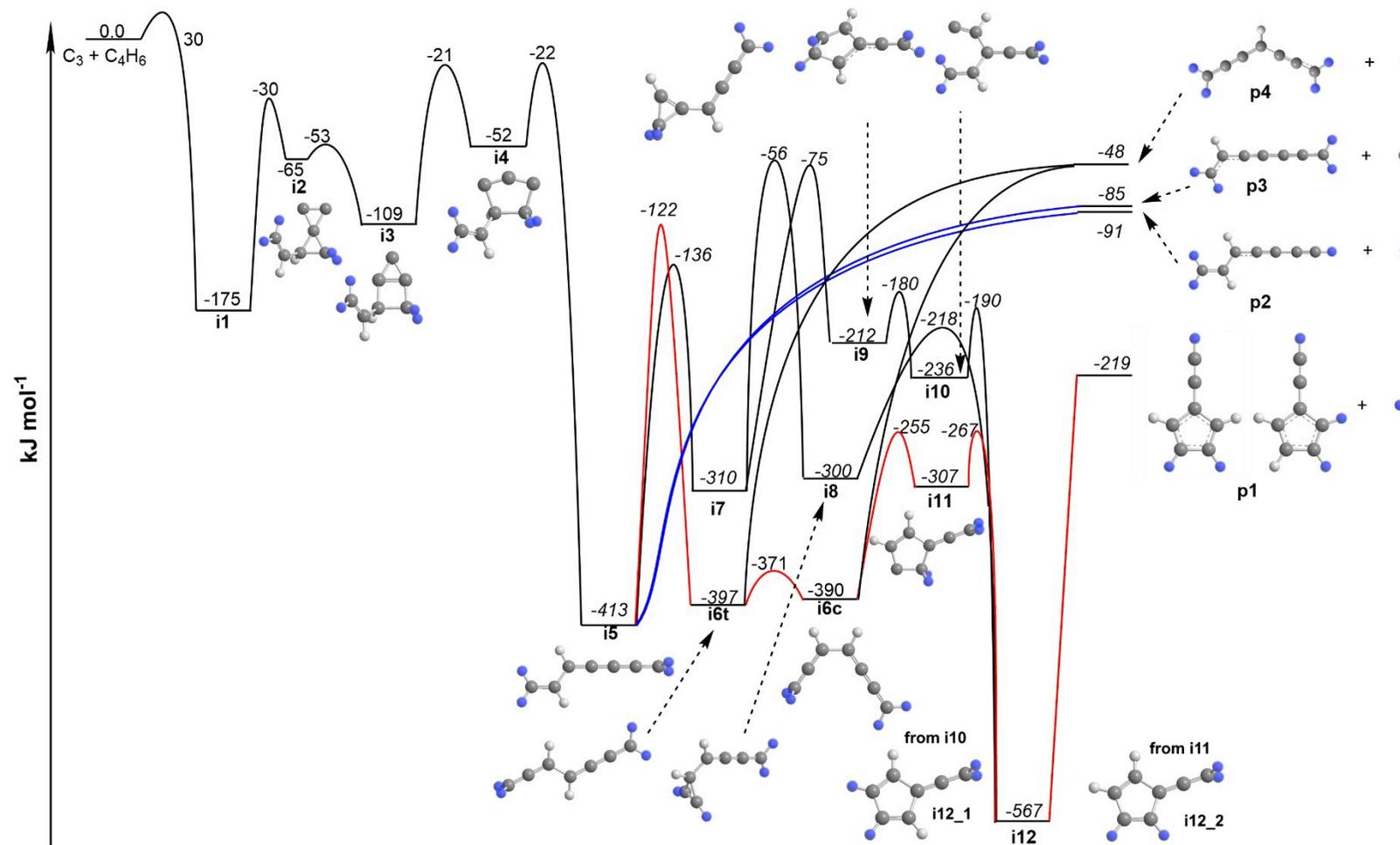


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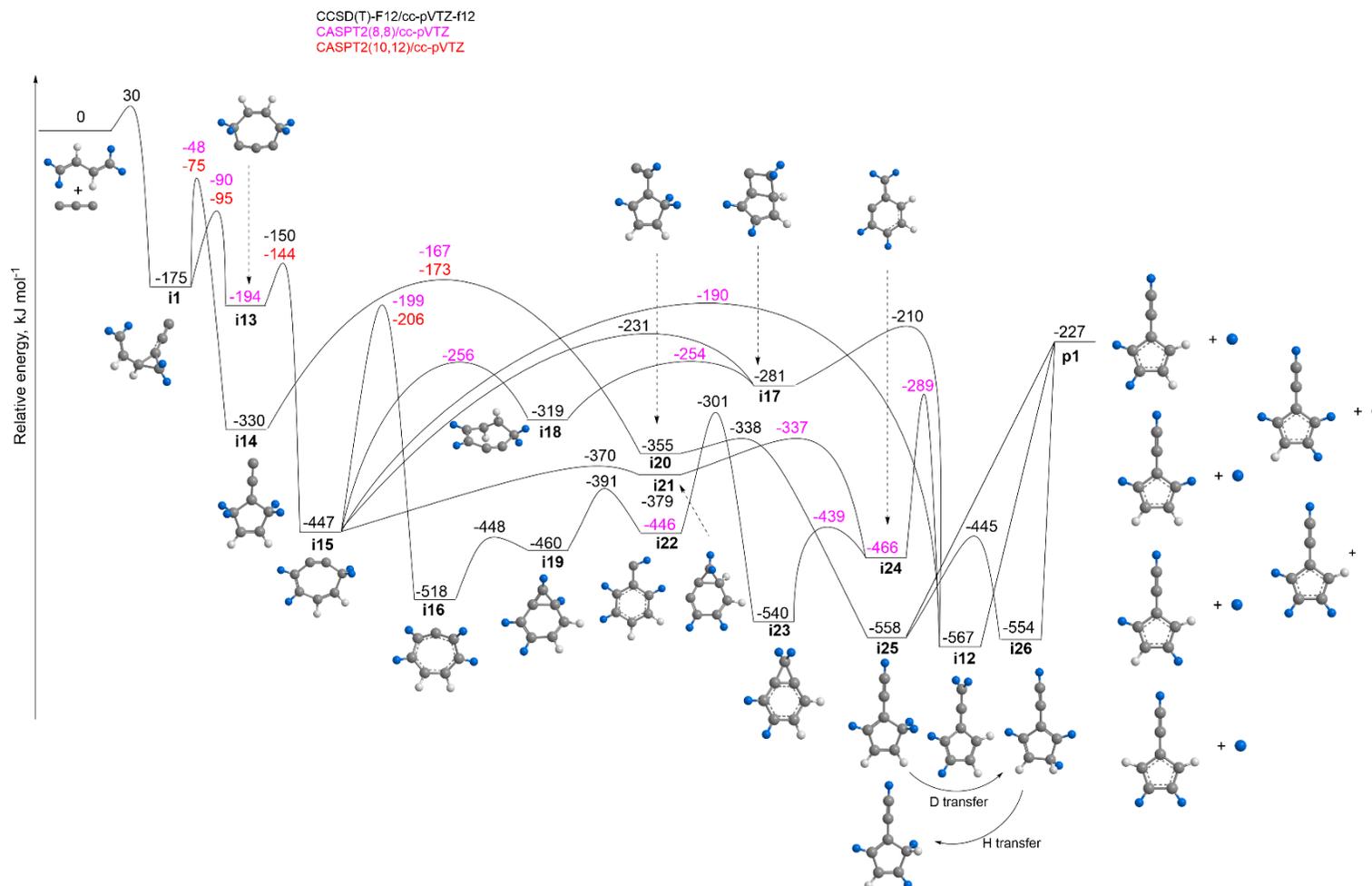


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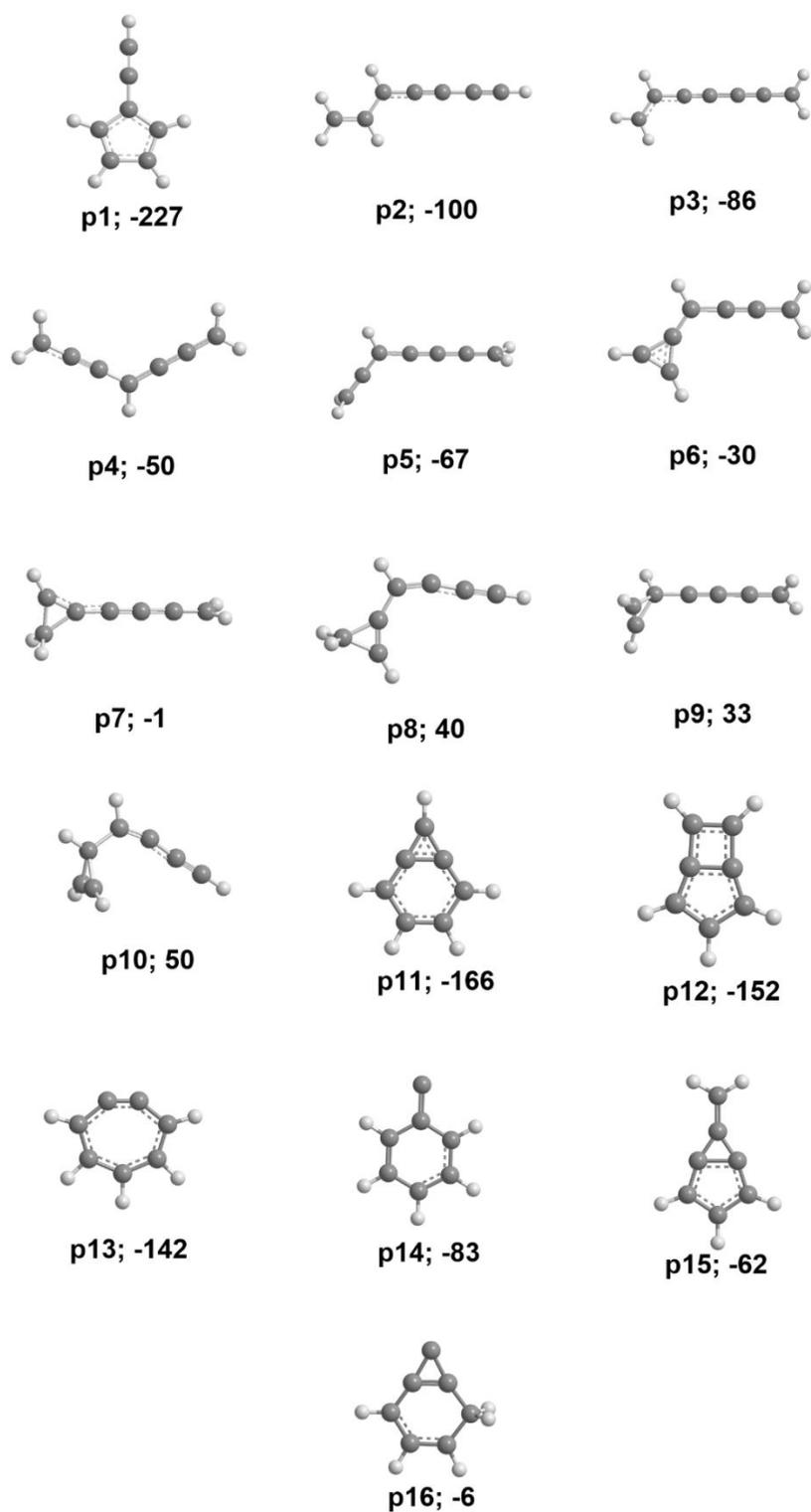


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Table S1. RRKM calculated statistical product branching ratios (%) for the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with 1,3-butadiene (C_4H_6 , X^1A_g) with **i1** as an initial intermediate at different collision energies (E_{col} , kJ mol^{-1}).

Products	Branching ratios, %				
	E_{col} , kJ mol^{-1}				
	0	15	30	44	48
p1+H	98.28	98.05	97.81	97.60	97.54
p2+H	0.00	0.00	0.00	0.00	0.00
p3+H	0.00	0.00	0.00	0.00	0.00
p4+H	0.00	0.00	0.00	0.00	0.00
p11+H	1.10	1.18	1.26	1.32	1.33
p12+H	0.33	0.39	0.44	0.49	0.51
p13+H	0.30	0.38	0.48	0.59	0.62
p14+H	0.00	0.00	0.00	0.00	0.00
p15+H	0.00	0.00	0.00	0.00	0.00
p16+H	0.00	0.00	0.00	0.00	0.00

Table S2. Contributions of selected channels connected to **i13** or **i14** for the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with 1,3-butadiene (C_4H_6 , X^1A_g) with **i1** as an initial intermediate at different collision energies (E_{col} , kJ mol^{-1}).

Channels	Branching ratios, %				
	E_{col} , kJ mol^{-1}				
	0	15	30	44	48
from i1 to fulvenallene (i12) and p1+H	68.13	61.29	55.42	50.65	49.38
from i1 to 1-/2-ethynyl-1,3-cyclopentadiene (i25 , i26) and p1+H	31.87	38.71	44.58	49.35	50.62

Table S3. Contributions of selected channels starting from **i15** for the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with 1,3-butadiene (C_4H_6 , X^1A_g) at different collision energies (E_{col} , kJ mol^{-1}).

Channels from i15	Branching ratios, %				
	E_{col} , kJ mol^{-1}				
	0	15	30	44	48
i15 → i21 → i24 → i12 (i)	97.85	97.06	96.06	94.94	94.58
i15 → i17 → i12 (ii)	0.17	0.22	0.27	0.32	0.33
i15 → i18 → i17 → i12 (iii)	0.20	0.25	0.30	0.36	0.37
i15 → i16 → i19 → i22 → i23 → i24 → i12 (iv)	0.24	0.31	0.39	0.47	0.49
i15 → i12 (v)	1.53	2.17	2.98	3.92	4.22

Table S4. RRKM calculated statistical p1+D/H branching ratios (%) for the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with 1,3-butadiene-1,1,4,4-d₄ ($CD_2CHCHCD_2$; X^1A_g) with i1 as an initial intermediate at different collision energies (E_{col} , kJ mol^{-1}).

Products	Branching ratios, %				
	E_{col} , kJ mol^{-1}				
	0	15	30	44	48
p1+D	86.51	83.25	80.39	78.02	77.38
p1+H	13.49	16.75	19.61	21.98	22.62

Table S5. RRKM calculated rate constants ($k(E)$, s^{-1}) of the reaction of tricarbon (C_3 ; $X^1\Sigma_g^+$) with 1,3-butadiene (C_4H_6 , X^1A_g) for unimolecular reaction steps at different collision energies (E_{col} , $\text{kJ}\cdot\text{mol}^{-1}$).

Step	E_{col}				
	0	15	30	44	48
i1-i2	2.28E+04	1.47E+05	6.23E+05	1.87E+06	2.47E+06
i2-i1	9.85E+09	2.47E+10	4.75E+10	7.56E+10	8.48E+10
i2-i3	3.71E+11	4.59E+11	5.40E+11	6.08E+11	6.27E+11
i3-i2	3.77E+09	8.19E+09	1.52E+10	2.45E+10	2.77E+10
i3-i4	4.09E+06	2.69E+07	1.04E+08	2.76E+08	3.53E+08
i4-i3	1.47E+10	4.58E+10	9.72E+10	1.63E+11	1.85E+11
i4-i5	1.45E+10	4.14E+10	8.44E+10	1.39E+11	1.57E+11
i5-i4	5.80E-05	9.07E-04	7.91E-03	4.28E-02	6.62E-02
i5-i6	6.23E+03	1.53E+04	3.44E+04	6.89E+04	8.32E+04
i6-i5	1.55E+04	3.66E+04	7.99E+04	1.55E+05	1.86E+05
i5-i7	1.06E+05	2.45E+05	5.24E+05	1.00E+06	1.20E+06
i7-i5	5.45E+07	1.07E+08	1.95E+08	3.25E+08	3.73E+08
i5-p2	3.14E+06	7.90E+06	1.82E+07	3.72E+07	4.51E+07
i5-p3	2.45E+05	7.02E+05	1.81E+06	4.05E+06	5.04E+06
i6-i11	1.59E+08	2.07E+08	2.66E+08	3.30E+08	3.50E+08
i11-i6	2.59E+11	2.97E+11	3.37E+11	3.76E+11	3.87E+11
i6-p4	2.88E+03	1.24E+04	4.42E+04	1.28E+05	1.69E+05
i7-i8	1.61E+03	7.16E+03	2.57E+04	7.32E+04	9.66E+04
i8-i7	8.43E+02	3.66E+03	1.29E+04	3.60E+04	4.73E+04
i7-i9	1.16E+03	3.88E+03	1.11E+04	2.65E+04	3.33E+04
i9-i7	1.72E+07	4.50E+07	1.02E+08	2.00E+08	2.38E+08
i8-i12	1.05E+11	1.34E+11	1.68E+11	2.05E+11	2.17E+11
i12-i8	1.57E+07	2.86E+07	5.01E+07	8.19E+07	9.38E+07
i9-i10	1.72E+12	1.97E+12	2.23E+12	2.48E+12	2.55E+12
i10-i9	1.48E+10	1.81E+10	2.16E+10	2.51E+10	2.62E+10
i10-i12	4.34E+10	5.06E+10	5.82E+10	6.56E+10	6.78E+10
i12-i10	5.30E+04	1.04E+05	1.95E+05	3.37E+05	3.92E+05
i11-i12	5.98E+11	6.55E+11	7.12E+11	7.66E+11	7.82E+11
i12-i11	5.94E+06	9.03E+06	1.34E+07	1.90E+07	2.09E+07
i12-p1	5.93E+08	9.82E+08	1.58E+09	2.40E+09	2.69E+09
i1-i21	2.36E+02	1.96E+03	9.93E+03	3.40E+04	4.65E+04
i21-i1	4.31E-02	6.11E-01	5.08E+00	2.67E+01	4.10E+01
i21-i15	7.32E+12	7.44E+12	7.55E+12	7.65E+12	7.68E+12

i15-i21	8.18E+10	9.07E+10	1.00E+11	1.09E+11	1.12E+11
i21-i24	1.30E+12	1.39E+12	1.49E+12	1.58E+12	1.61E+12
i24-i21	5.79E+09	6.88E+09	8.10E+09	9.37E+09	9.75E+09
i24-i23	4.08E+12	4.21E+12	4.34E+12	4.46E+12	4.49E+12
i23-i24	1.60E+12	1.78E+12	1.98E+12	2.17E+12	2.22E+12
i24-i12	1.80E+09	2.38E+09	3.09E+09	3.89E+09	4.14E+09
i12-i24	1.12E+07	1.63E+07	2.31E+07	3.15E+07	3.43E+07
i23-i22	6.27E+08	8.64E+08	1.17E+09	1.53E+09	1.65E+09
i22-i23	8.26E+09	1.03E+10	1.28E+10	1.54E+10	1.62E+10
i22-i19	4.66E+11	4.99E+11	5.33E+11	5.64E+11	5.74E+11
i19-i22	3.34E+11	3.64E+11	3.96E+11	4.26E+11	4.35E+11
i19-i16	7.15E+12	7.26E+12	7.38E+12	7.48E+12	7.51E+12
i16-i19	1.11E+12	1.20E+12	1.28E+12	1.37E+12	1.39E+12
i15-i16	4.39E+06	7.30E+06	1.17E+07	1.77E+07	1.98E+07
i16-i15	5.05E+05	8.99E+05	1.54E+06	2.47E+06	2.81E+06
i15-i12	5.10E+07	9.20E+07	1.59E+08	2.55E+08	2.91E+08
i12-i15	2.54E+05	5.10E+05	9.76E+05	1.72E+06	2.01E+06
i1-i27	1.02E+07	2.21E+07	4.25E+07	7.19E+07	8.26E+07
i27-i1	4.62E+11	7.17E+11	1.03E+12	1.37E+12	1.48E+12
i27-i18	1.24E+08	4.36E+08	1.15E+09	2.42E+09	2.91E+09
i18-i27	3.43E+00	2.61E+01	1.38E+02	5.19E+02	7.34E+02
i15-i18	3.53E+08	4.98E+08	6.87E+08	9.12E+08	9.86E+08
i18-i15	4.34E+11	5.08E+11	5.88E+11	6.68E+11	6.92E+11
i16-i18	1.02E-01	6.64E-01	3.41E+00	1.32E+01	1.90E+01
i18-i16	1.09E+03	5.50E+03	2.21E+04	6.93E+04	9.37E+04
i1-i14	1.43E+08	3.36E+08	6.88E+08	1.23E+09	1.43E+09
i14-i1	3.03E+04	1.12E+05	3.47E+05	8.84E+05	1.13E+06
i14-i20	7.10E+07	1.11E+08	1.67E+08	2.38E+08	2.62E+08
i20-i14	7.59E+06	1.23E+07	1.93E+07	2.84E+07	3.16E+07
i20-i25	2.21E+12	2.28E+12	2.36E+12	2.42E+12	2.44E+12
i25-i20	2.64E+08	3.44E+08	4.43E+08	5.55E+08	5.91E+08
i14-i29	1.59E+06	3.42E+06	6.81E+06	1.22E+07	1.43E+07
i29-i14	9.39E+06	1.98E+07	3.86E+07	6.82E+07	7.95E+07
i29-i25	1.71E+09	2.70E+09	4.10E+09	5.87E+09	6.47E+09
i25-i29	3.71E+03	7.83E+03	1.57E+04	2.87E+04	3.39E+04
i1-i13	3.08E+08	5.38E+08	8.68E+08	1.29E+09	1.43E+09
i13-i1	1.50E+09	2.90E+09	5.14E+09	8.22E+09	9.30E+09
i27-i13	7.98E-04	1.81E+00	2.17E+03	8.86E+04	1.88E+05
i13-i27	8.60E-08	3.02E-04	5.27E-01	2.96E+01	6.87E+01
i15-i13	4.02E+04	8.60E+04	1.73E+05	3.16E+05	3.72E+05
i13-i15	1.92E+11	2.44E+11	3.01E+11	3.60E+11	3.78E+11
i20-i31	1.51E+06	2.84E+06	5.02E+06	8.20E+06	9.37E+06
i31-i20	7.92E+06	1.51E+07	2.71E+07	4.50E+07	5.16E+07
i15-p13	1.19E+07	2.18E+07	3.85E+07	6.29E+07	7.20E+07
i23-p11	1.16E+07	2.02E+07	3.39E+07	5.33E+07	6.03E+07
i22-p14	3.12E+04	7.90E+04	1.83E+05	3.78E+05	4.61E+05

i16-p13	8.77E+05	1.80E+06	3.50E+06	6.26E+06	7.34E+06
i25-p1	1.64E+08	2.48E+08	3.67E+08	5.19E+08	5.72E+08
i31-p12	8.96E+07	1.72E+08	3.11E+08	5.17E+08	5.95E+08
i18-i17	1.22E+11	1.42E+11	1.63E+11	1.84E+11	1.90E+11
i17-i18	4.19E+12	4.37E+12	4.53E+12	4.68E+12	4.72E+12
i12-i17	3.57E+04	6.39E+04	1.10E+05	1.78E+05	2.03E+05
i17-i12	3.02E+11	3.62E+11	4.27E+11	4.93E+11	5.13E+11
i30-i17	1.02E+06	1.77E+06	2.96E+06	4.64E+06	5.24E+06
i17-i30	4.82E+10	6.19E+10	7.78E+10	9.48E+10	1.00E+11
i30-i33	1.65E+08	2.48E+08	3.62E+08	5.05E+08	5.54E+08
i33-i30	1.27E+08	1.92E+08	2.82E+08	3.96E+08	4.35E+08
i31-i30	1.21E+11	1.44E+11	1.69E+11	1.95E+11	2.03E+11
i30-i31	5.57E+08	7.71E+08	1.05E+09	1.38E+09	1.48E+09
i16-i30	2.70E+09	3.43E+09	4.31E+09	5.28E+09	5.58E+09
i30-i16	1.26E+10	1.55E+10	1.88E+10	2.24E+10	2.35E+10
i15-i17	3.08E+07	4.60E+07	6.68E+07	9.28E+07	1.02E+08
i17-i15	7.76E+11	8.90E+11	1.01E+12	1.13E+12	1.16E+12
i30-p12	1.37E+07	2.42E+07	4.12E+07	6.55E+07	7.44E+07
i33-p12	8.37E+06	1.53E+07	2.67E+07	4.36E+07	4.99E+07
i25-i26	1.87E+11	2.09E+11	2.34E+11	2.58E+11	2.65E+11
i26-i25	2.25E+11	2.52E+11	2.80E+11	3.08E+11	3.16E+11
i26-p1	2.43E+08	3.66E+08	5.40E+08	7.60E+08	8.36E+08

Optimized Cartesian coordinates (Å) and vibrational frequencies (cm⁻¹) for all reactants, intermediates, transition states, and products involved in the C₃+C₄H₆ reactions.

Reactants

C₄H₆

Cartesian coordinates

C -1.838912 -0.110778 0.000026
C -0.609780 0.401525 0.000080
C 0.609781 -0.401527 -0.000042
C 1.838912 0.110779 0.000035
H -2.718610 0.521982 0.000114
H -2.003266 -1.184255 -0.000485
H -0.476875 1.481589 -0.000224
H 0.476876 -1.481591 0.000263
H 2.718610 -0.521980 -0.000053
H 2.003265 1.184257 -0.000203

Vibrational frequencies

154.5481 304.2800 524.5559
530.7604 788.9380 902.6179
947.1043 951.2222 1006.3630
1009.6451 1053.4804 1235.2147
1328.4726 1329.7492 1421.3049
1475.6592 1685.3408 1752.8546
3148.8774 3151.4242 3163.1706

3168.1714 3242.8677 3243.1637

C₃

Cartesian coordinates

C	-0.486711	0.188336	0.000000
C	-1.774828	0.188336	-0.000000
C	0.801406	0.188336	0.000000

Vibrational frequencies

91.8051 91.8051 1258.7608
2174.2960

Intermediates

i1

Cartesian coordinates

C	-0.672830	0.696189	0.551547
C	-0.022922	1.624028	-0.491430
C	0.685933	0.467676	0.055873
C	-1.785150	-0.218813	0.170337
C	-1.624368	-1.466238	-0.249458
C	1.754714	-0.293880	0.050763
C	2.780032	-1.056659	0.037116
H	-0.732639	1.115632	1.553982
H	0.296653	2.613371	-0.180436
H	-0.356273	1.542128	-1.521815
H	-2.780646	0.210831	0.249821
H	-2.477530	-2.073998	-0.527078
H	-0.642025	-1.921782	-0.322959

Vibrational frequencies

74.3487 103.0731 167.5953
228.8059 280.8434 382.7533
468.5179 568.0938 655.7278
700.5529 777.5717 873.2456
986.6658 992.1991 1027.8100
1043.9062 1045.8112 1061.3643
1102.0252 1149.8563 1324.8514
1332.6947 1420.2747 1453.4355
1545.8704 1730.6633 2087.9230
3126.2355 3137.6338 3153.5998
3169.6345 3219.5023 3249.1017

i2

Cartesian coordinates

C	-0.361277	0.744718	0.554747
C	0.527233	1.450355	-0.409046
C	-1.693156	0.223433	0.144497
C	-1.930663	-0.990667	-0.331309
C	0.900830	0.066583	0.058850
C	2.136452	-0.646790	-0.370726
C	1.327872	-1.299511	0.471953
H	-0.275616	1.050862	1.595071

H	1.186589	2.241347	-0.069518
H	0.228192	1.494565	-1.451034
H	-2.505820	0.936880	0.261317
H	-2.933703	-1.283145	-0.619126
H	-1.143385	-1.729234	-0.430514

Vibrational frequencies

65.4710 123.2690 159.0080
219.9043 309.5700 389.7502
533.0851 593.1736 669.4866
700.3359 767.4792 835.5551
926.0124 996.8522 997.6819
1027.3911 1047.8304 1069.6912
1099.9573 1141.7855 1260.1961
1333.0611 1381.3144 1453.2169
1457.7329 1601.6362 1733.8904
3137.4260 3145.3616 3154.8520
3168.4519 3236.6629 3256.0357

i3

Cartesian coordinates

C	-0.221970	0.526753	0.568759
C	0.756727	1.288207	-0.352630
C	-1.640403	0.360478	0.132363
C	-2.163750	-0.770283	-0.319759
C	0.686868	-0.700591	0.437923
C	1.624941	0.044623	-0.348747
C	1.884979	-1.302093	-0.028907
H	-0.178030	0.882853	1.602095
H	1.252284	2.176978	0.038544
H	0.379424	1.497501	-1.354576
H	-2.245153	1.262813	0.191141
H	-3.201116	-0.824542	-0.627875
H	-1.571764	-1.678165	-0.383343

Vibrational frequencies

108.2893 127.3351 229.1675
293.5202 325.5228 376.9814
568.2684 648.2856 706.4890
775.6592 886.1563 933.0203
982.2134 1007.8969 1030.8514
1075.0374 1117.8076 1136.7898
1194.6503 1230.6766 1259.5285
1321.8167 1328.9304 1448.8708
1453.4461 1608.9362 1734.4558
3081.3332 3091.1068 3149.6783
3154.9090 3164.2267 3247.7864

i4

Cartesian coordinates

C	-0.123389	0.159884	0.589942
C	1.045226	1.044969	-0.064748

C	-1.495029	0.550317	0.129848
C	-2.393116	-0.258342	-0.412549
C	0.256250	-1.341438	0.351171
C	2.183297	0.080608	-0.501177
C	1.393066	-0.908293	-0.138360
H	-0.057290	0.269738	1.680797
H	1.434838	1.828525	0.591284
H	0.690867	1.527408	-0.981781
H	-1.718396	1.609183	0.257462
H	-3.361865	0.113443	-0.725105
H	-2.185983	-1.314528	-0.547420

Vibrational frequencies

88.6146 139.4588 248.1811
318.9766 343.4191 522.2578
554.5954 590.9164 661.8368
716.2475 887.3671 910.3235
932.3317 984.5319 1011.4519
1029.3318 1077.5086 1136.4855
1175.7853 1209.2035 1241.6943
1274.1131 1327.5296 1417.1103
1445.2537 1565.6111 1736.6864
3036.7681 3057.5118 3116.9953
3138.4617 3160.1128 3251.7173

i5

Cartesian coordinates

C	3.588983	-0.233680	-0.000037
C	2.276453	-0.464812	0.000002
C	1.275260	0.595434	0.000029
C	-0.022917	0.380336	0.000051
C	-1.275574	0.166982	0.000143
C	-2.533436	-0.044029	-0.000238
C	-3.821190	-0.260753	0.000024
H	4.304258	-1.047069	-0.000006
H	3.986095	0.776707	-0.000070
H	1.901539	-1.484102	0.000092
H	1.630252	1.624526	-0.000179
H	-4.373593	-0.353384	0.929801
H	-4.374024	-0.353549	-0.929484

Vibrational frequencies

81.5648 89.3821 178.4480
214.1884 329.5156 381.5241
447.1701 494.2974 522.9587
556.7554 684.1524 805.9386
871.4790 883.7470 953.4235
964.7630 1013.1613 1039.1272
1181.3892 1253.9817 1324.2024
1391.8310 1454.1955 1534.8314
1709.9792 1980.1148 2272.9615
3138.6597 3146.9800 3153.1173

3181.1601 3222.7632 3248.5327

i6

Cartesian coordinates

C	-2.242873	1.535126	-0.000007
C	-1.897200	0.284242	0.000107
C	-1.535323	-0.975287	-0.000116
C	-0.148365	-1.450380	-0.000020
C	0.922613	-0.681123	0.000073
C	1.939070	0.068633	0.000147
C	2.996893	0.844817	-0.000089
H	-2.390305	2.076325	-0.929733
H	-2.390433	2.076452	0.929625
H	-2.312979	-1.733740	-0.000171
H	-0.010753	-2.528459	0.000016
H	2.896984	1.924966	-0.000206
H	3.998594	0.428286	-0.000103

Vibrational frequencies

70.0306 81.8348 187.7421
217.2170 317.1671 328.8266
459.9688 468.3643 563.2329
647.8646 722.8303 835.4317
878.9827 888.1341 892.6870
919.7851 1009.7689 1024.9429
1032.5584 1169.5227 1329.3986
1373.7737 1452.8393 1479.7812
1711.7058 2063.2768 2235.4374
3135.7422 3145.5109 3160.8778
3175.9294 3217.3099 3231.5419

i7

Cartesian coordinates

C	-1.927079	1.080236	0.000049
C	-2.889925	-0.078945	0.000415
C	-1.384200	-0.096091	-0.000630
C	-0.224151	-0.946386	-0.000222
C	1.013023	-0.483054	-0.000115
C	2.192840	-0.033008	0.000090
C	3.418750	0.433700	0.000172
H	-1.827943	2.150996	-0.000598
H	-3.431343	-0.328217	-0.913654
H	-3.430119	-0.328110	0.915248
H	-0.389874	-2.019880	0.000128
H	4.273074	-0.234936	0.000584
H	3.610666	1.501437	-0.000265

Vibrational frequencies

60.5088 86.0189 223.4069
259.2366 290.4852 350.1725
477.6420 520.3765 594.6905
764.0837 798.6694 887.1952

903.5770 908.9957 993.6425
1018.9703 1034.5505 1053.5985
1092.1841 1102.7267 1164.3488
1336.0357 1451.7382 1523.1625
1702.1098 1845.2980 2233.9481
3050.8307 3120.1255 3146.1145
3171.8604 3232.9235 3303.4868

i8

Cartesian coordinates

C	-1.849501	0.852228	0.642455
C	-1.849320	0.852303	-0.642430
C	-1.710675	-0.508136	-0.000039
C	-0.400732	-1.219998	-0.000001
C	0.776312	-0.631544	0.000003
C	1.897367	-0.044559	-0.000015
C	3.064701	0.553503	0.000028
H	-1.845344	1.371982	1.584335
H	-1.845097	1.372028	-1.584306
H	-2.570001	-1.177614	-0.000156
H	-0.435752	-2.307785	0.000058
H	3.987441	-0.017202	0.000102
H	3.139836	1.635810	-0.000038

Vibrational frequencies

36.9626 89.9114 207.5577
258.9284 322.4963 374.1032
534.4719 600.2735 611.8125
712.9204 810.8163 814.9917
871.4911 881.1370 898.7552
945.2827 1021.4421 1032.0304
1034.6417 1062.8792 1175.5079
1315.2491 1382.8892 1453.5540
1717.9619 1753.6129 2236.2103
3105.9377 3143.4018 3151.5823
3228.1115 3275.3986 3325.9207

i9

Cartesian coordinates

C	-0.772887	-0.770530	-0.463319
C	-1.927648	-0.795116	0.372625
C	-1.837429	0.705634	-0.049540
C	-0.576064	1.244384	0.017813
C	0.353616	0.133561	-0.057950
C	1.639874	-0.048748	0.029816
C	2.927464	-0.218064	0.110216
H	-0.857754	-1.031892	-1.512346
H	-1.799160	-0.885089	1.448311
H	-2.799366	-1.314713	-0.008621
H	-0.355573	2.307912	0.024252
H	3.567495	-0.098196	-0.759112
H	3.402807	-0.484740	1.049549

Vibrational frequencies

112.4929 160.1906 296.8106
391.7301 427.0895 462.3284
540.8214 592.3807 637.1987
714.3175 817.6572 851.5436
905.2053 933.8451 1009.1418
1020.5562 1075.4634 1129.9828
1172.2754 1223.7911 1244.2404
1327.2856 1407.5080 1496.2923
1512.0041 1518.6254 2096.3074
3128.0974 3131.8972 3171.6160
3197.0670 3212.3304 3218.0735

i10**Cartesian coordinates**

C	0.630521	-1.205577	0.000030
C	1.958161	-1.215086	-0.000040
C	1.716469	1.720948	0.000034
C	0.479558	1.321183	-0.000004
C	-0.192617	0.014006	0.000003
C	-1.506616	-0.054437	0.000072
C	-2.801625	-0.135214	-0.000039
H	0.075151	-2.137891	0.000100
H	2.549013	-0.297844	-0.000085
H	2.515762	-2.143577	-0.000072
H	-0.119067	2.244237	-0.000124
H	-3.362041	-0.169991	0.929600
H	-3.361924	-0.169875	-0.929753

Vibrational frequencies

126.8689 145.3487 157.2312
186.1421 288.6447 358.0736
447.5762 513.3401 558.7142
584.7398 684.0145 729.4206
745.9431 912.4609 930.6727
944.5149 1006.3099 1012.8128
1047.3841 1255.9829 1263.7338
1332.6834 1454.3575 1482.7219
1721.7518 1781.6770 2070.3943
3068.1982 3098.7489 3134.1888
3189.3377 3216.1932 3234.4043

i11**Cartesian coordinates**

C	-0.644449	1.221770	0.000045
C	-2.053320	0.709778	-0.000116
C	-1.915153	-0.723753	0.000002
C	-0.613274	-1.135076	0.000008
C	0.274663	0.007275	0.000048
C	1.584959	-0.033607	0.000044
C	2.883288	-0.052762	-0.000048

H	-0.485792	1.864446	-0.873369
H	-0.486073	1.864277	0.873640
H	-2.757369	-1.406491	0.000011
H	-0.257055	-2.160287	-0.000016
H	3.443060	-0.061939	0.929952
H	3.442951	-0.061761	-0.930115

Vibrational frequencies

62.9193 157.2647 195.3169
337.9330 447.4049 541.1281
567.4402 606.3439 768.5902
802.0929 867.1889 874.7791
888.9201 949.1260 1002.1113
1018.4902 1087.2316 1127.4049
1143.0565 1200.7915 1231.2332
1297.7095 1398.2350 1402.6833
1473.7972 1532.1380 2064.1391
3056.4128 3093.6798 3140.6525
3191.4609 3211.5655 3223.9667

i12

Cartesian coordinates

C	0.595948	1.178718	0.000134
C	1.867722	0.732950	-0.000043
C	1.867779	-0.732955	-0.000099
C	0.596084	-1.178754	0.000129
C	-0.284411	0.000079	0.000112
C	-1.598249	-0.000070	0.000074
C	-2.895123	0.000012	-0.000124
H	0.246976	2.200463	-0.000002
H	2.757347	1.348175	-0.000401
H	2.757505	-1.348024	-0.000280
H	0.246778	-2.200382	0.000040
H	-3.453715	-0.000077	0.930491
H	-3.453396	-0.000042	-0.930941

Vibrational frequencies

132.9156 154.4220 372.5398
492.9374 564.3579 569.0156
631.7739 653.5685 747.3159
786.2341 826.2030 887.3958
907.4456 947.9196 959.5097
999.3331 1011.1699 1095.6049
1107.8588 1201.4962 1295.4804
1325.7101 1402.6978 1482.8892
1558.1926 1641.2221 2067.7097
3142.2132 3222.5622 3225.8492
3234.1836 3257.5085 3262.0318

i13

Cartesian coordinates

C	0.669443	1.277146	-0.060400
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C	1.708461	0.178458	0.106452
C	1.269174	-1.238456	-0.130765
C	-0.669431	1.277152	-0.060398
C	-1.708456	0.178470	0.106454
C	-0.000006	-1.383906	0.029450
C	-1.269188	-1.238451	-0.130768
H	1.128353	2.250468	-0.224940
H	2.077306	0.185063	1.143237
H	2.589274	0.413205	-0.498376
H	-1.128340	2.250475	-0.224939
H	-2.077304	0.185079	1.143238
H	-2.589267	0.413226	-0.498376

Vibrational frequencies

95.6358 201.8216 205.9772
304.2458 407.4394 467.3543
629.6950 731.0395 795.5884
795.6326 864.0672 874.6880
929.5409 930.5620 1028.0376
1070.4679 1150.8403 1196.7826
1286.2742 1352.5440 1369.5806
1383.9729 1427.7389 1434.5752
1439.4977 1698.7961 1727.4570
3023.4350 3025.0788 3080.1596
3080.3231 3132.0199 3157.1227

i14

Cartesian coordinates

C	1.791121	0.663997	0.000166
C	0.395127	1.227704	-0.000152
C	-3.085050	0.000000	0.000274
C	1.791122	-0.663997	0.000167
C	0.395127	-1.227704	-0.000152
C	-1.812801	0.000000	-0.000072
C	-0.481091	0.000000	-0.000141
H	2.673500	1.290908	0.000339
H	0.173087	1.848853	-0.875586
H	0.172751	1.849159	0.874974
H	2.673500	-1.290907	0.000340
H	0.173088	-1.848852	-0.875588
H	0.172750	-1.849161	0.874973

Vibrational frequencies

58.5220 150.9822 182.0958
360.6215 472.0069 519.0872
546.5465 702.5649 800.6299
809.3411 822.7146 963.2237
987.3306 988.3841 996.1833
1123.3472 1142.7074 1162.2224
1198.8057 1257.2722 1303.9643
1368.8547 1424.1726 1428.7151
1436.9881 1712.6540 2079.1038

3047.9568 3050.8783 3080.6357
3080.7886 3211.1654 3234.7320

i15

Cartesian coordinates

C	-1.164691	0.973290	-0.000023
C	-1.793488	-0.418287	0.000036
C	-0.640711	-1.320155	-0.000022
C	0.118950	1.390977	-0.000010
C	1.448213	0.742160	0.000028
C	0.561788	-1.399803	-0.000030
C	1.727846	-0.575044	0.000002
H	-1.906494	1.770717	-0.000070
H	-2.436875	-0.544559	-0.877968
H	-2.436749	-0.544541	0.878137
H	0.209432	2.474704	-0.000051
H	2.281599	1.438985	0.000067
H	2.741651	-0.954143	0.000008

Vibrational frequencies

115.5574 286.0492 381.8016
382.6956 429.1791 552.1391
632.6445 689.2890 812.0315
819.2611 846.0834 928.8118
961.6207 980.9806 997.1379
1027.7812 1177.5607 1215.2145
1218.2869 1296.5073 1362.5690
1410.4161 1456.4060 1486.7379
1633.1313 1692.0561 2310.3484
3040.1093 3066.4587 3143.2908
3166.9719 3185.8008 3226.0982

i16

Cartesian coordinates

C	-0.695547	1.280585	-0.211027
C	-1.596181	0.266206	-0.185675
C	-1.216131	-1.035828	0.354504
C	0.695535	1.280592	0.211022
C	1.596175	0.266220	0.185682
C	0.000008	-1.401672	-0.000001
C	1.216144	-1.035818	-0.354506
H	-1.067909	2.252571	-0.525583
H	-2.618238	0.459259	-0.503082
H	-1.842618	-1.572710	1.058605
H	1.067885	2.252583	0.525578
H	2.618228	0.459278	0.503100
H	1.842633	-1.572686	-1.058615

Vibrational frequencies

298.0630 308.9250 373.2856
428.9443 497.3122 612.3624
692.5612 702.5909 807.0001

827.8891 848.6446 897.3964
937.7255 984.3456 1003.2286
1048.9903 1049.0525 1124.7240
1227.1852 1247.4339 1304.2145
1407.6196 1413.5415 1463.2779
1605.1425 1655.4638 1947.6252
3153.6123 3160.7944 3174.7232
3183.8911 3192.3780 3192.6688

i17

Cartesian coordinates

C	-1.128876	-1.036779	0.043161
C	-1.671313	0.188353	0.280302
C	-0.727549	1.214240	-0.073241
C	0.240151	-0.892840	-0.474296
C	1.474723	-0.561137	0.483126
C	0.391924	0.618196	-0.618539
C	1.578131	0.927788	0.111494
H	-1.664449	-1.976162	0.110927
H	-2.656839	0.373559	0.687573
H	-0.773485	2.254703	0.220234
H	0.519227	-1.572714	-1.276627
H	1.271758	-0.693297	1.548267
H	2.360642	-1.133013	0.197578

Vibrational frequencies

203.3713 249.5821 390.2887
559.6560 667.3156 721.3275
745.0139 787.8896 843.6871
859.6964 885.4387 900.7815
955.8047 980.3762 985.9591
1045.0207 1093.6709 1115.6267
1132.8111 1175.8489 1235.6197
1264.5160 1321.0187 1394.6863
1423.6641 1478.0264 1587.9875
3070.6912 3142.0552 3157.5721
3213.6915 3233.6965 3245.9148

i18

Cartesian coordinates

C	0.244648	-1.255529	-0.332967
C	1.559413	-0.657607	0.023537
C	1.566535	0.703521	0.081419
C	-0.793405	-0.948301	0.458240
C	-1.878757	-0.001604	-0.056758
C	0.287936	1.376978	-0.040680
C	-0.901273	1.139658	-0.135284
H	0.065324	-1.297989	-1.409770
H	2.499411	-1.195476	0.094919
H	2.499813	1.240401	0.202412
H	-0.592353	-0.803751	1.518375
H	-2.288301	-0.247645	-1.038023

H -2.694483 0.161775 0.647042

Vibrational frequencies

235.9034 296.4165 336.2411
422.6467 449.3726 528.9336
581.7555 671.5184 741.3015
790.9188 844.6189 908.9569
974.1815 1002.0295 1039.0381
1065.4569 1090.4490 1144.8531
1188.5061 1241.8354 1311.1599
1362.9860 1373.5686 1482.0795
1539.3783 1652.4976 2213.4961
3097.0285 3105.6220 3145.3576
3159.8408 3190.4277 3221.2380

i19

Cartesian coordinates

C 1.217435 0.922547 0.240214
C 1.538637 -0.481961 0.053813
C 0.590171 -1.416891 -0.185024
C 0.004254 1.454476 -0.046565
C -1.099276 0.575721 -0.466187
C -0.735206 -0.884381 -0.134528
C -1.739049 -0.384100 0.506004
H 2.030346 1.583404 0.522369
H 2.581812 -0.775027 0.103075
H 0.812618 -2.459944 -0.370060
H -0.112871 2.534910 -0.072147
H -1.628030 0.833605 -1.384132
H -2.345661 -0.429413 1.394530

Vibrational frequencies

234.9539 326.3932 392.0902
551.5607 575.1434 619.5952
650.7342 718.8529 780.6737
804.5762 914.0772 949.2870
960.4963 980.1627 1004.4032
1014.6807 1023.9805 1051.6969
1144.6508 1181.2466 1214.7529
1347.1916 1401.0025 1454.1731
1574.2458 1666.1475 1862.3189
3099.6920 3167.8851 3190.2892
3204.1701 3222.3661 3280.4558

i20

Cartesian coordinates

C -1.616265 0.843739 -0.016060
C -0.199145 1.093152 0.222572
C 1.940173 -0.262152 0.344169
C -1.813679 -0.477632 -0.154606
C -0.505394 -1.197978 -0.044182
C 2.254164 0.391590 -0.734971

C	0.468343	-0.085007	0.245326
H	-2.376669	1.611910	-0.055454
H	2.462558	-0.870824	1.067892
H	0.255981	2.063068	0.367516
H	-2.763803	-0.973630	-0.300217
H	-0.514453	-1.972915	0.731064
H	-0.232797	-1.691887	-0.984283

Vibrational frequencies

115.6706 151.6638 255.4524
346.0889 399.9322 541.6582
633.3431 704.3603 735.2291
830.0638 897.9301 910.1399
939.8375 976.2956 988.1819
1022.8382 1037.3932 1141.1706
1142.3655 1197.1120 1271.3387
1328.4369 1405.2442 1426.6033
1569.3197 1654.4479 1707.1161
3059.6041 3098.3691 3227.2721
3241.7648 3252.1822 3254.4246

i21

Cartesian coordinates

C	-0.941915	0.671727	-0.457443
C	-1.796868	-0.215884	0.519417
C	-0.802562	-0.851107	-0.297850
C	0.295645	1.326371	-0.044282
C	1.437050	0.655047	0.280052
C	0.377862	-1.358856	-0.152392
C	1.569417	-0.763251	-0.000998
H	-1.547457	1.178035	-1.204240
H	-2.836245	-0.250667	0.208818
H	-1.633314	-0.127194	1.590343
H	0.335750	2.409332	-0.107099
H	2.308624	1.218625	0.599170
H	2.540860	-1.212410	-0.166012

Vibrational frequencies

237.0229 318.2253 450.3814
519.6775 539.1701 582.8438
618.7026 768.8387 820.3857
841.3509 872.9066 926.4092
961.5185 983.8888 1011.5717
1045.9014 1079.0220 1089.0595
1111.6682 1196.0693 1280.9118
1335.8304 1421.2486 1452.8777
1507.1974 1588.2378 1900.3975
3116.2124 3159.9239 3176.9507
3196.9951 3206.9665 3207.9800

i22

Cartesian coordinates

C	0.360353	1.185331	0.000037
C	2.467450	-0.172156	-0.000005
C	1.038249	-0.053972	0.000051
C	-1.022365	1.239954	0.000026
C	-1.758820	0.056983	-0.000044
C	0.264906	-1.233576	0.000057
C	-1.118375	-1.179248	-0.000043
H	0.942231	2.101343	0.000043
H	2.956663	0.816255	-0.000502
H	0.790134	-2.181757	0.000123
H	-1.533047	2.195978	0.000043
H	-2.842623	0.100915	-0.000090
H	-1.701748	-2.092629	-0.000089

Vibrational frequencies

191.1503 211.8030 388.0682
 458.7947 469.3844 544.6962
 631.8819 699.0204 780.5653
 845.1288 869.1084 949.6882
 969.9936 1012.7285 1024.1329
 1032.3716 1055.3033 1109.6837
 1188.8515 1203.2753 1291.2307
 1325.7403 1348.8427 1478.9125
 1520.6023 1629.3563 1657.3006
 3014.0469 3190.0493 3195.6438
 3207.7637 3219.4490 3225.2981

i23

Cartesian coordinates

C	0.333811	-1.448417	-0.000006
C	-2.142287	-0.000009	0.000013
C	-0.799102	-0.671876	-0.000020
C	1.522261	-0.698602	0.000009
C	1.522231	0.698646	0.000008
C	-0.799131	0.671833	-0.000011
C	0.333749	1.448412	-0.000009
H	0.347913	-2.532159	-0.000023
H	-2.737275	-0.000001	-0.912376
H	-2.737230	-0.000033	0.912461
H	2.474809	-1.217454	0.000023
H	2.474747	1.217555	0.000017
H	0.347833	2.532166	-0.000013

Vibrational frequencies

190.7624 349.5337 444.6497
 456.0731 587.9690 686.6329
 717.3168 750.2552 885.2926
 901.1642 939.1451 1004.1451
 1018.0582 1020.6308 1021.1422
 1033.1940 1102.7279 1136.9173
 1143.3909 1187.5547 1302.2800
 1394.7131 1469.6922 1501.9129

1502.5040 1649.1385 1772.6189
3078.0524 3154.8084 3191.1634
3202.3701 3211.6682 3219.8702

i24

Cartesian coordinates

C	-0.311496	1.154593	-0.000223
C	-2.427580	-0.143011	0.000564
C	-1.020894	-0.077741	-0.000544
C	1.073794	1.190122	0.000031
C	1.821476	0.016381	0.000325
C	-0.194143	-1.210438	-0.000666
C	1.163155	-1.228722	0.000206
H	-0.880722	2.079214	0.000469
H	-3.019373	0.763900	0.000332
H	-2.937850	-1.096534	0.000432
H	1.581253	2.147993	-0.000322
H	2.905021	0.054246	0.000068
H	1.725801	-2.155920	0.000863

Vibrational frequencies

198.3891 343.9673 353.0349
461.9443 505.6846 525.3584
628.7497 668.8477 697.7941
745.8881 840.7040 844.4288
933.5086 963.6453 983.7321
985.7434 1043.7160 1134.5494
1178.1260 1261.0533 1270.8158
1328.9717 1452.3905 1462.0134
1489.1206 1562.9725 1624.6653
3170.5552 3182.4919 3191.6089
3205.2966 3220.7759 3281.7791

i25

Cartesian coordinates

C	-1.848329	0.729686	-0.000077
C	-0.452797	1.158315	0.000065
C	1.765720	0.041770	0.000078
C	-1.901878	-0.611983	-0.000093
C	-0.511587	-1.166399	0.000053
C	2.966882	-0.011987	-0.000030
C	0.348446	0.071180	0.000136
H	-2.694396	1.404182	-0.000161
H	-0.114481	2.185871	0.000052
H	-2.794103	-1.222891	-0.000165
H	-0.312655	-1.789911	0.879622
H	-0.312446	-1.789933	-0.879447
H	4.029328	-0.050818	-0.000698

Vibrational frequencies

153.2970 161.0212 327.3155
481.0484 528.0433 538.2210

557.8712 646.1791 701.7100
708.3750 828.9620 900.8750
909.9603 919.7028 973.8423
981.1054 1021.5838 1123.2722
1138.6823 1186.9766 1257.7797
1327.8635 1389.4681 1410.7187
1590.9160 1672.1033 2236.7034
3055.9679 3093.8155 3221.2168
3236.3787 3248.5957 3483.9403

i26

Cartesian coordinates

C	1.766086	0.808239	0.000000
C	0.477095	1.169329	0.000000
C	-1.787762	-0.028320	0.000000
C	1.865775	-0.688326	0.000000
C	0.435579	-1.128197	-0.000001
C	-2.988235	0.009926	0.000000
C	-0.363303	-0.042279	-0.000001
H	2.620156	1.471289	0.000001
H	0.079375	2.175251	0.000000
H	2.405952	-1.063836	0.878350
H	2.405953	-1.063836	-0.878348
H	0.108293	-2.158261	0.000000
H	-4.051139	0.037166	0.000002

Vibrational frequencies

154.6548 163.1152 341.3546
430.8312 531.9398 555.7492
625.9737 663.7011 700.5160
724.6858 784.3464 827.4270
920.9302 932.1233 948.8889
970.0631 1003.0778 1101.2647
1131.9963 1213.2847 1249.6880
1309.3445 1385.0987 1420.3712
1605.4156 1680.9985 2246.1060
3047.7195 3080.7454 3229.6295
3246.7534 3253.8287 3483.6806

i27

Cartesian coordinates

C	-0.545027	-1.107498	0.392718
C	-1.757346	-0.334816	-0.073610
C	-1.280656	1.131789	-0.022966
C	0.545066	-1.107561	-0.392623
C	1.757363	-0.334767	0.073578
C	-0.000027	1.297588	0.000328
C	1.280631	1.131824	0.022542
H	-0.392326	-1.058913	1.471954
H	-2.671367	-0.463947	0.506745
H	-2.008484	-0.506740	-1.127450
H	0.392383	-1.059228	-1.471872

H	2.008360	-0.506439	1.127501
H	2.671412	-0.464085	-0.506674

Vibrational frequencies

223.8777	294.8249	323.9687
340.3029	388.1524	493.3728
506.2927	655.3970	767.4183
803.2228	825.2276	860.3333
892.0209	1000.3933	1041.2271
1072.0553	1113.6287	1183.5995
1234.8006	1249.2348	1341.4081
1342.0512	1363.1000	1434.1317
1444.0328	1638.6517	1692.2325
3060.9962	3062.5045	3120.5921
3125.2282	3141.9080	3142.3212

i28

Cartesian coordinates

C	1.438617	-0.667606	-0.000112
C	0.200537	-1.552480	0.000136
C	-2.245433	0.000002	-0.000219
C	1.438620	0.667603	-0.000112
C	0.200540	1.552479	0.000136
C	-0.978738	-0.662108	0.000023
C	-0.978736	0.662109	0.000024
H	2.394603	-1.182862	-0.000301
H	0.189619	-2.214249	0.872919
H	0.189551	-2.214764	-0.872242
H	2.394607	1.182858	-0.000302
H	0.189622	2.214249	0.872919
H	0.189555	2.214763	-0.872242

Vibrational frequencies

95.6198	263.6305	393.2381
444.7038	446.1507	510.3816
664.1305	664.1938	826.9562
878.6298	927.2249	942.1215
961.2888	1002.7810	1027.4730
1206.7739	1214.4348	1227.6261
1240.4871	1274.4854	1361.8831
1413.2177	1432.0214	1444.8895
1445.4226	1722.3580	1814.5636
3053.7246	3054.9289	3085.9243
3087.0904	3177.2668	3199.5361

i29

Cartesian coordinates

C	-0.500352	1.289075	0.179377
C	0.575878	0.418443	0.706924
C	2.083463	0.335156	-0.667065
C	-1.496325	0.567006	-0.329642
C	-1.271416	-0.916619	-0.182368

C	1.259586	-0.586632	-0.380438
C	0.127209	-1.008551	0.427893
H	-0.426413	2.367611	0.179980
H	1.149128	0.653586	1.592988
H	-2.365830	0.973851	-0.830600
H	-2.005191	-1.362634	0.496458
H	-1.345575	-1.444674	-1.135993
H	0.325618	-1.775004	1.169078

Vibrational frequencies

179.2357 194.5234 284.4572
437.2994 496.3253 668.0980
732.4084 760.1721 800.1233
844.4551 910.5404 955.3470
962.0724 981.2298 1019.4000
1034.7799 1114.7434 1134.7234
1152.2740 1202.9406 1297.0400
1316.7495 1363.3688 1390.1529
1477.6697 1693.3800 1936.2121
3066.4754 3117.2750 3183.6233
3223.3625 3228.0951 3252.6727

i30

Cartesian coordinates

C	1.125997	-1.068055	-0.108660
C	1.766118	0.119482	-0.225900
C	0.858356	1.234015	0.039317
C	-0.236326	-0.810933	0.442138
C	-1.570504	-0.677365	-0.331113
C	-0.321679	0.702540	0.425683
C	-1.697141	0.640026	-0.107728
H	1.590360	-2.041569	-0.200216
H	2.801723	0.241317	-0.523199
H	1.042018	2.256423	-0.264216
H	-0.389563	-1.273118	1.422556
H	-2.436552	1.385940	-0.364125
H	-2.156907	-1.407247	-0.873215

Vibrational frequencies

245.1443 315.2378 465.7217
555.5016 694.4819 739.1234
746.5138 787.4494 856.6973
872.4357 893.2013 938.9151
958.0383 967.6962 1021.6040
1062.8041 1071.4527 1100.8518
1128.0847 1176.1861 1260.7424
1291.3491 1326.1703 1394.3486
1558.4103 1593.1854 1661.1297
3073.4723 3204.3929 3226.0833
3228.5110 3234.5259 3260.5450

i31

Cartesian coordinates

C	1.029039	1.198469	0.019750
C	-0.301090	0.683460	-0.238704
C	-1.812592	-0.664538	0.089425
C	1.854105	0.130069	0.120102
C	1.075429	-1.164320	0.028903
C	-1.833196	0.666894	0.094605
C	-0.293738	-0.658570	-0.286726
H	1.329148	2.236700	0.069475
H	-2.591445	1.423418	0.236200
H	-2.554339	-1.437705	0.233938
H	2.934877	0.168071	0.173552
H	1.509076	-1.874172	-0.683732
H	1.064949	-1.665091	1.006436

Vibrational frequencies

164.0647	296.7818	394.5300
416.6908	605.4703	657.3514
671.2573	718.9987	757.7964
865.1617	877.3524	901.1569
913.4665	936.6150	952.3668
1070.4209	1104.1285	1114.7201
1167.2077	1225.7643	1260.1635
1295.3849	1395.5035	1417.2690
1544.8718	1636.3463	1657.9472
3046.4458	3087.0047	3217.5068
3223.3833	3240.7137	3259.3538

i32**Cartesian coordinates**

C	0.084446	0.761848	-0.000133
C	2.679431	-0.001528	0.000464
C	1.196309	-0.007382	0.002993
C	-1.236683	1.166830	-0.000267
C	-2.030310	0.003443	-0.000310
C	0.079981	-0.766130	-0.000183
C	-1.244973	-1.163686	-0.000282
H	3.049444	0.661482	0.784820
H	3.065212	-1.008037	0.159674
H	3.044795	0.373986	-0.958486
H	-1.598828	2.184548	0.000014
H	-3.116968	0.006932	0.000312
H	-1.612863	-2.179285	-0.000024

Vibrational frequencies

63.5840	153.6707	270.1140
463.2690	566.1365	593.5059
605.9476	641.1965	766.5525
798.9585	802.4605	898.9884
907.5278	975.9809	1038.6226
1061.6113	1084.5201	1123.9772
1217.6918	1286.4802	1374.1115

1399.8852	1437.4724	1482.0458
1484.5339	1572.0358	1944.2745
3063.4075	3138.0569	3167.2954
3192.3172	3241.7285	3246.5314

i33

Cartesian coordinates

C	-0.937745	-1.241609	0.000002
C	-1.868004	-0.079868	-0.000001
C	-1.210203	1.111177	-0.000002
C	0.291163	-0.703413	0.000001
C	1.824747	-0.622284	-0.000003
C	0.194541	0.746487	0.000004
C	1.537585	0.896382	-0.000001
H	-1.250326	-2.276562	0.000004
H	-2.946745	-0.186241	-0.000002
H	-1.653606	2.095027	-0.000004
H	2.325387	-1.011931	-0.891012
H	2.325394	-1.011935	0.891001
H	2.207388	1.750412	0.000013

Vibrational frequencies

120.7354 282.8195 484.3790
541.2711 676.0116 717.0498
752.3983 791.4802 849.1154
867.2491 874.7420 945.6489
949.7675 969.2506 1022.3122
1025.4652 1114.8721 1121.2694
1187.8505 1234.3640 1252.6948
1326.0392 1371.0653 1501.4477
1540.7925 1678.6329 1720.5350
3061.8592 3108.2198 3199.6261
3213.7275 3237.3779 3268.6653

Transition states

C₃+C₄H₆ - i1

Cartesian coordinates

C	0.731112	0.751652	-0.293820
C	-0.190932	1.572730	0.287848
C	1.512507	-0.228349	0.477946
C	2.581467	-0.843790	-0.014472
H	1.106349	0.988594	-1.282801
H	-0.662648	2.371852	-0.269662
H	-0.506470	1.419597	1.312632
H	1.172298	-0.429553	1.490039
H	3.149886	-1.548700	0.579958
H	2.920831	-0.662969	-1.029423
C	-0.837669	-0.325553	-0.834715
C	-1.942507	-0.445498	-0.133793
C	-3.050684	-0.837663	0.377549

Vibrational frequencies

-386.1431 41.6994 96.2723
156.7244 185.1679 242.4112
293.6746 329.9911 449.1887
529.8076 621.4116 742.1831
892.1868 959.0351 985.7437
1005.9458 1025.1857 1074.7345
1228.0256 1246.7243 1307.3783
1327.6387 1414.3893 1475.5996
1607.0294 1734.5132 2038.5361
3156.3584 3171.3277 3177.3555
3201.5314 3252.4437 3274.8578

i1-i2

Cartesian coordinates

C	-0.290146	0.709750	0.574923
C	0.497610	1.505345	-0.460856
C	-1.650981	0.205170	0.242397
C	-1.939010	-0.945959	-0.348400
C	0.975127	0.180866	-0.007665
C	2.114896	-0.629164	-0.125257
C	1.224019	-1.519241	0.240406
H	-0.164761	1.034874	1.606520
H	1.085628	2.370766	-0.173253
H	0.075612	1.529821	-1.461530
H	-2.448532	0.894432	0.510111
H	-2.967365	-1.204181	-0.573616
H	-1.169667	-1.666312	-0.601514

Vibrational frequencies

-381.3683 89.2110 154.5485
194.6960 286.7118 350.8110
377.1331 553.1203 663.9056
717.3938 754.9556 843.3026
936.1001 991.2892 1026.7090
1043.8251 1046.2831 1079.0243
1108.9901 1154.3625 1329.0436
1337.6379 1418.0492 1450.2513
1487.0921 1644.6615 1732.5420
3124.5174 3132.4174 3153.5303
3168.0195 3221.4963 3254.8154

i2-i3

Cartesian coordinates

C	-0.335329	0.689538	0.565908
C	0.657547	1.273884	-0.392856
C	-1.705572	0.325326	0.092621
C	-2.062170	-0.884424	-0.315346
C	0.741010	-0.278579	0.361781
C	2.034171	-0.253994	-0.483366
C	1.576213	-1.341465	0.308183
H	-0.312487	1.134297	1.560487
H	1.329052	2.049784	-0.052254

H	0.401794	1.284995	-1.443968
H	-2.418851	1.145181	0.087608
H	-3.069422	-1.079420	-0.663767
H	-1.365300	-1.716557	-0.309654

Vibrational frequencies

-446.7311 95.1753 146.3871
182.4100 335.7362 394.7504
484.6630 579.5959 683.5431
772.0190 832.4825 837.5623
916.7806 993.8058 1027.6600
1033.4776 1057.3804 1098.9884
1138.1445 1172.2580 1230.2418
1331.9923 1353.8296 1453.2926
1460.1239 1684.6673 1733.3768
3122.2690 3154.4896 3167.7608
3173.9350 3250.1076 3279.2884

i3-i4

Cartesian coordinates

C	-0.130839	0.191098	0.564697
C	0.884721	1.177800	-0.165789
C	-1.565901	0.446215	0.211410
C	-2.365441	-0.419715	-0.396249
C	0.423494	-1.209136	0.224657
C	1.910407	0.155706	-0.534760
C	1.786971	-0.971853	0.057704
H	-0.010660	0.314653	1.652154
H	1.279523	1.999056	0.438454
H	0.417216	1.608514	-1.054219
H	-1.941634	1.432368	0.481682
H	-3.393570	-0.165043	-0.627143
H	-2.011346	-1.410241	-0.660945

Vibrational frequencies

-294.1521 99.3344 125.0790
210.6075 261.8615 351.0220
528.3913 590.3746 672.3103
749.9113 860.8868 945.5331
988.9441 997.6828 1013.4546
1039.0206 1041.9287 1090.0131
1129.8181 1189.2628 1238.9153
1307.2524 1333.2019 1442.2018
1462.6009 1553.3870 1732.0198
3007.3515 3072.0160 3122.2385
3138.8664 3158.3382 3249.7048

i4-i5

Cartesian coordinates

C	-0.262705	0.026759	0.593772
C	1.321328	1.098611	-0.231226
C	-1.618634	0.507135	0.289698

C	-2.481681	-0.146791	-0.482548
C	0.204731	-1.307606	0.253649
C	2.293000	0.029002	-0.294382
C	1.401327	-0.913068	-0.091154
H	0.170573	0.390966	1.524050
H	1.591731	2.051909	0.221809
H	0.671844	1.184473	-1.098229
H	-1.887508	1.466710	0.724006
H	-3.473040	0.244978	-0.676015
H	-2.217792	-1.103288	-0.922482

Vibrational frequencies

-642.8499 94.7536 200.8055
247.3763 356.0960 397.4355
492.2676 540.7890 601.2180
658.3093 704.6134 809.5473
916.2906 978.7247 986.4170
1028.7099 1045.2434 1052.5525
1127.4001 1160.0123 1249.9952
1328.7102 1372.7009 1443.7719
1450.1592 1637.2659 1712.1988
3108.8182 3148.9558 3153.9920
3172.9064 3208.4089 3252.9100

i5-i6

Cartesian coordinates

C	-3.378186	-0.616858	-0.012108
C	-2.169524	-0.107722	-0.175851
C	-1.292541	0.953880	-0.045883
C	-0.130338	0.242832	0.196584
C	1.161739	0.146559	0.135538
C	2.404534	-0.088716	0.026939
C	3.690742	-0.307875	-0.092020
H	-3.639764	-1.590519	-0.406978
H	-4.125024	-0.088514	0.574717
H	-0.979755	-0.871974	0.055192
H	-1.454660	2.022038	-0.137289
H	4.309057	0.315576	-0.729458
H	4.171593	-1.119210	0.444627

Vibrational frequencies

-1828.2844 90.2429 111.7052
233.5454 244.7985 343.3237
395.3639 503.2195 524.9428
545.0784 579.4110 665.5794
860.7970 864.2770 879.8815
912.9405 986.0957 1017.2311
1059.6475 1101.7897 1205.8159
1349.8568 1447.3202 1470.5920
1796.2287 1811.5756 1851.9925
2208.3426 3137.6439 3141.9137
3206.1041 3226.7011 3237.8254

i5-i7**Cartesian coordinates**

C	3.593649	-0.138728	0.266489
C	2.373519	-0.387381	-0.215378
C	1.304059	0.559244	0.065136
C	0.006892	0.298027	-0.156959
C	-1.278805	0.135890	-0.046309
C	-2.528060	-0.041212	0.040327
C	-3.822865	-0.226168	0.137849
H	4.395721	-0.864450	0.184115
H	3.798117	0.793832	0.780930
H	2.170132	-1.325176	-0.732746
H	0.489076	0.805957	-1.138459
H	-4.272634	-0.519043	1.079566
H	-4.470736	-0.089149	-0.720340

Vibrational frequencies

-651.6678 58.3498 86.7706
145.8607 183.4496 340.2866
379.7988 446.1939 484.2026
503.0530 563.1381 665.2229
757.9693 812.2434 912.6716
976.6156 1009.4598 1018.1362
1029.5005 1127.4668 1325.5902
1362.8872 1433.1425 1491.5578
1681.8290 1872.5775 2241.0224
2380.6781 3121.7384 3154.0532
3158.2221 3241.0782 3255.4421

i6-i11**Cartesian coordinates**

C	-0.680798	1.357899	-0.212788
C	-1.842967	0.804258	0.268896
C	-1.990605	-0.542754	0.147057
C	-0.739495	-1.193921	-0.069029
C	0.342396	-0.364335	-0.187385
C	1.614222	-0.224107	-0.040453
C	2.873809	0.065924	0.158825
H	-0.619550	1.492038	-1.295546
H	-0.106894	2.082306	0.360100
H	-2.918585	-1.093707	0.240526
H	-0.642306	-2.267704	-0.196387
H	3.167487	0.833399	0.868472
H	3.660469	-0.464122	-0.367903

Vibrational frequencies

-643.2056 129.3430 143.4629
299.7909 375.0135 463.7981
502.6706 538.3664 562.9833
654.9896 778.1825 854.0207
885.1005 919.7630 961.8512

969.6412 1005.8394 1031.5747
1093.4799 1114.3504 1292.7507
1330.4652 1407.3951 1443.0809
1554.4360 1614.6222 2084.1036
3102.8653 3138.4876 3190.2808
3191.8708 3213.9660 3222.4239

i7-i8

Cartesian coordinates

C	-1.712507	0.879799	0.250056
C	-2.921714	0.491807	-0.270170
C	-1.427506	-0.463852	0.457880
C	-0.245864	-1.136452	-0.069278
C	0.947375	-0.566038	-0.090629
C	2.075726	0.001507	-0.049206
C	3.252785	0.580877	-0.020625
H	-1.088902	1.752624	0.127267
H	-3.177125	0.791541	-1.294164
H	-2.719138	-0.732963	0.243069
H	-0.336246	-2.192273	-0.309577
H	4.157839	0.019821	-0.228212
H	3.353800	1.635369	0.213440

Vibrational frequencies

-1453.2075 57.6222 107.2434
211.8889 243.3488 269.5433
358.2547 450.1804 540.6595
589.1981 642.9859 790.4829
864.0899 883.9641 896.9422
906.3272 982.7703 1031.4471
1034.3284 1140.6943 1185.3491
1312.0114 1413.9345 1444.5484
1492.1111 1684.6730 2205.1497
2220.5452 3073.6192 3145.3456
3165.6054 3231.6881 3261.0800

i7-i9

Cartesian coordinates

C	-1.023882	-0.624714	-0.696515
C	-1.953559	-0.910732	0.471277
C	-1.581784	0.447837	-0.058277
C	-0.565286	1.385822	0.171618
C	0.509318	0.598759	-0.213628
C	1.662305	0.071455	-0.013748
C	2.821144	-0.516578	0.162415
H	-0.800067	-1.013523	-1.674235
H	-1.533407	-1.249027	1.417862
H	-2.941899	-1.303361	0.245138
H	-0.581272	2.384388	0.586068
H	3.733416	-0.095674	-0.250818
H	2.913698	-1.433895	0.737131

Vibrational frequencies

-796.7563 95.2767 158.4934
234.7304 317.1261 378.2894
467.7155 555.5366 612.0613
677.3172 778.7832 838.3337
886.8639 910.8612 957.5585
971.0525 1023.8369 1028.1397
1033.8494 1074.1568 1164.2055
1342.0639 1418.5536 1469.5715
1529.9053 1561.3204 2105.0418
3087.2428 3124.1239 3175.3593
3203.3380 3229.3519 3299.4210

i8-i12**Cartesian coordinates**

C -2.046710 -1.172752 -0.607906
C -1.768326 -0.750948 0.588169
C -1.628143 0.653540 0.214996
C -0.390223 1.256487 -0.091576
C 0.803523 0.629698 -0.037017
C 1.904496 0.035045 -0.018359
C 3.070335 -0.595662 0.004779
H -2.279712 -0.896754 -1.620690
H -1.584459 -1.274270 1.518950
H -2.524244 1.259765 0.144342
H -0.402594 2.302411 -0.389163
H 3.990958 -0.077959 -0.240340
H 3.130330 -1.645646 0.268390

Vibrational frequencies

-778.3991 81.7270 111.6427
184.4529 259.4213 284.7663
381.7004 451.6948 467.3351
541.1842 604.1601 693.0940
794.9602 831.2677 853.2738
871.5269 903.4066 1013.6279
1033.3160 1171.2171 1235.9358
1330.3511 1377.7882 1442.2875
1598.6238 1673.2942 2042.8032
3148.6969 3156.2859 3187.7516
3193.8482 3238.4131 3337.9376

i9-i10**Cartesian coordinates**

C 0.744650 -0.896355 -0.419269
C 1.834741 -1.029136 0.365185
C 1.860202 1.047159 -0.107948
C 0.545632 1.308044 0.024726
C -0.291736 0.118829 -0.049451
C -1.584435 -0.041316 0.031151
C -2.873613 -0.200626 0.096699

H	0.723779	-1.313887	-1.421147
H	1.825976	-0.753826	1.411511
H	2.703484	-1.567999	0.007210
H	0.199287	2.334003	0.105306
H	-3.363950	-0.448769	1.033516
H	-3.501229	-0.089114	-0.782946

Vibrational frequencies

-330.7750	104.8918	156.2827
255.5091	336.4517	383.8351
553.0755	563.3290	586.9237
626.7405	783.4536	816.5481
840.0813	911.3090	982.2785
1007.0808	1021.1637	1055.2536
1094.8090	1212.3891	1291.2063
1316.0131	1442.6623	1488.6293
1601.9064	1641.6664	2094.2256
3130.5121	3173.6980	3187.1646
3192.6639	3210.8291	3269.7773

i10-i12

Cartesian coordinates

C	0.599134	-1.167216	0.000024
C	1.895791	-0.903852	0.000011
C	1.886040	1.151387	-0.000018
C	0.563010	1.218283	0.000045
C	-0.270877	0.006262	0.000054
C	-1.584387	-0.021775	-0.000008
C	-2.881588	-0.042220	-0.000058
H	0.194702	-2.172866	0.000259
H	2.627212	0.242532	-0.000499
H	2.716526	-1.613509	-0.000147
H	0.102686	2.199889	0.000243
H	-3.441968	-0.050680	0.929941
H	-3.441903	-0.050581	-0.930097

Vibrational frequencies

-998.2421	133.1686	155.2802
339.9900	400.1784	427.7229
531.6784	563.9356	618.8269
637.9703	654.0353	746.7076
750.6520	844.6163	906.2448
928.5632	929.0903	1005.9040
1054.7805	1184.2166	1215.3924
1262.5104	1339.8266	1474.9295
1629.0263	1672.6956	2071.3225
2622.3316	3137.4234	3193.0428
3206.2357	3218.9985	3220.1219

i11-i12

Cartesian coordinates

C	0.604704	-1.162761	0.029312
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C	1.970237	-0.794513	0.110554
C	1.906142	0.689230	-0.000532
C	0.645073	1.167669	-0.002660
C	-0.280031	0.036514	0.003340
C	-1.591962	0.040516	-0.000396
C	-2.888762	0.019262	0.001111
H	1.351596	-1.339726	-0.970789
H	0.225465	-2.167240	0.188683
H	2.795782	1.305863	-0.029961
H	0.327647	2.201898	-0.036215
H	-3.444880	0.000431	0.932833
H	-3.448021	0.023268	-0.928913

Vibrational frequencies

-1014.4456 127.5409 155.7873
 372.2307 445.1510 551.7255
 567.3957 587.0503 651.3101
 794.9780 830.6913 861.5862
 889.8742 919.4173 990.1860
 993.8651 998.1955 1110.6797
 1161.9175 1203.4004 1279.2713
 1314.4863 1343.4237 1398.4603
 1484.7120 1583.8349 2066.7613
 2207.9254 3144.8826 3193.8033
 3211.3683 3229.7757 3236.0041

i1-i21

Cartesian coordinates

C	-0.950880	0.539088	-0.565849
C	-1.766333	-0.174804	0.572394
C	-0.793749	-0.886506	-0.229965
C	0.228630	1.352668	-0.132249
C	1.421991	0.954005	0.278150
C	0.415590	-1.355441	-0.053603
C	1.683235	-1.189530	-0.089685
H	-1.541177	0.941400	-1.381942
H	-2.819380	-0.284001	0.332806
H	-1.544878	0.066188	1.609735
H	0.049422	2.427554	-0.104270
H	2.161368	1.606942	0.734746
H	2.263744	-0.194966	0.133762

Vibrational frequencies

-1166.3276 212.7060 276.6388
 325.0932 397.5015 429.2329
 529.6666 553.9755 599.7374
 690.9228 732.4007 768.5823
 856.5102 887.0463 932.6975
 963.2368 1018.9816 1061.0327
 1079.6050 1098.4669 1100.9536
 1238.2127 1310.7153 1460.4446
 1527.6728 1633.6934 1974.7344

2554.4434 3110.3340 3142.2118
3185.0375 3190.6573 3207.8308

i21-i15

Cartesian coordinates

C	-1.002507	0.800460	-0.336199
C	-1.770877	-0.268820	0.460641
C	-0.784425	-0.964551	-0.308981
C	0.263413	1.340613	-0.039225
C	1.434811	0.649249	0.274608
C	0.402077	-1.374048	-0.188752
C	1.591904	-0.723036	0.002098
H	-1.627278	1.367314	-1.022118
H	-2.808361	-0.328404	0.141152
H	-1.653859	-0.263189	1.544539
H	0.392211	2.395485	-0.267444
H	2.316021	1.235113	0.519600
H	2.574888	-1.165521	-0.100872

Vibrational frequencies

-452.3244 226.6498 353.4273
435.6497 518.6282 538.2277
604.0433 741.9922 813.3997
842.7684 859.0806 948.5273
984.5087 996.2264 1044.2022
1073.9122 1094.3921 1157.0282
1164.5947 1241.7930 1283.1380
1386.5905 1419.5603 1493.9963
1505.9526 1557.2762 1977.0550
3088.2387 3154.5430 3168.8856
3175.0832 3185.6681 3208.3210

i21-i24

Cartesian coordinates

C	-0.626961	0.959316	-0.388781
C	-2.029225	-0.229716	0.439612
C	-0.908030	-0.473563	-0.341441
C	0.648561	1.339887	0.039584
C	1.599349	0.363268	0.290089
C	0.068148	-1.436457	-0.286063
C	1.346477	-0.996362	-0.001841
H	-1.331493	1.698982	-0.750597
H	-2.793810	0.478329	0.147134
H	-2.153414	-0.718230	1.403428
H	0.906110	2.390707	0.091969
H	2.589182	0.670858	0.618211
H	2.193512	-1.678886	-0.017102

Vibrational frequencies

-461.3886 227.4416 353.4602
439.9419 514.9479 607.8953
629.8056 715.5850 757.3241

883.3911 907.6166 919.7243
949.7063 959.4429 1006.5763
1018.3031 1062.7843 1123.7952
1184.1115 1216.3591 1307.3862
1353.0921 1411.8997 1492.2799
1535.5835 1554.8194 1617.8222
3139.6118 3149.4029 3178.6763
3195.7741 3219.3466 3253.3621

i24-i23

Cartesian coordinates

C	-0.102672	1.325193	-0.030856
C	-2.348734	-0.094736	0.078268
C	-0.943904	0.217653	-0.121009
C	1.261081	1.054749	-0.007346
C	1.743457	-0.259702	0.032172
C	-0.453667	-1.043774	-0.118249
C	0.877104	-1.356741	0.068001
H	-0.481811	2.338840	0.043689
H	-2.881669	0.216762	0.971504
H	-2.873538	-0.688857	-0.655714
H	1.972013	1.873129	0.014616
H	2.815695	-0.428234	0.044633
H	1.253321	-2.367497	0.175394

Vibrational frequencies

-540.6177 152.8276 284.0069
433.7139 466.0500 523.8226
608.1766 682.2322 698.3317
756.8787 831.1679 886.2560
950.0436 973.8711 1008.8634
1019.5775 1034.8117 1125.5850
1182.5040 1222.8295 1291.9025
1348.3176 1449.7111 1475.7953
1499.0054 1609.0502 1686.2937
3155.4973 3184.7785 3195.3140
3206.2057 3216.4391 3282.7109

i24-i12

Cartesian coordinates

C	-0.241130	1.073887	-0.214841
C	-2.437377	-0.121671	0.268530
C	-1.137647	-0.164934	-0.039253
C	1.090993	1.145421	0.024231
C	1.859003	-0.048114	0.236495
C	-0.131806	-0.970895	-0.519290
C	1.131955	-1.186014	0.047661
H	-0.832646	1.957841	-0.428139
H	-2.920692	0.826507	0.461170
H	-3.011648	-1.032194	0.365090
H	1.565793	2.120087	0.040878
H	2.900333	-0.045111	0.524711

H 1.494915 -2.193209 0.215098

Vibrational frequencies

-1290.8836 142.1141 303.5582
415.9392 469.8834 561.3550
579.2674 633.0271 664.1223
718.2322 761.8998 775.0633
821.6813 879.8932 927.1938
962.9839 1027.3357 1084.2923
1108.1890 1192.0742 1227.4942
1346.1317 1425.6594 1454.3786
1486.6852 1610.1607 1733.0728
3182.8216 3190.8253 3214.3421
3218.9088 3243.4725 3281.7763

i23-i22

Cartesian coordinates

C 0.119501 1.418059 -0.022682
C -2.283774 0.051896 0.054388
C -0.904480 0.499142 -0.159566
C 1.403491 0.869051 0.012724
C 1.619991 -0.511909 0.055879
C -0.680028 -0.841791 -0.194390
C 0.550147 -1.414833 0.062023
H -0.042585 2.484169 0.074470
H -2.543667 0.100638 1.126076
H -1.965538 -1.163107 -0.343053
H 2.261746 1.531343 0.050684
H 2.636412 -0.888714 0.080665
H 0.704537 -2.482014 0.160896

Vibrational frequencies

-1359.9608 159.5803 352.4301
389.9575 467.6955 569.4246
625.2516 690.2079 757.6091
824.3980 889.0412 922.4442
947.8024 989.8904 1011.9159
1034.5658 1040.9532 1133.6202
1181.1549 1186.8296 1216.0158
1313.1444 1384.5738 1478.9467
1495.0243 1625.9216 1710.0237
2234.4793 2997.9139 3191.4776
3206.7347 3220.7437 3224.4497

i22-i19

Cartesian coordinates

C -1.600837 -0.398715 0.210030
C -1.292446 0.981835 0.015669
C -0.011246 1.391645 -0.194279
C -0.651738 -1.366749 0.047939
C 0.675917 -0.998676 -0.329581
C 1.002445 0.390997 -0.250268

C	2.168909	0.026968	0.352341
H	-2.624774	-0.676980	0.432755
H	-2.089849	1.712988	0.088142
H	0.245866	2.441183	-0.272228
H	-0.924763	-2.415205	0.093779
H	1.331773	-1.716423	-0.790956
H	2.315724	0.490609	1.337397

Vibrational frequencies

-367.9131 270.4969 391.1411
440.2907 564.9646 597.7565
693.7709 743.2675 761.7523
807.8649 866.5321 897.6401
926.9328 990.9144 1016.5202
1023.0993 1024.9184 1095.6257
1192.1270 1197.7519 1244.5157
1353.7049 1392.5354 1470.1942
1530.2062 1612.6777 1677.4817
3058.0665 3189.9678 3200.1780
3212.4625 3222.9804 3287.7370

i19-i16

Cartesian coordinates

C	-1.084576	1.019837	-0.291908
C	-1.570316	-0.294933	-0.101497
C	-0.758082	-1.344726	0.276803
C	0.176363	1.432320	0.105904
C	1.248462	0.558012	0.400961
C	0.586959	-1.091970	0.072752
C	1.596873	-0.556508	-0.509866
H	-1.815152	1.786305	-0.527152
H	-2.644397	-0.447652	-0.139483
H	-1.136536	-2.259307	0.714493
H	0.293109	2.480754	0.373926
H	1.905338	0.793322	1.238019
H	2.223541	-0.685607	-1.378694

Vibrational frequencies

-461.4857 289.8138 348.8916
422.7644 510.8071 605.9594
640.9500 702.0911 734.7281
817.1698 877.3434 917.0509
926.0877 985.3252 995.5236
997.1122 1064.0979 1113.1133
1160.1108 1203.2581 1231.7238
1354.2076 1421.1600 1467.3340
1529.9527 1611.7839 1930.9287
3122.4025 3159.8746 3185.1718
3203.6650 3219.2921 3255.2620

i15-i16

Cartesian coordinates

C	1.408151	0.730729	0.159797
C	1.406383	-0.643719	-0.325171
C	0.264698	-1.385475	-0.085095
C	0.250649	1.437955	0.152339
C	-1.093392	1.018941	-0.207455
C	-0.898608	-1.310673	0.507651
C	-1.633278	-0.233706	-0.124394
H	2.336164	1.204210	0.460652
H	1.364213	-1.833503	0.441413
H	2.194238	-1.020082	-0.972514
H	0.339120	2.490992	0.410052
H	-1.777461	1.832956	-0.428944
H	-2.683893	-0.358882	-0.376689

Vibrational frequencies

-1400.4601 267.1827 300.0980
 375.7243 427.4144 542.4396
 562.1359 684.2236 727.6165
 805.9570 831.6259 881.7471
 928.9125 984.9299 1007.9157
 1015.5202 1044.7848 1195.1351
 1225.6638 1239.5120 1267.8098
 1400.1732 1422.0566 1457.9651
 1552.9788 1650.7167 1726.7261
 2027.2724 3160.1017 3167.7535
 3169.8901 3187.5416 3206.7641

i15-i12

Cartesian coordinates

C	0.099579	1.659904	0.000003
C	2.374349	0.130389	0.000047
C	1.347083	-0.772150	-0.000059
C	-1.154894	1.230596	-0.000005
C	-1.753403	-0.108490	0.000038
C	0.279694	-1.376854	-0.000083
C	-1.139673	-1.307845	0.000014
H	0.493938	2.667577	0.000005
H	2.832055	0.447254	0.929934
H	2.831639	0.447948	-0.929805
H	-1.902054	2.031443	-0.000050
H	-2.839327	-0.111517	0.000111
H	-1.732658	-2.216003	0.000077

Vibrational frequencies

-238.4863 121.7825 174.1579
 208.6855 278.9485 348.1379
 382.4700 457.5980 489.1212
 656.9508 740.3094 743.6566
 781.7970 837.8180 896.3780
 922.4488 996.8985 1001.7816
 1035.2446 1221.3269 1280.8390
 1307.4823 1433.3204 1472.0842

1620.4557 1664.8690 2047.9431
3065.6260 3156.0879 3177.6629
3197.7054 3238.9227 3253.6758

i1-i27

Cartesian coordinates

C	-0.438434	-1.222382	0.372259
C	-1.674751	-0.869309	-0.117180
C	-1.439038	1.527673	0.090802
C	0.692623	-0.989755	-0.403043
C	1.836480	-0.217700	0.113276
C	-0.142901	1.473203	-0.082737
C	1.051768	1.056580	0.037167
H	-0.318366	-1.333599	1.448089
H	-2.569160	-0.939679	0.488621
H	-1.829001	-0.753412	-1.184937
H	0.559967	-0.941933	-1.481620
H	2.101341	-0.391939	1.159073
H	2.740740	-0.189303	-0.492484

Vibrational frequencies

-246.2733 176.7890 276.0069
299.3631 335.1597 371.0019
387.9141 508.3454 515.7080
747.8972 760.6090 863.8268
906.6111 949.7633 970.6647
1018.9234 1116.2364 1185.2932
1225.6505 1276.4253 1314.6492
1361.3249 1388.3496 1445.5937
1512.0577 1579.4428 1961.2829
3086.1898 3148.4852 3152.2569
3163.0272 3165.8025 3260.5294

i27-i18

Cartesian coordinates

C	0.390454	-1.209091	-0.360911
C	1.650653	-0.479932	-0.001012
C	1.503743	0.938239	-0.007845
C	-0.684660	-1.027615	0.422022
C	-1.831780	-0.146666	-0.063708
C	0.160648	1.292058	-0.049736
C	-1.066224	1.169113	-0.054316
H	0.224546	-1.122267	-1.438588
H	2.649514	-0.907691	0.039821
H	1.789776	0.282009	1.081614
H	-0.534015	-0.969570	1.500055
H	-2.165154	-0.359697	-1.081955
H	-2.701675	-0.139415	0.592089

Vibrational frequencies

-1211.5948 244.6554 323.6833
339.0881 419.1802 451.4848

529.9266 608.0435 709.4398
801.6239 833.9227 848.1330
888.5514 988.3291 1008.5094
1056.7089 1076.5473 1150.8783
1223.1107 1261.7674 1293.8499
1315.1917 1351.9220 1380.7019
1471.9055 1633.6206 2027.6055
2147.1387 3087.1024 3089.2088
3128.0421 3150.0747 3169.0794

i15-i18

Cartesian coordinates

C -0.363202 1.351547 -0.172034
C -1.546158 0.600040 -0.067134
C -1.539374 -0.789695 0.113268
C 0.865659 0.932405 0.479809
C 1.871801 -0.001840 -0.169183
C -0.264875 -1.410536 0.001088
C 0.920007 -1.145270 -0.164791
H -0.368662 2.246912 -0.791098
H -2.500076 1.071990 -0.289722
H -2.466460 -1.345992 0.172431
H 0.744706 0.695351 1.537712
H 2.159326 0.267366 -1.187993
H 2.768015 -0.155534 0.432531

Vibrational frequencies

-540.5858 251.1958 296.1214
371.1519 403.1321 429.7089
459.9918 620.0325 714.1631
719.1206 801.2049 843.7105
884.7694 909.2078 1009.6498
1058.5789 1096.3312 1142.0945
1166.2522 1208.7182 1237.7931
1310.7913 1363.5036 1415.9806
1449.4096 1471.6809 2045.6435
3083.7509 3117.3599 3136.6486
3143.7977 3171.3296 3216.6359

i16-i18

Cartesian coordinates

C -0.357870 -1.260832 0.339674
C -1.601040 -0.553494 0.040633
C -1.452100 0.823395 -0.113870
C 0.725444 -1.056501 -0.467713
C 1.796460 -0.140541 -0.033719
C -0.153925 1.323680 -0.088770
C 1.075873 1.114566 0.175611
H -0.179009 -1.479784 1.392585
H -2.599895 -0.976834 0.057496
H -2.322088 1.451749 -0.268985
H 0.536092 -0.957760 -1.540329

H	1.496902	0.693388	1.217016
H	2.870948	-0.232393	0.031138

Vibrational frequencies

-1859.8894 151.4257 233.8518
289.0861 382.8701 417.0208
493.7574 508.3794 621.1678
639.3739 725.2296 794.2415
831.8186 900.1417 924.0562
931.8022 1016.3844 1072.0984
1129.3985 1166.6698 1245.7960
1265.6078 1312.9560 1373.2127
1386.6600 1521.9344 1757.9387
2331.6901 3090.3206 3119.1619
3191.5604 3214.4264 3241.4462

i1-i14

Cartesian coordinates

C	1.968698	0.483275	0.156480
C	1.061905	1.509585	-0.189257
C	-3.272153	0.402666	0.093772
C	1.651871	-0.833779	0.083091
C	0.237969	-1.251928	-0.192381
C	-2.028640	0.023897	0.072985
C	-0.778677	-0.233698	0.116868
H	2.935178	0.764266	0.567510
H	0.380165	1.413875	-1.024600
H	1.184107	2.510722	0.207478
H	2.381664	-1.607043	0.288867
H	0.094392	-1.518968	-1.251412
H	-0.021342	-2.162959	0.362800

Vibrational frequencies

-437.6869 72.2040 115.6338
167.0095 264.4054 350.7041
403.5206 436.6066 531.9275
648.7315 689.3477 774.8283
793.5671 841.1267 928.7325
981.6514 1024.5722 1128.8859
1147.0305 1221.8086 1290.1772
1407.8692 1410.3496 1427.0017
1511.3762 1561.1182 1920.1290
3000.9535 3048.8922 3159.3547
3165.0558 3215.5924 3252.7751

i14-i20

Cartesian coordinates

C	1.447755	0.915408	-0.041974
C	0.020385	1.058459	0.294210
C	-2.013446	0.352435	-0.675449
C	1.747652	-0.377931	-0.210805
C	0.545891	-1.254915	0.017328

C	-1.949312	-0.473053	0.325472
C	-0.543268	-0.268371	0.337334
H	2.140868	1.741292	-0.127512
H	-1.006279	1.286550	-0.666553
H	-0.351771	1.844480	0.943573
H	2.728813	-0.772194	-0.440267
H	0.267339	-1.868507	-0.844930
H	0.687086	-1.943812	0.858991

Vibrational frequencies

-1482.8468 199.8977 278.9191
396.6153 445.7428 539.0591
613.7803 664.0717 721.0989
819.3361 829.1118 888.7330
945.3783 968.3261 984.5567
1032.1508 1128.3939 1144.7939
1158.2434 1223.0833 1252.2105
1344.5683 1383.3843 1418.9360
1439.6416 1596.1974 1656.2851
1757.4100 3055.1180 3100.7498
3192.2770 3221.4459 3244.2316

i20-i25

Cartesian coordinates

C	1.633365	0.805976	-0.045632
C	0.228652	1.125487	0.180016
C	-1.975181	-0.255213	0.619396
C	1.781155	-0.525084	-0.151531
C	0.445216	-1.188712	0.001015
C	-2.150169	0.158032	-0.550384
C	-0.488761	-0.026720	0.229128
H	2.423818	1.542255	-0.109947
H	-0.179500	2.118113	0.313610
H	2.707643	-1.060895	-0.305896
H	0.154805	-1.759751	-0.888548
H	0.417544	-1.885708	0.845009
H	-2.369972	0.483392	-1.546273

Vibrational frequencies

-312.3986 174.9753 207.6931
362.1572 368.8637 530.6698
570.0502 587.5116 701.4374
824.1867 868.8205 885.9014
907.5576 929.6847 971.9321
974.8241 1024.1516 1105.3152
1129.8200 1140.3738 1257.2030
1313.7352 1393.8915 1422.7669
1539.6303 1647.9083 1818.9195
3057.7689 3099.0382 3217.9813
3236.3004 3246.5074 3403.3565

i14-i29

Cartesian coordinates

C	1.792789	-0.721450	-0.088388
C	0.443300	-1.172634	-0.012729
C	-3.103208	0.010790	-0.136681
C	1.814152	0.634130	-0.073782
C	0.435458	1.192086	0.027583
C	-1.854417	-0.037008	-0.034976
C	-0.459962	-0.049061	0.147889
H	2.653963	-1.373531	-0.128197
H	0.100429	-2.199710	-0.006605
H	2.708596	1.243869	-0.070502
H	0.319409	1.892726	0.860384
H	0.148395	1.739000	-0.875507
H	-0.339458	-0.443481	1.246938

Vibrational frequencies

-1062.8417 123.2841 136.5564
266.4889 436.2949 471.5177
531.3503 574.7002 707.3754
814.0518 850.5620 907.8485
922.7836 965.6579 994.0177
1020.4551 1060.4593 1130.3066
1154.8520 1172.6600 1218.3262
1284.2490 1399.9551 1415.1542
1440.0280 1577.4937 2036.5630
2475.3417 3070.2915 3108.2100
3223.8539 3236.2574 3251.5868

i29-i25**Cartesian coordinates**

C	-1.795825	-0.735534	0.026560
C	-0.445496	-1.177827	0.012878
C	3.106088	0.011034	0.025334
C	-1.842355	0.623377	0.013453
C	-0.458971	1.189924	0.005510
C	1.843665	-0.037548	0.124398
C	0.422407	-0.054302	-0.053638
H	-2.653236	-1.394653	0.040398
H	1.044057	-0.168128	-1.086948
H	-0.105526	-2.204161	0.025397
H	-2.738444	1.228471	-0.002955
H	-0.281535	1.877780	-0.826350
H	-0.242398	1.745943	0.923484

Vibrational frequencies

-1031.2195 138.7850 145.7391
290.3011 423.7769 462.8164
532.5206 562.6636 703.1177
754.5107 822.9785 861.4139
872.7187 942.8180 975.4393
980.3323 1055.2935 1124.0839
1157.8895 1170.2972 1241.9376

1300.1815 1380.7964 1407.8434
1438.4884 1554.4705 1932.1620
2338.9403 3067.8120 3108.0378
3226.3260 3241.8861 3252.0915

i1-i13

Cartesian coordinates

C	-0.848962	-1.262471	-0.291703
C	0.198216	-1.610007	0.548758
C	2.291435	-0.150668	-0.276847
C	-1.475255	-0.033162	-0.355418
C	-1.053151	1.190432	0.380797
C	1.357133	0.754652	-0.231375
C	0.357046	1.518592	-0.012537
H	-1.160110	-2.000545	-1.025365
H	0.658251	-2.586574	0.476410
H	0.460222	-1.020774	1.417530
H	-2.211129	0.115095	-1.139355
H	-1.731916	2.029987	0.236485
H	-0.974095	1.018598	1.464247

Vibrational frequencies

-216.5410 161.0878 201.3363
277.8778 296.0975 341.2591
433.5393 491.8323 600.4468
611.7399 777.9489 828.7882
868.5813 883.7008 962.3339
1002.9691 1048.2279 1135.6304
1200.9247 1262.9567 1292.3344
1366.5078 1430.4578 1451.0659
1514.6773 1541.1515 1926.4902
3024.2718 3133.0689 3168.3459
3178.5567 3191.8987 3274.6949

i27-i13

Cartesian coordinates

C	0.664483	-1.220714	-0.301987
C	1.745606	-0.228545	0.082412
C	1.280375	1.209506	0.051116
C	-0.664327	-1.220723	0.302099
C	-1.745557	-0.228772	-0.082569
C	-0.000106	1.338468	0.000078
C	-1.280586	1.209389	-0.051121
H	0.857240	-1.845388	-1.174084
H	2.650108	-0.351036	-0.518207
H	2.067384	-0.379351	1.125375
H	-0.856875	-1.844881	1.174612
H	-2.066970	-0.379555	-1.125644
H	-2.650208	-0.351444	0.517784

Vibrational frequencies

-911.4151 98.8006 210.6678

233.1494 243.6159 271.5735
406.6635 450.2191 607.3647
661.3019 782.1499 805.1150
836.8707 931.7190 938.4410
988.3185 1125.9044 1140.3966
1152.1552 1244.6796 1250.7408
1303.4874 1341.5799 1358.4413
1404.6959 1426.8387 1662.4423
3005.9702 3006.5225 3104.8324
3105.1603 3125.1413 3127.9013

i15-i13

Cartesian coordinates

C 1.013179 1.091658 -0.005954
C 1.780645 -0.218256 0.010697
C 0.846011 -1.374096 0.013761
C -0.303801 1.373107 -0.012423
C -1.547051 0.532877 -0.026465
C -0.374359 -1.342569 -0.016455
C -1.682057 -0.877399 -0.105595
H 1.662718 1.967673 -0.008690
H 2.440902 -0.241968 0.885090
H 2.453594 -0.258108 -0.853256
H -0.537301 2.435081 -0.012542
H -1.956056 -0.132976 0.988817
H -2.459260 1.118360 -0.144811

Vibrational frequencies

-1135.1863 129.2804 291.4804
300.1412 333.1936 473.1289
547.5823 691.0110 720.7795
800.0488 844.6618 877.4918
922.6958 948.9207 958.8825
1046.7961 1153.0322 1239.9568
1249.3789 1284.5858 1356.3415
1378.2681 1443.1883 1448.7366
1466.2624 1695.0742 2113.7281
2157.3705 3042.3979 3068.8740
3122.7251 3129.2371 3164.1397

i20-i31

Cartesian coordinates

C -1.391636 -0.960328 -0.002900
C -0.012539 -1.043662 -0.526073
C 1.886002 0.421226 -0.161812
C -1.767721 0.308440 0.233677
C -0.609812 1.243632 0.051500
C 1.769241 -0.620558 0.633512
C 0.469906 0.285801 -0.399717
H -2.052866 -1.816727 0.054960
H 1.307057 -1.634298 0.517674
H 2.604436 1.217165 -0.271741

H	-2.774221	0.649036	0.452470
H	-0.807426	2.017304	-0.700283
H	-0.337626	1.760219	0.977792

Vibrational frequencies

-763.7358 148.4244 216.9312
321.6041 426.0859 518.1401
554.6116 663.0942 740.4974
801.0376 824.5778 871.8119
890.8343 942.9878 972.1330
1004.1395 1041.0183 1088.6298
1137.4395 1156.0765 1250.1815
1316.0003 1363.3208 1372.9875
1434.7563 1611.3944 1615.8212
2871.8715 3050.3516 3092.3180
3191.5625 3218.0353 3271.7557

i18-i17

Cartesian coordinates

C	0.525702	-1.303435	-0.143592
C	1.670825	-0.448877	-0.075158
C	1.412734	0.900315	0.086555
C	-0.562460	-0.711546	0.480522
C	-1.910538	-0.229106	-0.035192
C	0.019500	1.192479	0.034474
C	-1.142010	1.004088	-0.411106
H	0.447835	-2.085607	-0.889362
H	2.685963	-0.795537	-0.245119
H	2.177277	1.657638	0.186292
H	-0.403194	-0.346063	1.496336
H	-2.315983	-0.750185	-0.900388
H	-2.674412	-0.103767	0.733222

Vibrational frequencies

-524.9085 294.0877 312.6992
403.7277 470.3866 519.7302
584.8799 692.2642 744.1725
789.0942 855.0839 911.4432
943.2443 985.6770 1020.9176
1069.8509 1107.3657 1117.6571
1160.3438 1218.1533 1262.8344
1353.4578 1397.4131 1447.7458
1491.8891 1534.6501 1906.1930
3096.3329 3116.4609 3169.2608
3188.6765 3206.8154 3238.2217

i12-i17

Cartesian coordinates

C	-0.770187	1.252796	-0.088641
C	-1.773584	0.284476	-0.194019
C	-1.339389	-1.024860	0.075297
C	0.374553	0.597803	0.444920

C	2.177324	0.155987	-0.171635
C	0.044336	-0.917918	0.261527
C	1.196902	-0.781038	-0.392693
H	-0.895365	2.318270	-0.204494
H	-2.794249	0.513966	-0.481093
H	-1.919980	-1.929416	0.000660
H	0.800275	0.789500	1.427285
H	2.428736	0.839497	-0.975943
H	2.920861	0.064710	0.625048

Vibrational frequencies

-615.7182 197.6475 260.0571
379.6301 551.8444 578.7570
650.8092 680.4269 717.1150
792.0748 799.7772 830.8480
925.6184 951.5338 998.2341
1030.9182 1054.2039 1085.3599
1099.3152 1144.0952 1207.2242
1290.3240 1341.6081 1443.7469
1481.4546 1514.3764 1758.6479
3079.1827 3147.1305 3202.3464
3210.5077 3259.0519 3275.8952

i30-i17

Cartesian coordinates

C	-1.121012	1.071880	-0.091707
C	-1.747100	-0.121578	-0.237182
C	-0.826363	-1.217185	0.041504
C	0.241774	0.822393	0.445030
C	1.558659	0.592197	-0.338243
C	0.328805	-0.687263	0.500403
C	1.748520	-0.777887	-0.035831
H	-1.592793	2.042547	-0.177112
H	-2.774491	-0.250414	-0.556868
H	-0.975085	-2.243045	-0.271458
H	0.473658	1.376154	1.359647
H	1.546963	-0.339063	-1.253560
H	2.222054	1.318484	-0.804481

Vibrational frequencies

-1152.9653 227.3854 315.7757
452.9047 557.5540 709.9828
755.2936 774.6179 815.6582
874.5047 885.4278 896.7897
927.3904 970.1646 1020.2437
1046.6548 1065.2363 1085.2619
1123.6895 1162.9578 1244.3896
1272.8692 1326.0838 1353.0962
1402.9538 1545.7520 1642.2634
2184.7454 3096.4697 3164.9217
3210.4115 3228.1189 3237.5539

i30-i33

Cartesian coordinates

C	1.132164	-1.154718	-0.134811
C	1.834342	0.075558	-0.233424
C	0.990154	1.168987	0.033546
C	-0.059806	-0.808521	0.473730
C	-2.026480	-0.546461	-0.167260
C	-0.243452	0.616783	0.388657
C	-1.580049	0.728594	-0.096847
H	1.563332	-2.138679	-0.250919
H	2.906206	0.147917	-0.388273
H	1.242264	2.212627	-0.090034
H	-1.317352	-1.264363	0.585122
H	-2.621420	-1.046225	-0.920125
H	-2.054273	1.607388	-0.517318

Vibrational frequencies

-702.2802 173.9649 267.4767
406.3968 496.3987 560.2608
638.2687 687.3519 765.2543
796.0463 825.0695 859.3548
950.1957 959.0760 963.4893
989.7510 1072.4846 1077.7482
1146.8658 1200.0178 1240.7946
1294.9652 1363.7993 1392.3185
1487.7093 1521.4169 1546.0537
2050.3667 3196.7033 3218.0193
3238.2646 3246.8746 3255.7161

i31-i30

Cartesian coordinates

C	1.088503	-1.133071	-0.057531
C	1.859512	0.075849	-0.145198
C	1.011798	1.184643	-0.024837
C	-0.284878	-0.676997	0.155906
C	-1.807156	-0.661856	-0.108286
C	-0.277066	0.706912	0.228546
C	-1.796543	0.674051	-0.058134
H	1.400135	-2.130076	-0.337441
H	2.940209	0.105346	-0.150795
H	1.339165	2.215381	-0.062828
H	0.657323	-1.217098	1.104584
H	-2.550574	-1.423821	-0.284383
H	-2.551278	1.433079	-0.211932

Vibrational frequencies

-1291.9975 171.4718 357.5792
430.4107 555.2166 666.3585
686.7749 699.8270 738.4800
777.8616 882.8109 902.2116
904.8762 913.9082 952.1430
1037.5595 1074.3346 1091.3836

1167.0607 1225.1169 1255.9187
1288.4199 1389.4333 1421.1270
1491.4792 1532.2785 1616.4929
2202.0463 3224.3806 3228.9743
3237.1926 3251.2229 3271.5210

i16-i30

Cartesian coordinates

C -0.839403 1.175464 -0.249836
C -1.709944 0.152452 -0.227048
C -1.154424 -1.121548 0.277366
C 0.479802 0.989649 0.427094
C 1.711779 0.438393 -0.061465
C 0.158778 -0.971153 0.232591
C 1.419155 -0.890571 -0.321907
H -1.115828 2.157342 -0.622957
H -2.714936 0.206943 -0.634551
H -1.739757 -1.994494 0.534466
H 0.580063 1.687107 1.270655
H 2.684318 0.929048 -0.055313
H 1.911671 -1.622063 -0.953066

Vibrational frequencies

-748.7529 236.0280 303.5596
476.9005 525.5038 638.0596
689.4900 743.0950 780.0274
789.3595 856.9876 877.0744
892.6159 967.1770 983.1085
1016.0795 1034.0252 1116.6573
1144.4078 1183.2697 1262.9082
1345.8486 1353.7525 1455.8391
1514.0567 1636.4147 1808.6067
3024.7988 3147.6846 3178.2555
3201.9214 3202.9152 3217.4728

i15-i17

Cartesian coordinates

C -1.189806 -0.997831 -0.042850
C -1.626374 0.303284 0.280586
C -0.704642 1.263531 -0.049492
C 0.160734 -1.153275 -0.302592
C 1.364242 -0.579259 0.495797
C 0.510123 0.749977 -0.568250
C 1.724124 0.848736 -0.057847
H -1.898994 -1.774854 -0.310383
H -2.604963 0.537612 0.679219
H -0.778291 2.317737 0.184864
H 0.451680 -1.962076 -0.967626
H 1.189233 -0.489540 1.571548
H 2.210935 -1.239847 0.310265

Vibrational frequencies

-558.8587 189.3766 266.7347
381.3981 435.6069 543.9041
662.4338 746.5199 792.5949
830.7125 861.3478 896.5073
944.5110 979.0151 991.0872
1046.9857 1090.5928 1128.6279
1164.4126 1195.5685 1216.6749
1362.4595 1426.6361 1449.7998
1492.0655 1567.1005 1599.7603
3067.7254 3144.1947 3171.5074
3196.1492 3225.8774 3243.0631

i25-i26

Cartesian coordinates

C -1.811702 0.761026 -0.007151
C -0.477919 1.150038 -0.017683
C 1.774292 0.004532 -0.005141
C -1.864926 -0.645617 -0.028960
C -0.470545 -1.126674 -0.052439
C 2.975931 -0.002856 0.016759
C 0.353371 0.016661 -0.038190
H -2.669340 1.414586 0.047085
H -0.115430 2.166767 0.047414
H -2.727702 -1.281967 -0.163429
H -1.226766 -1.080160 1.025131
H -0.170517 -2.154315 -0.195407
H 4.038742 -0.007562 0.036041

Vibrational frequencies

-1183.1969 159.7197 162.4518
460.8610 534.5931 565.8021
601.7493 624.6257 642.4621
703.8788 764.4628 805.4851
862.4529 939.1957 949.2475
999.6393 1013.4712 1077.5087
1096.4363 1223.1222 1241.9706
1261.0894 1398.0900 1448.8459
1496.5612 1551.5753 2130.4708
2242.7051 3238.7631 3252.0698
3261.8013 3270.6375 3484.4387

i13-i28

Cartesian coordinates

C 0.424445 1.389489 0.162467
C -0.847579 0.920557 -0.469173
C -2.198526 -0.347700 0.403536
C 1.471357 0.574482 0.248395
C 1.385348 -0.865941 -0.190748
C -1.000329 -0.674590 0.042960
C 0.084581 -1.549529 0.088593
H 0.464288 2.402651 0.545055
H -0.773022 0.785078 -1.551078

H	-1.673711	1.606241	-0.287143
H	2.396712	0.912609	0.701902
H	1.440524	-0.931065	-1.295384
H	2.229425	-1.456119	0.170461

Vibrational frequencies

-243.9631	135.0576	171.4705
360.6869	421.7882	447.0599
521.9751	544.1450	710.4522
716.9780	831.0552	862.9551
921.2933	959.5731	990.5573
1019.0345	1074.4650	1163.2204
1171.9236	1235.3932	1253.4793
1336.0251	1397.3047	1429.0070
1479.9925	1719.4647	1829.4651
2951.5397	3079.0346	3104.9423
3145.4887	3187.7067	3210.8091

i24-i32

Cartesian coordinates

C	-0.448799	0.959139	0.000024
C	-2.398360	-0.049621	-0.000023
C	-0.927522	-0.333171	0.000026
C	0.886507	1.310906	0.000001
C	1.795826	0.246334	-0.000013
C	-0.000442	-1.336120	0.000016
C	1.355158	-1.084899	-0.000003
H	-1.836307	1.272072	-0.000018
H	-2.953889	-0.222661	-0.920197
H	-2.953964	-0.222617	0.920114
H	1.227509	2.338404	-0.000009
H	2.862114	0.450746	-0.000043
H	2.080326	-1.891354	-0.000016

Vibrational frequencies

-2385.8810	186.7822	373.4731
414.5146	421.6040	482.4242
538.8163	627.6782	668.9061
764.8991	836.7107	900.1221
955.5527	981.1157	993.3096
1046.9045	1056.9284	1132.5407
1155.1181	1176.2192	1225.2074
1326.7105	1422.1292	1435.4865
1466.5281	1609.6642	1639.0943
1826.2267	3105.8013	3184.1144
3205.7615	3206.8850	3222.7375

Products

p1

Cartesian coordinates

C	-1.717438	-0.000031	-0.000002
C	-0.321993	-0.000010	-0.000004

C	0.525830	-1.171569	0.000002
C	1.811623	-0.736475	-0.000001
C	1.811596	0.736510	0.000001
C	0.525775	1.171560	0.000000
C	-2.926409	0.000009	0.000002
H	0.169218	-2.190132	-0.000005
H	2.698913	-1.354297	0.000004
H	2.698861	1.354367	0.000006
H	0.169126	2.190109	-0.000004
H	-3.990023	-0.000013	0.000010

Vibrational frequencies

143.6144 156.9817 401.5705
 524.8528 529.8027 563.2349
 633.2168 643.9659 647.9939
 674.7398 727.0966 759.8823
 914.5762 915.8552 931.9939
 1002.3144 1044.0254 1080.3858
 1129.9068 1278.5189 1304.8588
 1416.5917 1532.1718 1550.9793
 2124.9272 3227.3528 3238.9177
 3265.6836 3269.6864 3475.3401

p2

Cartesian coordinates

C	3.526567	-0.224510	-0.000084
C	2.190257	-0.448829	0.000044
C	1.222096	0.586134	0.000041
C	-0.137873	0.354849	0.000076
C	-1.343042	0.155473	0.000051
C	-2.685372	-0.066882	0.000051
C	-3.875758	-0.264677	-0.000109
H	4.234717	-1.043437	-0.000073
H	3.927566	0.783856	-0.000198
H	1.821751	-1.470766	0.000157
H	1.559436	1.619366	-0.000159
H	-4.924726	-0.438363	-0.000146

Vibrational frequencies

82.4729 99.5269 192.8437
 223.3291 380.5836 403.9428
 476.9236 518.6578 557.0757
 598.5610 661.5995 690.9503
 778.1505 786.4228 894.7304
 976.0232 1017.3102 1188.0681
 1222.1407 1303.3258 1375.0690
 1464.7479 1560.4512 2122.3441
 2206.3242 3154.6872 3165.8219
 3179.5713 3256.0828 3483.4776

p3

Cartesian coordinates

C	-3.504583	0.590961	0.000000
C	-2.645816	-0.436766	0.000008
C	-1.242163	-0.288777	0.000003
C	-0.026579	-0.186134	-0.000003
C	1.309218	-0.064774	-0.000031
C	2.542907	0.047181	-0.000037
C	3.881208	0.168812	0.000033
H	-4.573898	0.418230	0.000029
H	-3.156936	1.617347	-0.000025
H	-3.021618	-1.456671	0.000056
H	4.349345	1.146322	0.000089
H	4.517957	-0.708235	0.000006

Vibrational frequencies

78.7857 94.5364 170.4604
 189.8914 241.6574 334.2733
 420.9727 473.9313 512.6016
 530.9582 626.7401 685.4749
 761.6852 959.8568 987.3361
 1007.1652 1024.8917 1121.3237
 1317.9580 1378.7549 1446.1073
 1503.7429 1640.9725 1997.2015
 2179.7849 3151.3840 3160.7701
 3170.2013 3246.0879 3263.1410

p4

Cartesian coordinates

C	3.496253	-0.728903	0.000118
C	2.313275	-0.116313	-0.000180
C	1.203425	0.447397	-0.000066
C	0.000036	1.089109	0.000101
C	-1.203566	0.447913	-0.000059
C	-2.313412	-0.115929	0.000035
C	-3.496122	-0.729171	0.000008
H	4.418622	-0.159478	0.000664
H	3.561596	-1.810900	-0.000605
H	0.000187	2.177315	0.000067
H	-3.560866	-1.811211	0.000602
H	-4.418872	-0.160343	-0.000474

Vibrational frequencies

68.0754 176.4359 191.5449
 202.3496 312.8227 388.0338
 406.9372 412.4022 500.9742
 535.6179 539.9888 821.3206
 821.5858 851.9296 855.0743
 871.6453 1033.8588 1034.3683
 1297.4919 1373.5025 1430.4507
 1521.6992 1582.9779 1837.2752
 2163.5646 3145.7078 3151.7048
 3152.5952 3244.7960 3244.8798

p11**Cartesian coordinates**

C	0.266310	1.466863	0.000049
C	-2.075696	-0.000064	0.000026
C	-0.874605	0.702022	-0.000129
C	1.459162	0.694668	-0.000004
C	1.459230	-0.694549	-0.000036
C	-0.874552	-0.702103	-0.000029
C	0.266496	-1.466880	0.000031
H	0.282861	2.548697	0.000256
H	-3.151744	0.000013	0.000099
H	2.413792	1.209389	0.000027
H	2.413947	-1.209116	-0.000078
H	0.283064	-2.548713	0.000254

Vibrational frequencies

267.4020 307.3954 463.5233
478.9545 508.9266 573.4255
701.4797 721.6207 729.2817
826.4301 878.6707 966.0947
978.5725 992.6685 1012.2058
1020.9679 1063.0439 1118.5973
1201.8934 1308.0111 1392.3230
1471.3983 1493.2136 1533.8000
1789.5931 3194.9761 3211.1551
3225.8064 3228.8898 3295.4782

p12**Cartesian coordinates**

C	-1.026366	1.184374	0.000001
C	0.263795	0.730255	0.000004
C	1.738346	-0.685910	-0.000002
C	-1.839451	0.000000	-0.000003
C	-1.026366	-1.184374	0.000001
C	1.738346	0.685910	-0.000001
C	0.263795	-0.730255	0.000004
H	-1.400956	2.197874	0.000000
H	2.525682	-1.428004	-0.000006
H	-2.922044	0.000001	-0.000011
H	-1.400958	-2.197874	0.000000
H	2.525682	1.428004	-0.000006

Vibrational frequencies

140.4688 330.8447 485.1679
522.8125 690.2187 714.3313
730.1531 757.2509 798.4675
827.9220 874.1655 904.6788
939.3613 953.4450 987.1729
1003.0280 1087.4184 1199.4455
1221.5884 1232.4294 1300.9182
1372.9675 1479.7838 1550.8169
1609.4984 3227.1044 3229.0253

3247.1948 3254.3735 3259.4252

p13

Cartesian coordinates

C	1.311786	0.830852	0.000023
C	1.710489	-0.487203	0.000086
C	0.606908	-1.379673	-0.000148
C	-0.000142	1.395428	-0.000045
C	-1.311761	0.830869	0.000007
C	-0.606792	-1.379564	0.000016
C	-1.710462	-0.487415	0.000026
H	2.110270	1.570048	-0.000021
H	2.750644	-0.779909	0.000167
H	-0.000144	2.480325	-0.000162
H	-2.110336	1.569978	0.000086
H	-2.750583	-0.780208	0.000133

Vibrational frequencies

235.2907 259.3185 379.1647
436.6072 453.3736 585.3884
648.0424 650.7731 701.4196
787.5425 861.8860 884.6153
910.8125 969.2224 992.0553
998.5877 1092.5893 1205.2261
1210.7334 1305.7583 1419.1853
1422.2045 1519.2008 1561.0932
2242.8127 3162.6761 3167.1890
3197.9005 3233.3459 3237.1430

p14

Cartesian coordinates

C	-0.376311	1.215976	-0.000013
C	-2.527111	0.000016	-0.000089
C	-1.094494	0.000527	-0.000020
C	1.007394	1.214072	0.000021
C	1.690959	-0.000494	0.000042
C	-0.377192	-1.215353	0.000008
C	1.006551	-1.214628	0.000033
H	-0.935027	2.145375	-0.000034
H	1.559066	2.146795	0.000028
H	2.775839	-0.001032	0.000066
H	-0.936605	-2.144372	0.000006
H	1.557958	-2.147460	0.000051

Vibrational frequencies

179.4225 292.4132 346.9125
450.8214 537.6265 626.5012
695.7097 780.1212 845.9351
869.2536 983.3326 1019.9571
1020.5907 1038.7299 1050.0360
1102.6471 1191.2933 1198.3864
1297.7244 1307.7800 1347.5638

1469.5869 1516.0780 1624.4671
1654.3391 3195.5111 3204.1781
3209.7232 3219.2346 3225.4558

p15

Cartesian coordinates

C	-0.143819	-0.759734	0.000001
C	-2.679310	0.000000	0.000000
C	-1.286253	0.000000	0.000001
C	1.169661	-1.169178	-0.000002
C	1.966478	0.000000	-0.000001
C	-0.143818	0.759734	0.000000
C	1.169661	1.169178	0.000001
H	-3.219152	0.937013	-0.000017
H	-3.219149	-0.937014	0.000013
H	1.534916	-2.185842	-0.000002
H	3.052864	-0.000001	0.000001
H	1.534917	2.185842	0.000002

Vibrational frequencies

152.1098	278.5404	404.8664
455.4818	566.0998	593.3950
594.8579	646.7112	723.1179
782.7878	798.9225	807.9047
873.2873	932.9778	952.3248
1031.5683	1074.3543	1103.5148
1247.4699	1264.4090	1349.4495
1418.3801	1479.3130	1570.5956
1753.6237	3182.5998	3195.9427
3241.6709	3246.6001	3299.9216

p16

Cartesian coordinates

C	-1.412375	0.745728	-0.000085
C	-0.228128	1.511450	0.000162
C	2.236952	0.049854	-0.000226
C	-1.436523	-0.635201	-0.000167
C	-0.198895	-1.505321	0.000172
C	0.956668	0.720219	0.000025
C	0.980005	-0.614964	-0.000017
H	-2.365678	1.264986	-0.000234
H	-0.243849	2.593863	0.000418
H	-2.397484	-1.138682	-0.000443
H	-0.189631	-2.174936	0.870344
H	-0.189578	-2.175822	-0.869271

Vibrational frequencies

106.7419	280.1699	429.2730
445.1115	489.4479	525.6196
655.8467	672.7785	770.8689
852.6857	911.9491	920.9203
989.8811	1007.4590	1073.3834

1184.9806	1189.7937	1233.6386
1251.4592	1350.4325	1421.9794
1428.6023	1442.6158	1511.8249
1754.9115	3025.5633	3050.7035
3189.4344	3207.6895	3223.8563