

Supplementary information

A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl (CH_3CC , X^2A_1) – Propylene (CH_3CHCH_2 , $\text{X}^1\text{A}'$) System and the Formation of 1,3-dimethylvinylacetylene ($\text{CH}_3\text{CCCHCHCH}_3$, $\text{X}^1\text{A}'$) under Single Collision Conditions

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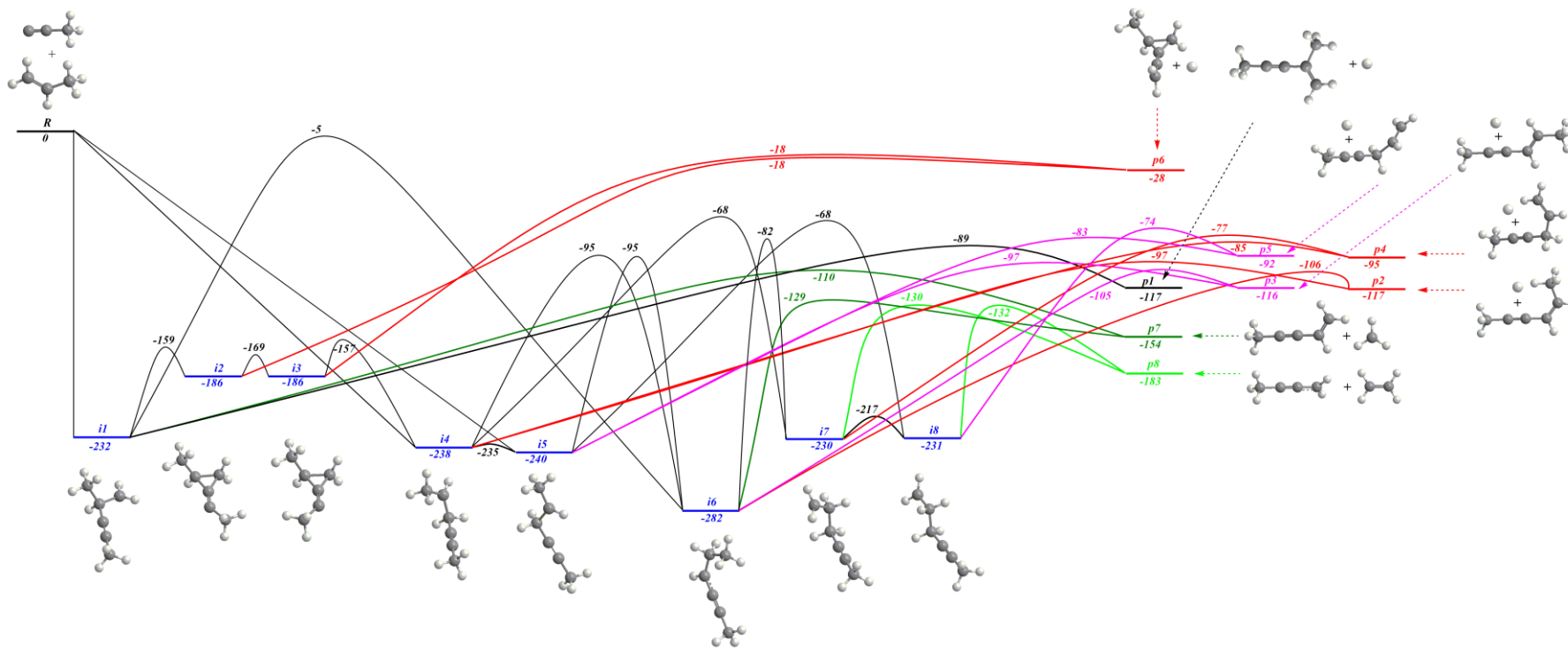


Figure S1. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH_3CC ; X^2A_1) radical with Propylene (CH_3CHCH_2 , X^1A') calculated at the CCSD(T)-F12/cc-pVTZ-F12// ω B97X-D/6-311G(d,p) level of theory. Relative energies of various species are shown in kJ mol^{-1} . Part I.

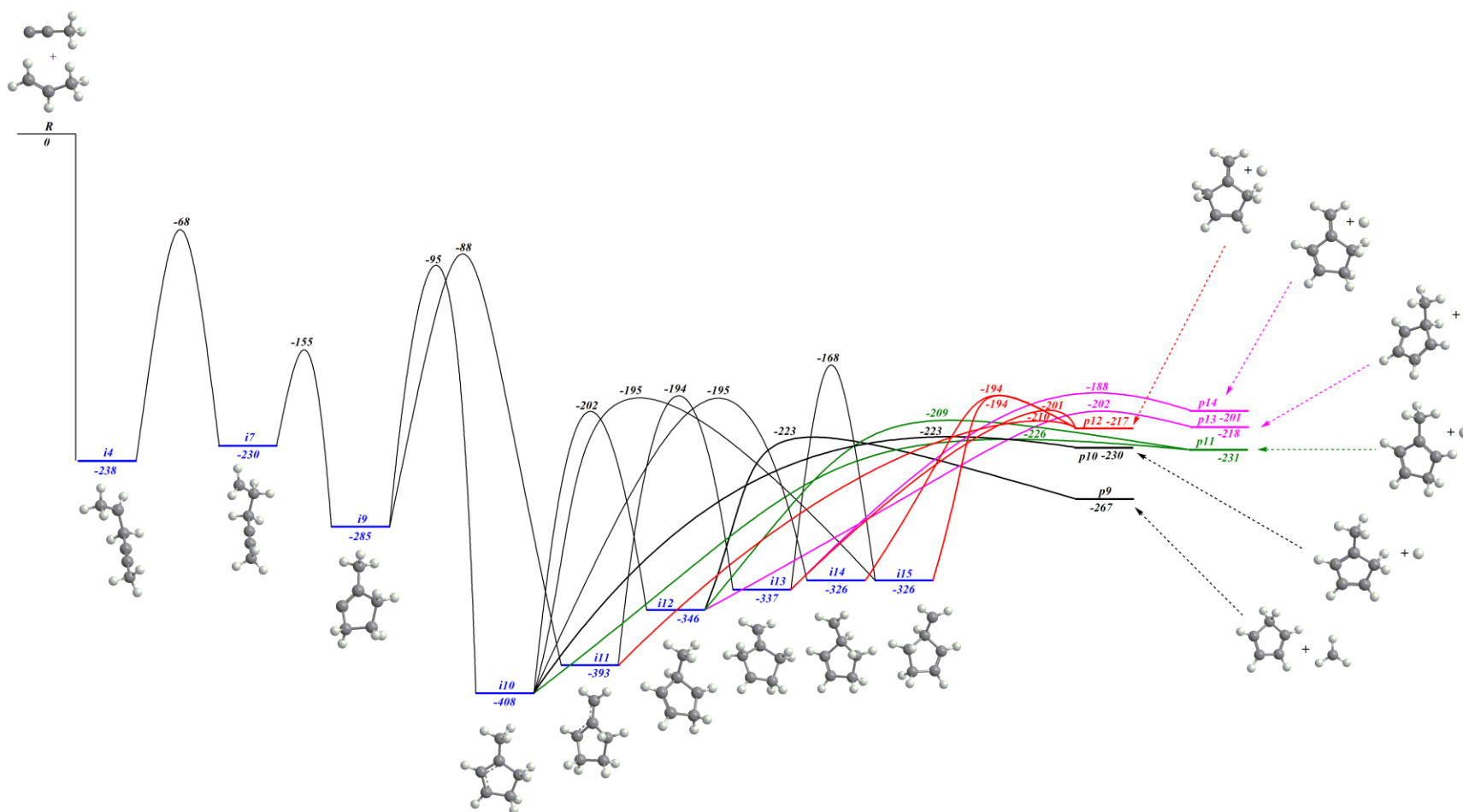


Figure S2. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH_3CC ; X^2A_1) radical with Propylene (CH_3CHCH_2 , X^1A') calculated at the CCSD(T)-F12/cc-pVTZ-F12// ω B97X-D/6-311G(d,p) level of theory. Relative energies of various species are shown in kJ mol^{-1} . Part II.

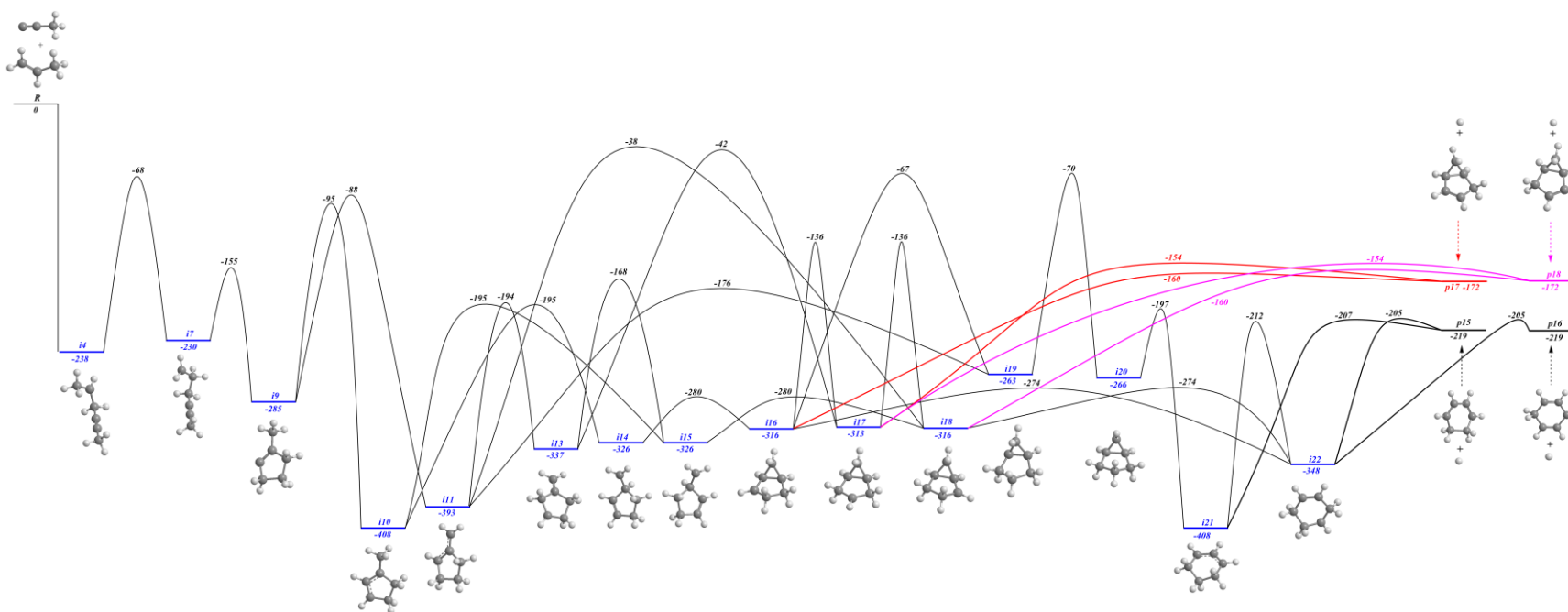


Figure S3. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH_3CC ; X^2A_1) radical with Propylene (CH_3CHCH_2 , X^1A') calculated at the CCSD(T)-F12/cc-pVTZ-F12// ω B97X-D/6-311G(d,p) level of theory. Relative energies of various species are shown in kJ mol^{-1} . Part III.

Table S1. Statistical branching ratios (%) for the reaction of 1-propynyl + propene with *iI* and *i4/i5* as initial intermediates at different collision energies (E_C , kJ mol⁻¹)

E_C	<i>iI</i>		<i>i4/i5</i>	
	0	37	0	37
<i>p1</i>	0.4	0.6	0.4	0.5
<i>p2</i>	4.3	4.6	5.4	7.7
<i>p3</i>	6.0	6.5	7.6	11.0
<i>p4</i>	0.9	1.4	1.2	2.4
<i>p5</i>	2.1	3.5	2.7	5.8
<i>p6</i>	0.0	0.0	0.0	0.0
<i>p7</i>	86.1	83.1	82.5	72.1
<i>p8</i>	0.2	0.3	0.2	0.5
<i>p9</i>	0.0	0.0	0.0	0.0
<i>p10</i>	0.0	0.0	0.0	0.0
<i>p11</i>	0.0	0.0	0.0	0.0
<i>p12</i>	0.0	0.0	0.0	0.0
<i>p14</i>	0.0	0.0	0.0	0.0
<i>p14</i>	0.0	0.0	0.0	0.0
<i>p15</i>	0.0	0.0	0.0	0.0
<i>p16</i>	0.0	0.0	0.0	0.0
<i>p17</i>	0.0	0.0	0.0	0.0
<i>p18</i>	0.0	0.0	0.0	0.0

Table S2. RRKM calculated rate constants ($k(E)$, s^{-1}) of the reaction of 1-propynyl + propene as functions of the internal energy (E , kJ mol^{-1}) of the intermediate states for unimolecular reaction steps at different collision energies (E_C , kJ mol^{-1})

E_C	0		37		E_C	0		37	
Reaction step	$k(E)$	E	$k(E)$	E	Reaction step	$k(E)$	E	$k(E)$	E
<i>i4 - i3</i>	2.63E+09	238	5.67E+09	275	<i>il4 - il0</i>	3.96E+08	326	8.99E+08	363
<i>i3 - i4</i>	2.83E+12	186	4.10E+12	223	<i>il3 - p12</i>	3.79E+09	337	9.33E+09	374
<i>il - i2</i>	1.49E+08	232	2.91E+08	269	<i>il3 - p14</i>	1.39E+09	337	3.85E+09	374
<i>i2 - il</i>	3.22E+12	186	4.56E+12	223	<i>il2 - p9</i>	1.01E+10	346	2.12E+10	383
<i>i5 - p3</i>	5.90E+06	240	4.11E+07	277	<i>il2 - p11</i>	1.09E+09	346	2.59E+09	383
<i>i5 - p5</i>	2.13E+06	240	2.22E+07	277	<i>il2 - p13</i>	1.52E+09	346	3.87E+09	383
<i>i5 - i6</i>	6.06E+06	240	3.62E+07	277	<i>i4 - i6</i>	8.61E+06	238	5.05E+07	275
<i>i6 - i5</i>	1.26E+05	282	9.90E+05	319	<i>i6 - i4</i>	5.14E+04	282	4.00E+05	319
<i>i6 - p7</i>	3.57E+07	282	1.79E+08	319	<i>i5 - i4</i>	2.27E+12	240	2.34E+12	277
<i>i6 - p3</i>	4.70E+05	282	3.68E+06	319	<i>i4 - i5</i>	7.89E+12	238	8.08E+12	275
<i>i5 - i8</i>	8.58E+04	240	1.02E+06	277	<i>i20 - il9</i>	6.55E+04	266	6.62E+05	303
<i>i8 - i5</i>	3.08E+05	231	3.45E+06	268	<i>il9 - i20</i>	1.12E+05	263	1.12E+06	300
<i>i8 - p5</i>	7.23E+05	231	9.01E+06	268	<i>il3 - il7</i>	4.18E+00	337	2.20E+02	374
<i>i4 - i7</i>	3.05E+05	238	3.54E+06	275	<i>il7 - il3</i>	1.33E+02	313	6.40E+03	350
<i>i7 - i4</i>	9.27E+05	230	1.02E+07	267	<i>il3 - il5</i>	2.20E+07	337	6.92E+07	374
<i>i4 - p4</i>	3.26E+06	238	3.12E+07	275	<i>il5 - il3</i>	2.28E+07	326	6.79E+07	363
<i>i4 - p2</i>	1.45E+07	238	9.92E+07	275	<i>i7 - p8</i>	9.04E+09	230	2.92E+10	267
<i>i9 - il0</i>	2.57E+06	285	1.95E+07	322	<i>il4 - il6</i>	7.59E+10	326	9.50E+10	363
<i>il0 - i9</i>	1.59E+02	408	1.96E+03	445	<i>il6 - il4</i>	1.30E+12	316	1.59E+12	353
<i>i7 - i9</i>	1.21E+09	230	2.41E+09	267	<i>il4 - p12</i>	4.47E+08	326	1.10E+09	363
<i>i9 - i7</i>	2.50E+09	285	7.60E+09	322	<i>il5 - p12</i>	4.52E+08	326	1.11E+09	363
<i>i9 - il1</i>	5.67E+05	285	4.19E+06	322	<i>il5 - il8</i>	7.66E+10	326	9.59E+10	363
<i>il1 - i9</i>	3.94E+02	393	4.52E+03	430	<i>il8 - il5</i>	1.30E+12	316	1.59E+12	353
<i>il1 - p12</i>	1.09E+09	393	3.09E+09	430	<i>il0 - il5</i>	5.79E+06	408	1.80E+07	445
<i>il0 - p10</i>	2.66E+08	408	7.22E+08	445	<i>il5 - il0</i>	4.00E+08	326	9.07E+08	363
<i>il0 - p11</i>	3.75E+08	408	9.96E+08	445	<i>i22 - p15</i>	2.34E+09	348	5.75E+09	385
<i>i3 - i2</i>	4.71E+12	186	5.81E+12	223	<i>i22 - p16</i>	3.02E+09	348	7.38E+09	385
<i>i2 - i3</i>	6.19E+12	186	7.66E+12	223	<i>il6 - i22</i>	9.41E+11	316	1.17E+12	353
<i>i3 - p6</i>	5.44E+02	186	1.49E+05	223	<i>i22 - il6</i>	6.48E+10	348	9.29E+10	385
<i>i8 - i7</i>	9.03E+11	231	1.01E+12	268	<i>il6 - il9</i>	1.15E+03	316	1.58E+04	353
<i>i7 - i8</i>	2.66E+12	230	2.97E+12	267	<i>il9 - il6</i>	1.29E+05	263	1.39E+06	300
<i>il1 - il8</i>	1.61E-01	393	1.41E+01	430	<i>il8 - il7</i>	8.67E+06	313	3.45E+07	350
<i>il8 - il1</i>	3.36E+01	316	2.21E+03	353	<i>il7 - il8</i>	1.57E+07	313	6.16E+07	350
<i>i2 - p6</i>	9.20E+02	186	2.44E+05	223	<i>il7 - il6</i>	1.57E+07	313	6.16E+07	350

<i>i1-p7</i>	1.63E+07	232	8.05E+07	269	<i>i16-i17</i>	8.68E+06	316	3.45E+07	353
<i>i1-p1</i>	8.39E+04	232	6.44E+05	269	<i>i16-p17</i>	1.81E+08	316	6.03E+08	353
<i>i1-i6</i>	2.06E-03	232	2.31E+00	269	<i>i20-i21</i>	6.67E+10	266	1.09E+11	303
<i>i6-i1</i>	1.90E-04	282	3.01E-01	319	<i>i21-i20</i>	5.36E+06	408	1.60E+07	445
<i>i8-p1</i>	1.77E+09	231	5.55E+09	268	<i>i11-i19</i>	1.99E+06	393	6.97E+06	430
<i>i11-i13</i>	3.32E+07	393	9.88E+07	430	<i>i19-i11</i>	4.69E+10	263	9.56E+10	300
<i>i13-i11</i>	3.94E+08	337	9.47E+08	374	<i>i18-p18</i>	1.80E+08	316	6.02E+08	353
<i>i10-i12</i>	3.59E+06	408	1.05E+07	445	<i>i17-p18</i>	1.85E+08	313	6.48E+08	350
<i>i12-i10</i>	2.93E+08	346	6.85E+08	383	<i>i17-p17</i>	1.85E+08	313	6.49E+08	350
<i>i7-p4</i>	1.93E+06	230	2.08E+07	267	<i>i21-p15</i>	4.00E+08	408	1.20E+09	445
<i>i18-i22</i>	4.70E+11	316	5.87E+11	353	<i>i21-i22</i>	1.68E+08	408	4.50E+08	445
<i>i22-i18</i>	3.24E+10	348	4.65E+10	385	<i>i22-i21</i>	1.09E+09	348	2.34E+09	385
<i>i6-p2</i>	4.90E+05	282	3.66E+06	319	<i>i6-i7</i>	5.67E+03	282	5.54E+04	319
<i>i10-i14</i>	5.79E+06	408	1.80E+07	445	<i>i7-i6</i>	1.44E+06	230	1.01E+07	267

Table S3. Margins of RRKM calculated rate constants for H-loss channels exit steps of the reaction of 1-propynyl + propene at the collision energy of 37 kJ mol⁻¹, taking into account the relative energy error bars of ± 4 kJ mol⁻¹.

Step	$k(E), \text{s}^{-1}$
<i>i1-p1</i>	2.80E+05 – 1.47E+06
<i>i4-p2</i>	4.42E+07 – 2.21E+08
<i>i6-p2</i>	1.71E+06 – 7.77E+06
<i>i5-p3</i>	1.83E+07 – 9.16E+07
<i>i6-p3</i>	1.71E+06 – 7.83E+06
<i>i4-p4</i>	1.35E+07 – 7.14E+07
<i>i7-p4</i>	8.82E+06 – 4.87E+07
<i>i5-p5</i>	9.54E+06 – 5.10E+07
<i>i8-p5</i>	3.77E+06 – 2.14E+07
<i>i2-p6</i>	7.66E+04 – 7.50E+05
<i>i3-p6</i>	4.68E+04 – 4.62E+05

Table S4. Total rates of formation for products **p2** and **p3** from **i6** ($E_{\text{col}} = 37 \text{ kJ mol}^{-1}$) depending on varying energies of critical transition states evaluated using steady-state approximation.

TS	Relative Energy, kJ mol^{-1}								
i4-i6	-95	-91	-99	-95	-95	-91	-99	-91	-99
i6-p3	-105	-105	-105	-101	-109	-101	-109	-109	-101
i6-p2	-106	-106	-106	-102	-110	-102	-110	-110	-102
	Rate of formation from i6 , s^{-1}								
p2	3.43E+06	3.05E+06	4.06E+06	2.16E+06	5.36E+06	1.92E+06	6.49E+06	4.77E+06	2.52E+06
p3	3.45E+06	3.07E+06	4.08E+06	2.15E+06	5.40E+06	1.91E+06	6.53E+06	4.80E+06	2.51E+06

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

Reactants

Propylene

Cartesian coordinates

C	-1.276382	0.221005	-0.000011
C	-0.134665	-0.454315	-0.000065
C	1.230687	0.162110	0.000007
H	-2.235678	-0.284449	0.000197
H	-1.291429	1.307503	-0.000032
H	-0.168945	-1.542399	0.000050
H	1.801146	-0.152652	0.879852
H	1.175233	1.253093	-0.000755
H	1.801836	-0.153898	-0.878900

Frequencies

182.1162	433.1258	584.8547
935.9596	946.6634	949.9833
1028.6424	1072.0149	1195.7127
1328.2170	1407.9844	1453.7623
1479.9109	1496.4392	1741.6231
3037.0031	3096.8473	3127.1773
3147.8498	3161.1106	3240.4142

1-propynyl

Cartesian coordinates

C	-1.123766	0.000034	0.000188
H	1.340902	0.037697	1.467468
H	1.347686	-2.105149	0.242483
H	2.849266	-1.203608	-0.055380
H	1.579875	-1.250168	-1.294258
H	-3.332371	0.942655	-0.480319
H	-3.470957	-0.236441	0.830178
H	-3.252125	-0.787978	-0.835980

Frequencies

10.9733	34.6698	116.4472
141.8784	256.3832	306.3587
312.1812	348.2153	473.6279
540.7418	555.8082	683.7224
911.8485	961.1275	1031.9362
1057.2417	1059.3318	1074.7197

C	0.336608	-0.000571	-0.000814
C	1.540300	0.000283	0.000377
H	-1.504993	0.615339	0.817821
H	-1.506845	-1.015014	0.124083
H	-1.507018	0.401203	-0.940410

Frequencies

200.1523	203.0213	952.8370
1014.5159	1022.1101	1413.0112
1478.5078	1483.7864	2276.0322
3059.2654	3134.4920	3139.5728

Intermediates

i1

Cartesian coordinates

C	1.739138	1.305471	-0.179151
C	1.129542	0.062640	0.388751
C	1.768851	-1.209168	-0.219553
C	-2.965290	-0.019316	-0.114031
C	-1.518072	0.011691	0.066691
C	-0.327596	0.040936	0.220705
H	2.771240	1.543793	0.050633
H	1.207050	1.905677	-0.905295

1137.6814	1192.4399	1296.4990
1364.5791	1402.1902	1420.1205
1455.4825	1486.4304	1486.5399
1494.9920	1501.7224	2393.4538
3004.8123	3046.2987	3046.9065
3119.0464	3119.5025	3130.0405
3136.8933	3154.8565	3273.5587

i2

Cartesian coordinates

C	-0.649455	1.296038	0.241734
C	-1.271471	0.110085	-0.479993
C	-2.172179	-0.845542	0.266939
C	2.727253	-0.249596	0.148314
C	1.325607	-0.451606	-0.248729

C	0.178613	0.129847	-0.201347
H	-0.540988	2.231783	-0.297107
H	-0.843457	1.397137	1.305804
H	-1.549054	0.294684	-1.515372
H	-2.191439	-1.822817	-0.221689
H	-3.196035	-0.462865	0.311848
H	-1.813700	-0.990333	1.289481
H	2.855582	0.723299	0.642534
H	3.392274	-0.278346	-0.719487
H	3.056608	-1.027898	0.842476

Frequencies

112.2219	140.4169	165.4283
206.5565	270.7874	379.8876
397.0406	515.0574	672.3557
789.5391	872.7166	917.0755
938.2932	1021.9402	1047.9501
1051.0883	1058.9764	1084.4035
1134.3762	1179.0772	1207.7772
1377.9219	1402.8031	1417.2836
1471.7812	1473.4013	1483.5413
1491.6475	1504.2983	1888.4381

Frequencies

102.7242	103.9810	166.3498
230.7671	262.1611	375.3720
1125.5009	1178.8839	1199.7254
1367.9962	1397.5528	1421.4529
1496.6825	1504.6616	1889.2052
3007.3565	3043.5077	3089.8039
3114.9880	3115.5328	3120.5487
3123.3403	3148.5662	3209.9268

i4

Cartesian coordinates

C	0.886531	-1.149581	-0.134235
C	1.962087	-0.201341	0.307520
C	1.956979	1.227612	-0.099878
C	-2.915688	0.438570	0.066023
C	-1.572154	-0.125428	-0.008122
C	-0.468211	-0.594070	-0.064617
H	0.930310	-2.064692	0.465591
H	1.071517	-1.469922	-1.174275
H	2.869084	-0.638362	0.710693
H	2.706341	1.803458	0.447111
H	0.975510	1.684083	0.066466

3004.5420	3046.9262	3086.9033
3112.4371	3120.5371	3124.0305
3126.9614	3145.7069	3214.7479

i3

Cartesian coordinates

C	-1.110861	-1.308704	-0.149491
C	-1.110161	0.061348	0.511354
C	-1.710390	1.251401	-0.197769
C	2.541468	0.463273	0.030306
C	1.419942	-0.459972	-0.202577
C	0.152341	-0.556565	-0.001449
H	-1.261561	-2.181615	0.477979
H	-1.538717	-1.383859	-1.145486
H	-1.225070	0.055835	1.592750
H	-1.261209	2.184319	0.152992
H	-2.789345	1.307281	-0.024224
H	-1.540125	1.182060	-1.275380
H	3.302540	0.005667	0.668716
H	2.194828	1.383357	0.520697
H	3.024622	0.742265	-0.910291

424.7671	496.1699	673.1810
787.7788	860.6261	904.8513
948.6809	1038.8483	1047.4609
1052.9777	1071.4325	1086.7954
1466.2992	1467.6031	1480.1392

H	2.174290	1.344534	-1.174253
H	-3.079363	0.928851	1.028892
H	-3.672263	-0.341799	-0.048226
H	-3.072692	1.179278	-0.722156

Frequencies

77.5373	108.7524	116.0638
124.6590	196.6229	268.8615
363.9338	398.7040	415.3855
564.7489	757.4051	869.7454
897.9663	996.5493	1063.1100
1067.6530	1085.8701	1141.1453
1185.6261	1236.3326	1347.6353
1381.0173	1426.7631	1428.6065

1453.9260	1476.3038	1487.9876
1493.7242	1496.0940	2396.1627
2955.0935	2975.8004	3047.4466
3064.4351	3067.8198	3118.6761
3120.3203	3127.0383	3194.2067

i5

Cartesian coordinates

C	0.709976	0.714347	0.023297
C	1.626312	-0.468860	0.017292
C	3.097422	-0.264266	-0.037827
C	-3.281887	-0.310692	-0.018314
C	-1.870636	0.059184	-0.002318
C	-0.710201	0.365646	0.008384
H	0.934019	1.361039	-0.838533
H	0.913781	1.344013	0.905788
H	1.210401	-1.450614	0.206077
H	3.485504	0.174071	0.895513
H	3.377525	0.430376	-0.840280
H	3.629761	-1.203016	-0.201475
H	-3.472895	-1.084197	-0.766423
H	-3.907682	0.552524	-0.258485
H	-3.596325	-0.696354	0.954736

Frequencies

56.5698	87.8388	101.1245
113.9284	191.9446	279.4111
312.8532	352.0986	392.0286
503.8801	774.5896	873.4386
920.6680	996.5961	1053.6613
1055.8276	1116.4775	1151.8521
1174.5530	1206.7091	1300.8623
1402.8727	1413.6239	1426.1516
1454.7246	1479.2305	1485.2174
1489.3415	1492.5686	2401.7622
2963.7787	2978.7649	3001.7746
3043.4469	3048.5679	3119.4467
3121.8581	3128.9798	3213.6564

i6

Cartesian coordinates

C	2.064420	-0.270690	-0.007546
C	0.822929	-1.113597	0.003611
C	-2.939304	0.384333	-0.002803
C	-1.586315	-0.151271	0.003344
C	-0.454461	-0.607712	0.002816

H	2.662314	-0.541712	-0.888970
H	2.685205	-0.552053	0.854270
H	0.946169	-2.192509	0.010160
H	-2.934171	1.459322	0.194637
H	-3.555472	-0.098796	0.761047
H	-3.421595	0.221995	-0.971853
C	1.818446	1.233945	0.003911
H	1.235542	1.542298	-0.867474
H	2.765530	1.778336	-0.007529
H	1.262183	1.533065	0.895716

Frequencies

10.5672	74.5177	98.7570
170.8492	239.5768	253.8688
391.0845	392.1188	554.4129
586.8031	779.2589	781.9899
909.4873	1038.8034	1048.9292
1052.7277	1073.7061	1108.4592
1234.8174	1286.0412	1369.9934
1406.9908	1418.9940	1443.5630
1477.7427	1480.0744	1484.3363
1497.1346	1504.6828	2173.9157
3006.7754	3028.5529	3038.6010
3052.0650	3102.5783	3119.9436
3126.3724	3132.6151	3176.8681

i7

Cartesian coordinates

C	0.900093	-1.057978	-0.232535
C	1.942051	-0.124253	0.412113
C	2.003871	1.223917	-0.209335
C	-2.937034	0.410701	0.098935
C	-1.581296	-0.114074	-0.023060
C	-0.467057	-0.550844	-0.123171
H	0.956663	-2.043281	0.240711
H	1.146765	-1.200313	-1.289938
H	2.924321	-0.608005	0.364860
H	2.892193	1.835472	-0.109797
H	1.109734	1.673934	-0.625107
H	-2.933007	1.385115	0.593728
H	-3.565118	-0.263136	0.687043
H	-3.399037	0.532842	-0.883947
H	1.703723	-0.037449	1.484763

Frequencies

89.2472	121.4913	139.8269
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172.1671	228.3987	286.5011
381.4652	410.2268	491.2544
542.3316	698.6650	822.8582
892.3367	1000.9843	1050.1922
1059.0707	1069.0258	1120.2145
1173.6043	1191.9268	1284.5800
1358.2753	1382.8876	1424.7568
1465.1254	1470.8070	1489.1638
1491.5262	1493.1072	2394.2088
2975.9896	3049.4265	3050.9876
3065.3949	3093.7709	3118.9104
3124.3965	3158.9718	3268.1187

i8

Cartesian coordinates

C	-0.755891	0.714192	0.052477
C	-1.661690	-0.527510	-0.016005
C	-3.108264	-0.188250	-0.012581
C	3.240171	-0.289305	-0.021859
C	1.827381	0.073767	0.004072
C	0.666255	0.379259	0.024162
H	-0.980300	1.274908	0.965896
H	-0.990779	1.379075	-0.786207
H	-1.421604	-1.198171	0.816200
H	-1.401305	-1.090651	-0.926985
H	-3.458360	0.743097	-0.444632
H	-3.849030	-0.920725	0.282925
H	3.645913	-0.357515	0.990657
H	3.823605	0.454190	-0.570702
H	3.384089	-1.257122	-0.508747

Frequencies

63.2833	93.3905	104.6956
171.2666	219.0875	286.7008
352.5769	403.6431	491.2758
508.0471	740.8569	779.9159
889.9860	994.2726	1058.7241
1060.7254	1093.6416	1113.8699
1175.9567	1192.0539	1301.2572
1319.2700	1395.5566	1421.9404
1468.1095	1472.1625	1483.3296
1486.6089	1490.0670	2397.6739
2977.2797	3047.1118	3050.1661
3065.9787	3090.1562	3120.3524
3123.6738	3153.7056	3262.5510

i9

Cartesian coordinates

C	1.515471	-0.854033	0.082589
C	1.494338	0.683639	-0.153684
C	0.042444	1.137514	0.130240
C	-2.272006	-0.124418	-0.040085
C	-0.779266	-0.139763	-0.006142
C	0.058911	-1.157526	-0.034095
H	1.890651	-1.113588	1.078729
H	2.134866	-1.379310	-0.647782
H	2.229214	1.207652	0.460252
H	1.733845	0.881026	-1.201069
H	-0.070677	1.542488	1.143962
H	-0.289884	1.916441	-0.563579
H	-2.674189	0.333372	0.870077
H	-2.680006	-1.132030	-0.128615
H	-2.633175	0.471465	-0.884912

Frequencies

138.0656	167.4496	220.8263
309.3299	443.6972	568.0702
660.9781	807.0807	868.7505
894.9661	915.6286	952.0725
995.1642	1028.9765	1086.1282
1091.6264	1150.0733	1202.5658
1224.1506	1242.0894	1303.0181
1320.6602	1344.3335	1418.3596
1484.3931	1487.2429	1490.5685
1493.7247	1511.4619	1754.5320
3030.7985	3039.1287	3055.0613
3071.7911	3084.3390	3095.3352
3108.3972	3134.0408	3142.0404

i10

Cartesian coordinates

C	-1.415045	0.872675	0.000038
C	-1.596170	-0.621252	-0.000163
C	-0.147078	-1.171798	0.000161
C	2.213491	-0.014731	-0.000088
C	0.727353	0.055938	0.000038
C	-0.068773	1.190295	0.000064
H	-2.232412	1.581261	0.000074
H	-2.161312	-0.959507	0.875877
H	-2.160758	-0.959258	-0.876664
H	0.055335	-1.799502	0.876957
H	0.055629	-1.800027	-0.876180

H	2.586324	-0.555442	0.879018
H	2.664234	0.980041	-0.000228
H	2.586113	-0.555572	-0.879211
H	0.324183	2.201237	0.000062

1297.0873	1329.3661	1353.9044
1392.2377	1426.1497	1481.4934
1488.7854	1514.2302	1520.7551
3003.0357	3044.6094	3063.4319
3080.2532	3106.5300	3121.2812
3158.0762	3210.5503	3255.4746

Frequencies

79.5707	110.7371	229.5052
320.9575	452.9457	598.2127
627.3528	773.8764	799.3093
868.8719	921.7955	924.5335
974.5469	977.7390	1011.7547
1043.1426	1079.5310	1155.6115
1230.3554	1231.4623	1287.5510
1309.7957	1322.5033	1418.1158
1436.0152	1468.1915	1473.1395
1475.6607	1492.7584	1530.5831
3015.6575	3021.8662	3038.8340
3045.1900	3061.4540	3068.8736
3127.5158	3204.2376	3238.2534

i11

Cartesian coordinates

C	-1.421329	0.805937	0.104599
C	-1.427752	-0.701392	-0.222168
C	-0.022105	-1.189157	0.169637
C	2.222328	0.033361	-0.065823
C	0.848168	0.048262	0.013541
C	0.028127	1.168943	-0.010116
H	-1.784140	0.990447	1.126750
H	-2.065415	1.388765	-0.560768
H	-2.226213	-1.244300	0.287254
H	-1.570842	-0.834050	-1.298444
H	0.001179	-1.517499	1.215401
H	0.324094	-2.026005	-0.441146
H	2.783879	0.955748	-0.160471
H	2.778558	-0.896299	-0.040270
H	0.394281	2.187467	-0.066323

Frequencies

156.6998	224.8161	354.1803
461.7221	550.3668	602.5655
651.2247	712.4640	776.9635
827.9779	883.6794	902.2337
929.1258	942.2519	1014.4986
1046.7218	1052.2646	1145.3093
1196.8000	1245.4278	1272.3533

i12

Cartesian coordinates

C	-1.345450	0.832883	0.163226
C	-1.531424	-0.665427	0.186858
C	-0.176889	-1.157885	-0.211037
C	2.035884	-0.048904	0.398794
C	0.767537	-0.022934	-0.471822
C	-0.114455	1.176013	-0.200100
H	-2.138419	1.527361	0.414681
H	-1.847739	-1.027095	1.177176
H	-2.320901	-0.989599	-0.509053
H	0.089414	-2.201962	-0.315707
H	1.094021	-0.018410	-1.525232
H	1.771627	-0.027515	1.459356
H	2.672186	0.815140	0.185038
H	2.618683	-0.953925	0.207915
H	0.249905	2.193521	-0.289685

Frequencies

121.0804	213.3671	273.2390
312.1859	385.8439	508.4487
693.6558	744.8337	778.4845
868.1262	920.6853	924.4116
949.9451	988.3672	1008.3625
1040.6609	1072.9947	1103.0955
1135.7070	1138.7871	1288.2934
1297.7361	1313.1752	1332.9784
1392.1266	1410.8774	1463.1540
1493.4208	1497.2080	1708.0931
2963.6301	2988.3330	3003.0637
3039.7211	3116.9452	3124.7157
3198.3043	3224.7363	3227.6868

i13

Cartesian coordinates

C	-1.387984	0.795646	-0.071805
C	-1.453830	-0.687554	-0.248097
C	-0.098470	-1.178848	0.297890
C	2.127176	-0.082872	-0.209841

C	0.834595	-0.010278	0.076961	119.7845	132.0009	292.7179
C	0.011888	1.261825	0.167811	336.4880	458.6359	536.9615
H	0.120611	1.722064	1.163269	585.7098	735.6350	766.3563
H	-2.236550	1.459064	-0.176350	852.7636	870.9209	910.9852
H	-2.309618	-1.144432	0.259816	950.3286	977.4537	1005.9040
H	-1.551142	-0.951643	-1.313238	1029.8507	1106.4345	1116.3103
H	-0.189115	-1.367002	1.374463	1148.1663	1195.2313	1228.6932
H	0.259646	-2.097004	-0.170937	1284.8842	1288.1170	1325.1715
H	2.720273	0.810478	-0.377029	1341.0723	1390.7056	1464.5697
H	2.636430	-1.037895	-0.286166	1484.5154	1505.2048	1712.1427
H	0.349216	2.018860	-0.551342	2912.0116	3035.2865	3062.7404

3094.7661	3126.2291	3152.1371
3197.6399	3223.8278	3260.2217

Frequencies

114.3180	178.6247	333.1038
379.1203	421.9321	623.8373
659.6981	732.1850	812.5915
852.6904	913.7651	927.2351
932.9705	938.7245	990.1970
1007.5591	1053.0783	1129.0701
1168.6247	1219.2614	1263.9452
1284.8203	1304.5372	1343.6957
1360.7292	1452.8918	1466.1308
1479.4152	1496.8104	1763.7632
2973.1444	2979.2592	3036.6464
3044.9247	3068.9787	3123.0410
3150.7656	3227.3285	3236.0721

i14

Cartesian coordinates

C	1.546214	-0.609854	-0.018109
C	1.318599	0.875944	-0.154510
C	0.051707	1.203414	0.066536
C	-2.153003	-0.010293	-0.233821
C	-0.801279	-0.006396	0.387966
C	0.113762	-1.178141	-0.049916
H	2.048049	-0.828636	0.933182
H	2.178878	-1.020996	-0.809575
H	2.115655	1.579329	-0.366215
H	-0.348199	2.211402	0.063328
H	-2.684058	-0.943623	-0.383047
H	-2.686553	0.916941	-0.408483
H	-0.143421	-1.449602	-1.078137
H	-0.012091	-2.066378	0.572314
H	-0.924260	-0.046485	1.487753

Frequencies

i15

Cartesian coordinates

C	-1.318536	0.875992	-0.154647
C	-1.546238	-0.609780	-0.018166
C	-0.113804	-1.178162	-0.049564
C	2.152937	-0.010376	-0.233976
C	0.801297	-0.006401	0.388010
C	-0.051654	1.203440	0.066463
H	-2.115541	1.579394	-0.366487
H	-2.048331	-0.828464	0.933009
H	-2.178721	-1.020950	-0.809763
H	0.011864	-2.066178	0.573020
H	0.143494	-1.450058	-1.077643
H	2.687612	0.916691	-0.406102
H	2.682876	-0.943932	-0.385719
H	0.924438	-0.046190	1.487792
H	0.348302	2.211406	0.063173

Frequencies

119.9794	132.7230	292.5866
336.7146	458.7335	537.0942
585.7519	735.6566	766.4120
852.6600	870.9442	910.9840
950.3780	977.4576	1005.9466
1029.7144	1106.4189	1116.3423
1148.1661	1195.3502	1228.7065
1284.9746	1287.9683	1325.1923
1341.0957	1390.6829	1464.5684
1484.4736	1505.1848	1712.1490
2912.0048	3035.3003	3062.7629
3094.7659	3126.2280	3152.1299
3197.6509	3223.8385	3260.2161

i16

Cartesian coordinates

C	-1.454619	0.142295	0.322887
C	-0.576154	1.248517	-0.174384
C	0.774446	0.749783	-0.435569
C	1.428551	-0.055243	0.694785
C	0.697517	-0.767457	-0.397838
C	-0.752285	-1.154442	-0.150495
H	-2.480893	0.216320	-0.050549
H	-1.534227	0.161073	1.420813
H	-0.849021	2.295557	-0.161692
H	1.433437	1.271952	-1.118909
H	0.982298	0.001970	1.681991
H	2.511113	-0.107729	0.687850
H	1.277616	-1.356991	-1.097782
H	-0.851952	-1.967614	0.573633
H	-1.193108	-1.495257	-1.091669

Frequencies

184.0464	269.1071	333.9701
443.2658	631.6640	704.7181
760.8951	799.0129	836.2046
886.0846	919.7847	945.5157
977.4763	992.1040	1028.0051
1043.0758	1067.6350	1101.8337
1108.6305	1174.3888	1205.3466
1239.8248	1297.2359	1311.1624
1352.5027	1372.5532	1394.8514
1476.8967	1493.0519	1506.6637
2985.4454	3060.3074	3073.4392
3107.8135	3137.6304	3188.3379
3196.6022	3221.7668	3230.3292

i17

Cartesian coordinates

C	1.426557	0.000004	0.319291
C	0.698955	-1.240077	-0.094466
C	-0.706672	-0.756471	-0.417189
C	-1.421027	-0.000011	0.669745
C	-0.706690	0.756477	-0.417204
C	0.698938	1.240081	-0.094456
H	2.410274	0.000012	0.770929
H	1.155087	-1.693753	-0.988709
H	0.712990	-2.014318	0.683049
H	-1.299871	1.310538	-1.134425

H	-1.299865	-1.310546	-1.134389
H	-2.504312	-0.000052	0.651076
H	-0.982705	0.000019	1.663741
H	1.155080	1.693785	-0.988678
H	0.712958	2.014296	0.683085

Frequencies

206.7791	306.6391	377.5426
410.1058	637.0973	734.3797
774.5162	824.5263	875.3523
884.5643	911.3458	932.9977
991.3202	1024.2446	1031.9774
1052.4250	1087.7936	1100.2428
1103.1339	1181.9219	1183.8779
1220.1189	1301.6311	1312.1054
1337.5880	1384.7555	1400.8378
1481.1453	1484.6672	1497.3530
2980.7348	2983.7311	3041.4531
3042.4028	3134.0659	3192.3998
3200.8561	3227.1714	3229.1234

i18

Cartesian coordinates

C	-1.454609	-0.142296	0.322925
C	-0.752301	1.154438	-0.150527
C	0.697518	0.767469	-0.397829
C	1.428550	0.055244	0.694790
C	0.774451	-0.749783	-0.435563
C	-0.576150	-1.248519	-0.174378
H	-2.480918	-0.216326	-0.050423
H	-1.534113	-0.161054	1.420870
H	-1.193118	1.495145	-1.091747
H	-0.852017	1.967667	0.573532
H	1.433430	-1.271942	-1.118922
H	1.277636	1.356987	-1.097772
H	2.511111	0.107732	0.687850
H	0.982306	-0.001973	1.682002
H	-0.849068	-2.295550	-0.161893

Frequencies

184.1010	269.0381	333.9451
443.2369	631.6516	704.6924
760.8939	799.0060	836.2091
886.0779	919.7762	945.5131
977.4643	992.1006	1028.0015
1043.0877	1067.6283	1101.8285
1108.6237	1174.3910	1205.3469

1239.8171	1297.2388	1311.1584
1352.4934	1372.5472	1394.8472
1476.8901	1493.0476	1506.6516
2985.3465	3060.2875	3073.4171
3107.8015	3137.6219	3188.3349
3196.6005	3221.7521	3230.3206

i19

Cartesian coordinates

C	0.537721	1.269567	-0.072462
C	1.358831	0.065376	0.439521
C	0.765636	-1.179834	-0.273148
C	-1.516178	-0.241950	0.579246
C	-0.662438	-0.783948	-0.492710
C	-0.820258	0.685504	-0.432266
H	0.991429	1.686788	-0.977383
H	0.482975	2.073453	0.667124
H	2.428909	0.179538	0.256960
H	1.225584	-0.042438	1.519344
H	1.256342	-1.335159	-1.239619
H	0.883801	-2.092317	0.315779
H	-1.183839	-0.285869	1.614743
H	-2.592776	-0.306956	0.456796
H	-1.472311	1.234664	-1.102829

Frequencies

231.0932	295.8665	374.7877
587.7283	627.4955	737.9793
813.5092	858.9471	892.4494
899.4128	925.7692	954.4308
981.2939	1000.1135	1032.0453
1064.0860	1110.8109	1139.0632
1181.6185	1208.4006	1258.2255
1280.3599	1323.2966	1333.7623
1354.0540	1387.0333	1486.6342
1495.1729	1500.1149	1522.6038
3055.4314	3057.1579	3070.3058
3100.0356	3108.6749	3112.7986
3128.6754	3176.7257	3196.3136

i20

Cartesian coordinates

C	-0.618020	-1.228052	-0.192759
C	-1.352192	-0.000229	0.378941
C	-0.618514	1.227903	-0.192581
C	1.425857	-0.000039	0.740745

C	0.825019	0.766271	-0.358384
C	0.825275	-0.765691	-0.358865
H	-1.020355	-1.495083	-1.175891
H	-0.716365	-2.104253	0.453932
H	-2.416118	-0.000542	0.134640
H	-1.272184	-0.000386	1.469750
H	-1.020668	1.494384	-1.175959
H	-0.717662	2.104395	0.453551
H	1.299275	-0.000708	1.815793
H	1.469685	1.316224	-1.038646
H	1.469843	-1.315018	-1.039745

Frequencies

234.4348	285.0007	375.9223
588.1507	630.0709	688.4609
817.9038	834.2980	838.0297
894.3708	903.0501	939.4623
984.6222	993.9080	1016.6022
1061.6683	1102.0199	1106.3957
1170.0855	1189.9409	1192.7755
1261.4180	1298.8105	1317.1695
1321.1823	1350.1152	1407.9882
1487.3203	1491.9252	1514.4595
3054.4130	3055.6557	3068.7077
3102.3332	3102.4899	3124.6116
3149.6436	3158.2952	3212.8751

i21

Cartesian coordinates

C	1.265642	0.673368	0.199238
C	0.000691	1.351477	-0.337199
C	-1.264965	0.674639	0.199199
C	-0.000744	-1.472434	-0.093628
C	-1.212898	-0.811239	0.004349
C	1.212072	-0.812455	0.004325
H	1.376355	0.896975	1.271365
H	2.154245	1.089402	-0.285844
H	0.001186	2.415202	-0.084451
H	0.000674	1.277591	-1.430108
H	-1.375491	0.898397	1.271314
H	-2.153112	1.091590	-0.285930
H	-0.001247	-2.548973	-0.237389
H	-2.141831	-1.369085	-0.038274
H	2.140434	-1.371236	-0.038387

Frequencies

187.3978	262.5621	435.9803
506.0276	516.4841	608.6322
697.4319	735.3708	848.5618
869.6494	901.7645	968.8429
979.4123	1019.6825	1068.2281
1069.4566	1147.2472	1156.3489
1167.6294	1228.8921	1281.2459
1352.3755	1358.5725	1385.3706
1405.3157	1446.3964	1484.6163
1484.7396	1499.7918	1526.3413
2998.6018	2999.2056	3050.9066
3079.5800	3083.5889	3101.4916
3174.1305	3194.9224	3206.1548

i22

Cartesian coordinates

C	-1.418746	0.374563	-0.192582
C	-0.978811	-1.022857	0.271043
C	0.399217	-1.346398	-0.193722
C	1.480355	-0.334895	-0.018192
C	0.960592	1.073889	0.088005
C	-0.326818	1.392358	-0.002552
H	-2.315578	0.683574	0.353814
H	-1.702148	0.341671	-1.252102
H	-1.008091	-1.035141	1.374470
H	-1.692881	-1.780008	-0.062989
H	0.666238	-2.367155	-0.442764
H	2.080301	-0.561750	0.881447
H	2.198456	-0.395175	-0.847411
H	1.700046	1.857212	0.229725
H	-0.621077	2.436815	0.053810

Frequencies

136.7393	210.7455	387.6386
392.2787	501.4251	544.2156
669.5546	755.9314	842.6229
898.4464	910.0809	934.0986
987.7728	1007.1774	1038.4710
1061.0827	1124.1739	1174.4948
1195.0368	1208.2970	1279.3835
1337.8687	1351.1153	1384.5950
1405.3800	1431.7657	1457.2965
1474.4669	1488.7794	1752.2125
2945.7881	2956.6884	3028.3109
3031.4873	3078.0085	3092.3067
3158.4744	3183.1988	3193.7711

Transition states

i3 – i4

Cartesian coordinates

C	1.048409	1.274643	-0.143840
C	1.297557	-0.033842	0.538769
C	1.843556	-1.209397	-0.204308
C	-2.640502	-0.502273	0.042539
C	-1.457157	0.331821	-0.147696
C	-0.269319	0.673645	-0.084607
H	1.184635	2.174744	0.454417
H	1.472656	1.382824	-1.142588
H	1.321724	-0.030657	1.621566
H	1.523127	-2.153188	0.244005
H	2.942528	-1.203641	-0.212944
H	1.507063	-1.203062	-1.245247
H	-3.405638	0.029694	0.614612
H	-2.398533	-1.427790	0.580177
H	-3.082830	-0.776499	-0.919144

Frequencies

-699.1291	77.8162	93.7249
145.2041	164.4424	229.7618
367.7382	386.9297	425.4444
682.4923	712.5842	884.7336
927.1618	1023.7610	1032.9377
1049.8760	1067.2749	1126.5157
1188.1644	1205.0107	1219.6997
1377.2602	1412.2715	1423.9545
1471.9859	1479.1346	1480.3625
1487.1743	1496.3749	2088.6927
3002.7644	3012.1936	3077.4842
3079.6561	3085.0179	3110.2455
3117.2119	3148.5136	3202.1612

i1 – i2

Cartesian coordinates

C	-0.893893	1.366048	0.231730
C	-1.240916	0.086594	-0.460786
C	-2.134585	-0.903542	0.264085
C	2.808935	-0.198450	0.149725
C	1.390964	-0.317877	-0.173197
C	0.192544	-0.025433	-0.263670
H	-0.713842	2.266952	-0.337731
H	-1.001687	1.433067	1.306413
H	-1.519620	0.215608	-1.507820

H	-2.083402	-1.887309	-0.207567
H	-3.171581	-0.557808	0.246012
H	-1.822305	-1.009200	1.305924
H	3.027274	0.760445	0.635935
H	3.422033	-0.267201	-0.753021
H	3.124832	-0.998588	0.824534

1005.8134	1051.3065	1059.4341
1063.0156	1137.5034	1201.0982
1308.0401	1313.6654	1418.1983
1421.0855	1479.4967	1485.0734
1487.7117	1490.8256	1648.8790
2383.0284	3035.3686	3050.6335
3094.4149	3120.6265	3127.1521
3130.9034	3164.5430	3182.8225

Frequencies

-695.9988	107.2175	108.0779
127.8839	218.0791	281.1172
366.3206	376.7097	435.8744
640.0211	689.4435	720.1451
874.4506	928.8520	1027.7771
1031.5309	1057.6249	1117.4000
1168.4390	1206.6463	1240.4102
1372.2354	1409.4239	1413.8481
1449.8150	1478.8762	1482.5776
1490.0220	1503.5961	2087.0975
3020.0545	3051.3073	3091.3532
3103.3066	3116.1959	3131.7746
3138.5196	3168.7912	3288.1728

i5 - p3

Cartesian coordinates

C	0.703559	0.512946	-0.145947
C	1.648135	-0.424659	0.099911
C	3.112278	-0.190089	-0.053382
C	-3.314403	-0.232338	0.016725
C	-1.882552	0.032171	-0.037007
C	-0.700263	0.247062	-0.073598
H	0.994190	1.444029	-0.626636
H	0.862538	1.594907	1.464595
H	1.330794	-1.388438	0.488307
H	3.618176	-0.266134	0.915677
H	3.319779	0.797723	-0.470283
H	3.563263	-0.943915	-0.706626
H	-3.853900	0.402393	-0.690453
H	-3.709038	-0.035887	1.016978
H	-3.526325	-1.275246	-0.231775

Frequencies

-834.3215	77.0959	107.4750
116.8883	159.0483	250.5067
295.5186	341.4073	393.6144
424.4582	498.2332	517.1030
810.4058	826.3433	948.0452

i5 - p5

Cartesian coordinates

C	0.733446	0.846674	0.006270
C	1.668929	-0.262127	-0.395463
C	2.748547	-0.620257	0.305905
C	-3.200807	-0.386617	0.039188
C	-1.810486	0.054350	0.030189
C	-0.667215	0.419864	0.025586
H	0.838874	1.676753	-0.704163
H	1.017669	1.237379	0.988298
H	1.444640	-0.756495	-1.336789
H	3.379947	-1.441214	-0.012947
H	2.959067	-0.185165	1.277940
H	4.240407	0.673725	-0.405518
H	-3.836742	0.316130	-0.504779
H	-3.578758	-0.465527	1.061485
H	-3.299595	-1.366910	-0.433576

Frequencies

-501.0733	52.1236	64.2258
108.4342	201.8422	211.8359
288.5688	338.5075	397.4075
414.5099	499.9457	655.7558
801.9088	917.0958	945.6182
977.2506	1027.4331	1056.0403
1061.6970	1136.3239	1172.7079
1250.8480	1317.2276	1334.2232
1420.9038	1454.3342	1468.3571
1484.3147	1490.6216	1679.6749
2399.3597	3034.5068	3051.8666
3088.4299	3122.4105	3126.4619
3153.7836	3181.0275	3247.8563

i5 - i6

Cartesian coordinates

C	0.659087	-0.617521	0.098288
C	1.702713	0.444424	0.219560
C	3.103506	0.167426	-0.219488

C	-3.321217	0.252725	-0.085012
C	-1.898612	-0.058955	-0.024601
C	-0.721269	-0.322782	0.014599
H	1.002325	-1.598165	-0.215804
H	1.340678	1.461263	0.311022
H	3.814046	0.860355	0.235791
H	3.201931	0.252467	-1.311175
H	3.408948	-0.849594	0.048133
H	-3.921736	-0.638988	0.112870
H	-3.603169	0.639958	-1.068241
H	-3.585991	1.006460	0.661520
H	1.197718	-0.325661	1.205809

Frequencies

-1923.2478	44.2974	91.1638
108.9628	177.4408	221.0054
286.7013	349.9913	410.0486
508.9369	665.6040	738.3316
810.4769	929.0596	1032.5831
1048.9725	1052.4473	1107.9229
1155.3771	1225.6355	1235.2765
1311.1415	1408.8634	1419.2881
1441.4474	1481.7483	1483.8793
1487.3265	1496.1630	2213.4835
2331.9864	2997.8133	3045.4068
3072.3139	3113.3171	3119.0266
3122.5915	3180.1516	3210.6045

ib - p7

Cartesian coordinates

C	0.647392	-1.019878	-0.336120
C	1.667296	-0.797556	0.526775
C	-3.097702	0.537746	0.106600
C	-1.759132	-0.015654	-0.049906
C	-0.652057	-0.477056	-0.172014
H	0.824373	-1.598357	-1.238336
H	2.614719	-1.304853	0.395452
H	1.489690	-0.316007	1.480349
H	-3.617141	0.578314	-0.854035
H	-3.054878	1.551562	0.512819
H	-3.694748	-0.073781	0.788620
C	2.711594	1.263627	-0.155431
H	3.064979	0.974458	-1.136715
H	3.444484	1.360471	0.636791
H	1.824185	1.880824	-0.104369

Frequencies

-369.9255	35.0273	59.8828
89.7500	146.2265	174.0204
260.1735	329.0223	413.9816
443.5247	468.2216	549.9982
724.0590	738.8529	749.8413
920.8985	971.2473	1052.2375
1056.3302	1058.0112	1202.7658
1294.6324	1414.2065	1417.0702
1420.6326	1438.6166	1483.3268
1484.0048	1588.5974	2343.3372
3044.0490	3101.9627	3114.4336
3119.8994	3163.3881	3171.4438
3263.0471	3271.2737	3280.0714

ib - p3

Cartesian coordinates

C	0.675835	-0.546485	0.134781
C	1.637695	0.361530	-0.123259
C	3.101775	0.040869	-0.141082
C	-3.332339	0.190046	-0.076742
C	-1.900592	-0.068507	-0.004121
C	-0.715908	-0.276393	0.053346
H	0.960556	-1.548369	0.448685
H	1.339268	1.339778	-0.490542
H	3.464464	-0.001787	-1.173713
H	3.303782	-0.923299	0.330382
H	3.684006	0.806799	0.375798
H	-3.640992	0.886209	0.707502
H	-3.899992	-0.735296	0.047179
H	-3.599985	0.628363	-1.041556
H	1.590096	1.341239	1.738729

Frequencies

-560.3207	65.2448	105.2136
106.4656	180.5638	269.1320
290.9406	322.3894	371.5233
396.6781	469.1946	520.6714
811.8631	825.8669	946.6847
987.4358	1051.4657	1057.9007
1061.6476	1130.6011	1209.5329
1306.8824	1325.4425	1415.2360
1418.4414	1483.1700	1485.5487
1486.2621	1494.1713	1668.8359
2365.5084	3044.9349	3052.6314
3111.5858	3123.3524	3128.9095

3136.7062 3161.7561 3182.4835

i5 – i8

Cartesian coordinates

C 0.727441 0.744113 -0.105872
C 1.655437 -0.437070 -0.186551
C 3.091269 -0.265824 0.161918
C -3.250183 -0.323468 0.076141
C -1.843545 0.058135 0.011976
C -0.686531 0.374103 -0.035951
H 0.886582 1.400584 -0.975287
H 0.985419 1.351582 0.770738
H 1.389456 -1.259551 -0.840095
H 2.203034 -0.846349 0.915774
H 3.426630 0.685581 0.555917
H 3.823216 -0.953925 -0.239099
H -3.769202 -0.060767 -0.849045
H -3.753720 0.183592 0.903095
H -3.354742 -1.400675 0.228044

Frequencies

-1916.6065 67.9055 79.8758
104.8935 209.3025 283.1195
346.9497 372.3873 400.4021
506.9519 693.0313 739.1469
775.7106 897.4126 939.2238
1061.9377 1064.2484 1115.5800
1172.3450 1175.2616 1228.1515
1292.2863 1308.2814 1409.1908
1426.2331 1436.9551 1464.7713
1486.2406 1492.2836 2249.8611
2401.3016 2987.5744 3042.0067
3049.3035 3119.3545 3123.7146
3154.1651 3199.2118 3272.1142

i8 – p5

Cartesian coordinates

C -0.770666 0.816887 0.032544
C -1.737079 -0.315080 0.308964
C -2.993676 -0.338997 -0.159675
C 3.183212 -0.340261 -0.039739
C 1.785747 0.075263 -0.010657
C 0.633165 0.410185 0.000792
H -0.897519 1.570032 0.820378
H -1.036540 1.306072 -0.909545
H -1.440043 -1.010102 1.089534

H -3.338132 0.384296 -0.892241
H -3.691815 -1.109671 0.144058
H 3.609560 -0.354911 0.966327
H 3.778995 0.343278 -0.649755
H 3.279980 -1.342463 -0.464544
H -0.868700 -1.634505 -0.897587

Frequencies

-771.1404 61.1491 83.6349
108.6926 210.9069 291.9399
367.0622 396.6837 403.2380
412.9232 502.9463 603.8353
789.5000 921.2714 930.0657
944.3487 1047.0829 1058.6435
1063.2494 1137.0786 1177.8222
1250.9848 1311.4292 1334.1370
1423.7724 1455.5945 1473.3679
1484.9963 1490.2520 1656.2243
2401.0510 3036.7998 3051.3805
3090.4865 3122.4741 3125.5956
3153.1659 3181.6508 3250.8491

i4 – i7

Cartesian coordinates

C -0.903509 -1.134169 0.147503
C -1.974552 -0.159040 -0.272322
C -1.924927 1.263983 0.156020
C 2.908317 0.424509 -0.069567
C 1.561235 -0.129895 0.008522
C 0.454776 -0.591748 0.070658
H -0.963013 -2.035805 -0.469783
H -1.086514 -1.454015 1.185576
H -2.949100 -0.563904 -0.519858
H -2.842942 1.833998 0.206616
H -1.041701 1.624501 0.666878
H 2.888146 1.436519 -0.481554
H 3.545325 -0.188701 -0.711792
H 3.369472 0.471156 0.920110
H -1.647705 0.834406 -1.041071

Frequencies

-1923.5998 50.8962 90.5074
120.6945 211.6436 268.3454
364.2132 389.3100 403.8913
558.1691 680.9987 740.5911
774.1830 903.3108 941.2407

1056.0304	1059.5341	1062.3945
1155.6500	1187.5083	1258.2670
1266.2559	1354.7301	1373.8283
1420.2841	1436.9904	1472.7118
1486.3203	1486.8431	2247.7511
2394.0731	2978.5722	3046.7453
3074.4535	3119.6023	3119.8876
3158.5357	3189.6586	3279.5952

i4 – p4

Cartesian coordinates

C	-0.907747	-1.156816	0.064754
C	-2.013962	-0.146501	-0.095888
C	-1.853879	1.175964	-0.192481
C	2.898545	0.415415	-0.027793
C	1.551471	-0.143296	0.002677
C	0.444456	-0.606463	0.029434
H	-1.010414	-1.920979	-0.715534
H	-1.056819	-1.686940	1.014220
H	-3.016270	-0.567083	-0.091264
H	-2.705640	1.829456	-0.339143
H	-0.864876	1.617807	-0.250579
H	-1.831871	1.805749	1.805501
H	3.096897	0.900247	-0.986772
H	3.647247	-0.367247	0.117157
H	3.028442	1.159171	0.762194

Frequencies

-508.0979	93.3225	107.6555
113.4363	204.4703	224.1620
286.4884	327.0945	397.4810
424.6579	577.4387	624.9624
773.5848	922.5294	958.4913
978.8930	1016.6760	1061.7473
1065.7985	1077.9815	1177.7145
1245.9314	1327.0350	1374.9109
1425.2465	1436.5731	1473.1694
1486.3406	1495.2085	1680.5136
2399.9208	3032.1633	3049.5496
3059.5001	3121.5680	3123.7302
3161.2066	3179.3129	3258.0792

i4 – p2

Cartesian coordinates

C	-0.866812	-1.043431	-0.104349
C	-1.977852	-0.267583	-0.139944

C	-2.010082	1.207461	0.067004
C	2.955841	0.410738	0.006813
C	1.591130	-0.098543	-0.031800
C	0.465745	-0.521602	-0.053476
H	-0.958231	-2.097641	-0.346331
H	-0.919963	-1.673953	1.727295
H	-2.932039	-0.769329	-0.272945
H	-2.533307	1.702704	-0.757269
H	-1.005219	1.625062	0.145270
H	-2.559152	1.451802	0.983740
H	3.372651	0.490542	-1.000474
H	3.599825	-0.253061	0.588949
H	2.987619	1.401631	0.466279

Frequencies

-855.1074	92.8434	101.2195
121.1859	167.2184	260.6799
275.3983	354.4520	416.7374
421.2538	558.6212	606.5063
775.3051	793.2318	937.7504
1010.4294	1055.3104	1056.2576
1061.0517	1104.7804	1175.9503
1266.9727	1400.3717	1420.7359
1440.8894	1483.4794	1485.9684
1488.1302	1489.3533	1632.1971
2379.8420	3033.7151	3050.9686
3090.1801	3121.5852	3126.4930
3141.2900	3174.1830	3192.2678

i9 – i10

Cartesian coordinates

C	-1.390448	-0.838444	-0.010626
C	-1.540846	0.672165	0.110920
C	-0.096832	1.173159	-0.103665
C	2.213048	-0.051767	0.082950
C	0.735886	-0.090449	-0.071101
C	-0.056527	-1.275387	-0.192754
H	-2.247562	-1.480864	-0.201015
H	-0.805141	-1.549198	0.888959
H	-2.240360	1.037675	-0.645735
H	-1.946018	0.967750	1.082644
H	0.012027	1.701680	-1.060278
H	0.230977	1.877864	0.668909
H	2.684242	0.514694	-0.731117
H	2.627069	-1.060118	0.088786
H	2.499078	0.454853	1.014505

Frequencies

-1208.3698	78.1449	96.2399
235.2373	336.3744	482.0818
592.4201	647.7504	748.9978
813.7492	839.5518	910.6587
940.1293	954.9539	1011.4699
1035.0114	1131.0988	1164.9968
1220.8409	1240.4153	1250.3721
1281.9127	1315.7668	1380.0633
1391.6214	1411.1356	1468.0505
1474.6117	1485.3547	1495.0008
2133.9609	3010.8856	3022.2563
3056.0451	3062.9577	3071.7803
3111.2918	3150.5992	3168.0361

i7 – i9**Cartesian coordinates**

C	1.405268	-0.958093	0.114021
C	1.636385	0.540154	-0.242207
C	0.447035	1.348178	0.193954
C	-2.418346	0.076384	-0.054548
C	-1.021778	-0.365114	-0.025119
C	-0.054320	-1.135069	-0.005182
H	1.715689	-1.169243	1.142987
H	1.981307	-1.619276	-0.537187
H	2.565799	0.901202	0.213425
H	1.752593	0.624213	-1.325879
H	0.306367	1.518072	1.257759
H	0.074706	2.132754	-0.456491
H	-2.669820	0.624402	0.857220
H	-3.086211	-0.785275	-0.130931
H	-2.605892	0.734519	-0.906416

Frequencies

-594.8183	82.2003	150.5413
207.5067	217.9262	386.1341
472.1948	513.3181	595.6353
755.8996	794.1820	850.5619
890.4803	928.7773	1014.6835
1055.2641	1058.5076	1105.6810
1149.1226	1209.9591	1235.5304
1326.9078	1351.2746	1407.5337
1466.5829	1477.7099	1483.1000
1485.8803	1503.3257	2091.7842
3043.9737	3050.0529	3058.8641

3095.2734	3113.2830	3121.3001
3128.2259	3135.3728	3234.5278

i9 – i11**Cartesian coordinates**

C	1.222683	-1.073356	0.095324
C	1.590315	0.431192	-0.128997
C	0.304110	1.288259	0.096693
C	-2.221950	-0.040262	-0.015468
C	-0.755236	0.235703	-0.032638
C	-0.276691	-0.990751	-0.051933
H	1.499484	-1.421412	1.095859
H	1.709642	-1.729392	-0.628939
H	2.410169	0.745265	0.520326
H	1.921577	0.558263	-1.162127
H	0.285955	1.744961	1.093124
H	0.223665	2.100798	-0.630491
H	-2.781836	0.143574	0.901866
H	-1.653728	-1.348876	-0.035358
H	-2.794311	0.102107	-0.932139

Frequencies

-2332.9522	120.1024	164.2551
371.9880	410.7193	463.9770
601.0801	695.0335	784.5478
868.7876	893.9307	909.8149
973.8135	987.3103	999.0119
1025.7364	1060.2253	1078.8298
1152.6102	1196.2816	1211.7452
1258.8682	1289.4141	1328.4435
1361.7904	1445.0438	1478.3607
1494.5108	1509.8872	1772.4832
1830.4717	3046.7797	3062.3663
3078.5044	3087.9399	3093.9287
3111.9630	3134.7840	3179.9119

i11 – p12**Cartesian coordinates**

C	-1.306247	0.801643	-0.123059
C	-1.439486	-0.699305	-0.210179
C	-0.025320	-1.199364	0.153979
C	2.200455	0.040332	-0.035559
C	0.867658	0.020880	0.015368
C	-0.017773	1.179885	-0.054261
H	-1.772577	0.998303	1.999841
H	-2.143728	1.475834	-0.254355

H	-2.213871	-1.094796	0.450383
H	-1.714152	-0.981701	-1.233344
H	-0.007282	-1.532647	1.196559
H	0.309886	-2.033210	-0.464860
H	2.744160	0.974964	-0.118701
H	2.782703	-0.873704	0.002627
H	0.339145	2.202528	-0.055885

	892.7419	917.3191	961.6873
	969.6447	1009.4396	1036.5281
	1054.4007	1123.9264	1153.4401
	1199.7426	1269.7519	1342.5791
	1396.7456	1424.5357	1427.0444
	1485.7363	1494.6964	1572.6440
	1685.3863	3036.3857	3048.5030
	3090.5899	3094.9873	3131.5507
	3217.2241	3232.1059	3256.0551

Frequencies

-507.4741	92.9921	192.8747
296.3680	349.2833	365.1531
504.3819	640.4791	684.4081
762.2027	822.7905	836.6024
880.9201	907.8986	924.9064
966.6050	978.1391	1019.5940
1032.1344	1111.0916	1176.3288
1242.1930	1275.1958	1296.8553
1343.0418	1372.1898	1454.2859
1467.0914	1494.1545	1615.8517
1722.9218	3046.1949	3061.9171
3108.5858	3125.9911	3155.5005
3212.9662	3234.8701	3244.2032

i10 – p10

Cartesian coordinates

C	1.438067	0.808793	-0.076078
C	1.551750	-0.536604	-0.117302
C	0.173079	-1.134855	-0.126882
C	-2.218147	-0.040819	0.061466
C	-0.731345	0.062305	-0.014557
C	0.028277	1.173488	0.005027
H	2.257683	1.515464	-0.090307
H	2.461687	-1.102601	-0.257367
H	2.005970	-0.844698	2.013104
H	-0.011336	-1.677352	-1.063621
H	0.013505	-1.850921	0.686641
H	-2.626774	-0.542309	-0.822139
H	-2.679059	0.946068	0.135004
H	-2.528131	-0.625883	0.933744
H	-0.343634	2.188380	0.074896

Frequencies

-443.3796	139.7059	190.1677
254.2093	287.8383	332.1658
386.6405	529.8779	623.9880
742.6135	827.6357	863.9938

i10 – p11

Cartesian coordinates

C	-1.437682	-0.832619	0.038087
C	-1.536239	0.655587	-0.114078
C	-0.098403	1.086087	-0.130239
C	2.195317	-0.037708	-0.057115
C	0.702715	-0.000718	-0.052523
C	-0.145411	-1.191179	0.067610
H	-2.292511	-1.491417	0.110157
H	-2.046230	0.929411	-1.046708
H	-2.104471	1.116846	0.701403
H	0.227443	2.104594	-0.293443
H	0.136765	1.631008	2.016419
H	2.618059	0.960301	-0.183839
H	2.567633	-0.675634	-0.864722
H	2.574108	-0.451994	0.882833
H	0.237416	-2.199815	0.167449

Frequencies

-376.9415	152.4716	197.6598
225.8240	271.7150	331.4853
376.0764	586.2397	624.0511
717.4059	806.0551	824.3442
923.1790	931.5820	949.0408
975.6547	986.1009	1024.4208
1068.5368	1103.3977	1137.7486
1225.9902	1261.6294	1314.2882
1397.5112	1422.1075	1427.5302
1487.6985	1495.7400	1591.0842
1684.2521	3041.5373	3050.1953
3088.1294	3102.5606	3136.0832
3211.7609	3237.3431	3243.8398

i2 – i3

Cartesian coordinates

C	0.941054	1.322845	-0.241132
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C	1.249448	0.030298	0.497592
C	1.996118	-1.082661	-0.196921
C	-2.777876	-0.360855	-0.050631
C	-1.379921	0.021396	0.027510
C	-0.153655	0.353947	0.088320
H	0.977497	2.255358	0.313254
H	1.249900	1.393621	-1.280478
H	1.460292	0.141034	1.558873
H	1.768116	-2.049855	0.258698
H	3.077674	-0.924750	-0.140869
H	1.712691	-1.135500	-1.251632
H	-2.914671	-1.448800	0.012877
H	-3.239512	-0.030440	-0.989869
H	-3.342994	0.089511	0.770719

Frequencies

-250.3310	30.0522	121.6512
191.4034	253.4147	338.1722
369.6877	451.5674	613.2516
731.0512	846.2867	887.8868
930.8552	997.3567	1021.5745
1046.0806	1051.9542	1078.4027
1125.1641	1177.7311	1207.3014
1372.2972	1411.2184	1420.2758
1463.2117	1464.9106	1479.5410
1493.1451	1503.1206	1953.4263
2993.9046	3036.5008	3039.8705
3096.9631	3108.7653	3113.5480
3116.8006	3139.5091	3205.9222

$i3 - p6$

Cartesian coordinates

C	0.976121	-1.332431	0.176722
C	1.199870	0.009848	-0.502025
C	1.907569	1.129286	0.223391
C	-2.666275	0.206147	0.124373
C	-1.397579	-0.133757	0.039707
C	-0.152516	-0.410849	-0.073312
H	1.036968	-2.233377	-0.424907
H	1.313351	-1.441202	1.203400
H	1.378358	-0.037450	-1.573453
H	1.593364	2.101381	-0.163804
H	2.990961	1.043795	0.101292
H	1.678558	1.102433	1.291803
H	-3.379213	-0.114432	-0.627510
H	-2.757371	2.094788	-0.760652

H	-3.058122	0.674599	1.020687
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Frequencies

-498.1264	110.9098	157.7737
203.3144	220.0018	291.9629
334.3670	376.0221	432.5511
576.7401	655.5658	700.3623
813.9454	891.0421	910.4444
954.1900	979.4000	1034.5131
1050.1062	1082.3470	1125.1270
1135.2300	1182.8452	1324.8218
1396.1939	1421.6465	1464.4285
1493.9417	1499.8662	1539.0065
2104.3795	3047.1170	3121.9613
3126.8881	3129.6315	3152.0614
3155.3038	3216.5369	3237.1685

$i7 - i8$

Cartesian coordinates

C	0.768475	-0.875371	-0.146581
C	-3.139281	0.424118	0.012978
C	-1.757901	-0.041432	-0.047555
C	-0.621774	-0.427245	-0.097646
H	0.835231	-1.871182	0.301102
H	1.063363	-0.998990	-1.193597
H	-3.763866	-0.276909	0.572384
H	-3.562048	0.528224	-0.989492
H	-3.200625	1.397245	0.506731
C	1.760204	0.087770	0.562481
C	2.806688	0.641815	-0.335432
H	2.232530	-0.423582	1.408373
H	1.183902	0.909457	1.014020
H	2.595579	0.817010	-1.384653
H	3.717475	1.060801	0.075663

Frequencies

-111.7367	89.7588	117.7146
183.4684	199.3957	307.6351
377.4459	394.9795	501.8228
529.8643	707.2031	843.6421
901.3377	957.3283	1057.5509
1062.9183	1079.1923	1116.2104
1172.4294	1214.0303	1253.9210
1345.0714	1376.1128	1422.8678
1470.0369	1475.7034	1487.7734
1492.5474	1493.4632	2395.7112

2989.1715	3049.8843	3054.0023
3061.8774	3094.8948	3119.9126
3122.8957	3149.8249	3256.7070

i11 – i18

Cartesian coordinates

C	-1.434695	0.789943	0.076236
C	-1.463217	-0.736949	-0.183928
C	-0.065396	-1.190669	0.100501
C	2.253025	0.004932	-0.156960
C	0.841513	-0.015735	0.137561
C	0.003590	1.165578	-0.099226
H	-1.752810	0.998302	1.111996
H	-2.115368	1.342836	-0.575580
H	-2.235073	-1.251994	0.393698
H	-1.685405	-0.919047	-1.248322
H	0.706094	-0.256026	1.288448
H	0.274780	-2.211694	0.196855
H	2.800081	0.932047	-0.041817
H	2.811683	-0.914173	-0.282729
H	0.387100	2.177148	-0.087657

Frequencies

-1270.2083	168.0489	196.9850
318.9162	350.1430	395.0285
428.6369	496.7140	598.1436
636.4686	705.9030	845.1635
877.9398	912.5178	924.9630
966.9915	997.8255	1043.0637
1054.6574	1133.9447	1183.9389
1243.4901	1253.0896	1301.2560
1324.6590	1341.2767	1419.8176
1472.8634	1476.4085	1489.7262
2304.9214	2959.6005	2971.3173
3088.9329	3097.4382	3166.1249
3231.8974	3249.0119	3273.0307

i2 – p6

Cartesian coordinates

C	-0.829304	1.337716	0.215314
C	-1.251122	0.056089	-0.486815
C	-2.044449	-0.997895	0.248129
C	2.628787	-0.509945	-0.020206
C	1.372660	-0.122632	-0.087219
C	0.163433	0.296712	-0.130055
H	-0.814677	2.259885	-0.356109

H	-1.089002	1.449787	1.263798
H	-1.484961	0.163720	-1.543190
H	-1.877168	-1.984871	-0.189930
H	-3.115027	-0.779652	0.201419
H	-1.747723	-1.041858	1.299149
H	3.308923	-0.340624	-0.847979
H	2.972262	-1.143090	0.790752
H	3.607335	1.056433	0.947200

Frequencies

-522.1474	108.3043	146.1332
203.8058	219.0416	281.0639
331.8723	374.2207	437.8201
572.9753	654.8110	689.3030
812.5767	893.5954	896.4898
960.6421	979.3364	1027.5365
1054.7222	1082.5854	1123.9427
1137.5980	1181.1357	1324.5265
1396.3793	1425.1900	1465.7305
1489.9358	1505.3120	1537.6545
2103.7757	3045.9241	3121.7995
3124.3176	3129.0194	3151.4447
3154.0170	3218.7649	3236.7811

i1 – p7

Cartesian coordinates

C	-1.809403	-1.319106	-0.297908
C	-1.078028	-0.448852	0.458892
C	-1.715354	1.625358	-0.171188
C	2.937589	0.094927	-0.132558
C	1.507122	-0.094222	0.074205
C	0.327884	-0.257016	0.243232
H	-2.831150	-1.558177	-0.029748
H	-1.412052	-1.731653	-1.217158
H	-1.442695	-0.184688	1.446850
H	-1.132575	2.213665	0.528765
H	-2.788099	1.600593	-0.017304
H	-1.371264	1.616493	-1.197968
H	3.392894	-0.804845	-0.553772
H	3.439615	0.318295	0.812086
H	3.126474	0.923775	-0.819800

Frequencies

-549.2019	23.8168	99.5625
119.0868	149.1404	207.1217
281.4614	333.6956	418.8519

534.6967	554.5683	568.9314
597.1917	726.5436	829.0534
882.7153	980.3503	1041.1732
1056.1156	1058.5452	1188.2579
1274.7163	1417.3808	1419.9315
1424.7233	1431.1179	1484.3703
1485.5756	1553.3703	2379.9645
3045.6660	3093.2540	3116.8467
3120.5590	3160.0223	3170.0325
3257.5224	3262.3824	3266.1785

iI - pI

Cartesian coordinates

C	1.766590	1.280430	-0.124669
C	1.106744	0.109315	0.060113
C	1.796747	-1.229700	-0.101095
C	-2.986930	-0.044187	-0.043286
C	-1.531905	0.017202	0.001358
C	-0.332312	0.080332	0.043618
H	2.847265	1.295715	-0.207017
H	1.239187	2.225697	-0.133415
H	1.226955	0.080194	1.943560
H	1.404633	-1.963284	0.604069
H	2.872352	-1.130390	0.053326
H	1.619621	-1.606934	-1.112720
H	-3.386972	0.716810	-0.717842
H	-3.412565	0.123941	0.949267
H	-3.324087	-1.022098	-0.395460

Frequencies

-972.7797	67.1775	115.7724
153.1547	239.3630	310.2274
350.1065	385.9753	436.3938
505.8191	558.4390	583.1891
667.3919	683.2304	893.5072
931.3286	1032.8342	1055.7251
1059.2338	1066.4225	1097.4812
1322.8947	1411.7639	1420.3745
1429.6836	1483.6737	1486.3157
1491.0019	1502.4047	1606.3619
2381.9913	3049.8341	3054.7066
3121.5356	3125.6534	3129.2066
3152.1844	3166.8858	3268.9621

iI - i6

Cartesian coordinates

C	1.923347	-0.789083	0.463281
C	0.955470	-0.382962	-0.572217
C	-3.012683	0.129673	0.200163
C	-1.594584	-0.061798	-0.077030
C	-0.424810	-0.252891	-0.317959
H	2.839631	-1.274357	0.150173
H	1.552700	-1.003038	1.457979
H	1.254337	-0.513457	-1.606853
H	-3.327548	-0.470607	1.058123
H	-3.619304	-0.170534	-0.658749
H	-3.239583	1.177140	0.420475
C	1.907145	1.028594	0.096459
H	1.557623	1.698737	-0.712419
H	2.996563	1.139951	0.114181
H	1.462264	1.386970	1.020910

Frequencies

-1346.7176	53.3118	102.7365
117.1537	144.7133	240.5830
315.6744	443.0186	533.4601
558.8148	634.1452	714.6995
787.3795	826.1206	995.5326
1015.5175	1036.9517	1051.8946
1056.7596	1147.1963	1237.9016
1341.1869	1395.1951	1421.2925
1431.2050	1462.8483	1480.3529
1490.2111	1497.6838	2305.2166
2862.3339	3023.6115	3035.7321
3101.0395	3111.2474	3144.2776
3181.5889	3184.0987	3266.1135

i8 - p8

Cartesian coordinates

C	-0.580174	1.067378	-0.001156
C	-1.827230	-0.711370	0.008482
C	-3.141506	-0.342465	-0.006411
C	3.187014	-0.475026	-0.002546
C	1.842844	0.086731	0.003320
C	0.739771	0.583896	0.001752
H	-0.948820	1.525153	0.910018
H	-0.947463	1.515543	-0.917650
H	-1.369759	-1.049894	0.931680
H	-1.355702	-1.071250	-0.899439
H	-3.665048	-0.159965	-0.938284
H	-3.680057	-0.137345	0.912117
H	3.582155	-0.558645	1.012919

H 3.868709 0.154186 -0.581477
H 3.191669 -1.472647 -0.450531

1481.8451 1500.3666 1693.4450
2197.1841 2998.7812 3039.2988
3097.7711 3130.0129 3159.4922
3221.1922 3238.4506 3248.6532

Frequencies

-642.7699 55.6481 81.1289
83.0050 208.5289 234.6463
249.5079 401.4416 411.5817
467.1405 640.1064 762.5485
818.2349 823.8769 868.8867
1004.8104 1030.2005 1046.6000
1055.9683 1074.3630 1218.0412
1243.2303 1283.9593 1417.5070
1465.1589 1473.0421 1482.4742
1487.8954 1571.8411 2288.4896
3046.2807 3114.2433 3121.5481
3147.8002 3148.6510 3157.6501
3229.8554 3235.0795 3255.9570

iI1 – iI3

Cartesian coordinates

C -1.424685 0.785187 -0.000752
C -1.446400 -0.701160 -0.234301
C -0.054080 -1.173404 0.233532
C 2.181866 -0.012136 -0.144935
C 0.855769 0.029657 0.035015
C 0.007763 1.208084 0.075062
H -0.722592 1.137268 1.103466
H -2.214106 1.474567 -0.265757
H -2.262975 -1.222833 0.269347
H -1.554170 -0.884552 -1.313801
H -0.085946 -1.418764 1.302428
H 0.300086 -2.057965 -0.296915
H 2.763501 0.895118 -0.264820
H 2.712949 -0.956329 -0.182424
H 0.341851 2.216120 -0.133244

Frequencies

-1929.3437 158.8175 280.4691
364.0083 463.4869 576.9606
630.9898 638.0247 731.6300
809.6627 834.7512 858.3561
886.9693 922.4710 942.8923
995.8331 1031.4056 1066.5694
1160.8882 1202.2165 1244.9033
1255.7420 1301.1788 1320.0267
1332.9555 1349.8795 1452.3013

iI0 – iI2

Cartesian coordinates

C 1.410625 0.835726 -0.077489
C 1.582013 -0.666920 -0.102032
C 0.169180 -1.159475 0.090130
C -2.199139 -0.020968 -0.157818
C -0.741242 0.022937 0.184236
C 0.120707 1.188193 0.073153
H 2.244853 1.523604 -0.132310
H 2.013670 -1.017211 -1.055360
H 2.277668 -1.018140 0.674793
H -0.193005 -2.153021 -0.136242
H -0.402082 -0.629605 1.208558
H -2.341605 -0.047607 -1.245522
H -2.724645 0.853736 0.232770
H -2.677289 -0.912789 0.256443
H -0.250427 2.204080 0.135795

Frequencies

-1947.6409 182.7158 203.6101
288.3022 317.3817 529.2305
587.8932 621.3746 720.8217
785.6965 884.5402 924.9155
943.3684 947.0282 969.9075
1018.7561 1053.2034 1098.7720
1141.5372 1187.4338 1254.6569
1288.2381 1316.3616 1329.0006
1418.0977 1430.7389 1477.8612
1492.9725 1497.5951 1606.7462
2203.9155 2941.7563 2985.9746
3022.7086 3094.3268 3127.8473
3208.8163 3231.2563 3234.4787

i7 – p4

Cartesian coordinates

C 0.920916 -1.094687 -0.129565
C 2.008108 -0.051164 0.027219
C 1.833823 1.268400 -0.133690
C -2.917336 0.387285 0.064466
C -1.557801 -0.135550 -0.014186
C -0.441044 -0.572309 -0.067611

H	1.048099	-1.867913	0.634242
H	1.072274	-1.594636	-1.094354
H	3.016572	-0.453991	0.072225
H	2.103974	-0.114636	2.001947
H	2.676076	1.949047	-0.099971
H	0.842338	1.691804	-0.252147
H	-3.013499	1.313643	-0.507104
H	-3.191216	0.598355	1.101050
H	-3.634617	-0.333524	-0.335680

602.0995	669.9235	830.5935
882.3546	896.5377	926.7036
934.8099	999.8779	1013.7683
1085.9705	1099.1705	1156.9502
1184.5337	1198.2825	1209.0614
1234.7392	1300.7654	1337.6541
1375.6716	1394.4405	1477.9623
1483.2912	1493.5885	1509.1803
3022.6344	3036.3538	3078.8945
3087.8079	3118.6214	3169.8228
3197.7137	3221.7517	3227.0242

Frequencies

-747.7299	82.7933	106.7592
111.7738	214.4768	282.2281
379.4408	400.5589	428.3946
446.5267	578.7933	599.7976
776.1759	917.2774	943.2322
964.8563	1040.1417	1057.0518
1063.7835	1078.4983	1179.2534
1250.3847	1318.4161	1376.4467
1421.6200	1441.4524	1480.9471
1487.0881	1489.2806	1658.3007
2399.5097	3040.5589	3049.8595
3081.0618	3120.8510	3124.9552
3157.5720	3176.3984	3255.8435

i18 - i22

Cartesian coordinates

C	1.376535	0.227021	0.397258
C	0.846773	-1.115449	-0.196743
C	-0.633565	-0.979064	-0.396291
C	-1.385264	-0.176552	0.593888
C	-0.841627	0.932699	-0.257220
C	0.491942	1.290163	-0.180263
H	2.431515	0.382592	0.165248
H	1.299343	0.191565	1.491604
H	1.334030	-1.309957	-1.156543
H	1.090972	-1.954100	0.467368
H	-1.145314	-1.456989	-1.220296
H	-2.466219	-0.276885	0.544435
H	-1.032046	-0.212436	1.626181
H	-1.531197	1.461061	-0.906474
H	0.890149	2.102241	-0.775307

Frequencies

-647.1418	234.6900	345.1516
430.6779	575.5384	580.3887

i6 - p2

Cartesian coordinates

C	1.945628	-0.306556	-0.069351
C	0.828567	-1.061158	-0.124272
C	-2.983408	0.386900	0.056415
C	-1.620945	-0.124019	-0.011809
C	-0.492935	-0.543778	-0.061967
C	1.972958	1.190687	-0.059508
H	2.898407	-0.814158	-0.188193
H	2.358037	-0.601776	1.985097
H	0.924959	-2.140010	-0.198312
H	-3.083721	1.309710	-0.520372
H	-3.262762	0.602599	1.091133
H	-3.692954	-0.343217	-0.340426
H	2.208389	1.564094	-1.062223
H	2.742346	1.565981	0.618355
H	1.008113	1.604312	0.237893

Frequencies

-552.0209	78.3353	96.3986
118.2148	157.6217	252.7276
270.4245	348.8121	379.7030
419.1780	508.7797	611.7388
780.9142	796.3402	937.7529
997.2084	1049.9715	1061.1570
1062.1326	1107.4300	1181.8967
1271.3214	1401.3220	1418.6069
1444.9781	1484.1127	1484.6916
1485.5735	1492.9683	1654.8126
2359.6306	3047.8912	3048.1543
3115.0620	3118.5112	3124.3665
3148.5691	3172.8912	3191.5166

i10 - i14

Cartesian coordinates

C	1.559841	-0.631403	0.076971
C	1.388164	0.861913	-0.062494
C	0.087376	1.205952	-0.025259
C	-2.232375	-0.010199	-0.046783
C	-0.760643	0.038205	0.094229
C	0.124915	-1.176485	-0.105447
H	1.954972	-0.876294	1.071388
H	2.259671	-1.050909	-0.650941
H	2.217277	1.555288	-0.119706
H	-0.294974	2.219458	-0.063974
H	-2.715262	-0.970548	-0.160969
H	-2.789087	0.902110	-0.214046
H	-0.019231	-1.544187	-1.130200
H	-0.111179	-2.002505	0.569688
H	-1.505860	0.039692	1.111456

Frequencies

-1952.2186	139.5529	290.7052
317.6876	387.7941	489.2837
588.0748	629.7995	714.8460
754.3857	833.3365	870.7910
919.1906	940.7317	955.4521
1006.5386	1025.8253	1110.3726
1136.9044	1196.9168	1226.9950
1272.4437	1287.2113	1319.5604
1332.6321	1428.9663	1449.8975
1479.2655	1503.0307	1609.3332
2207.4015	3022.6012	3030.4477
3083.8316	3102.4325	3168.6574
3206.2060	3233.1614	3291.1341

i13 – p12**Cartesian coordinates**

C	-1.313050	0.838089	-0.147288
C	-1.512243	-0.651242	-0.117616
C	-0.102900	-1.203892	0.194861
C	2.154088	-0.064482	-0.155916
C	0.834009	-0.027009	0.001213
C	-0.012753	1.178541	-0.012737
H	-2.128612	1.542001	-0.258831
H	-2.257518	-0.953425	0.624493
H	-1.881330	-1.002466	-1.088837
H	-0.050376	-1.528927	1.238467
H	0.170829	-2.056419	-0.428688
H	2.731283	0.846717	-0.268053

H	2.695809	-1.003691	-0.172156
H	0.050113	1.558777	1.915246
H	0.386891	2.177407	-0.136745

Frequencies

-760.5258	89.6188	248.6977
310.6227	359.2052	401.3347
536.6575	643.3387	705.8295
760.1385	793.2706	840.0660
875.3638	910.5005	924.2362
963.1937	1006.4589	1016.7207
1030.9191	1115.4945	1174.1463
1243.7439	1272.4415	1291.9988
1341.2161	1372.2200	1454.2533
1466.9148	1496.1009	1589.9533
1747.9862	3040.3754	3064.5554
3084.8721	3122.8517	3159.2310
3209.7511	3230.1570	3247.1900

i13 – p14**Cartesian coordinates**

C	-1.409843	0.739676	-0.022074
C	-1.455588	-0.602473	-0.026105
C	-0.081295	-1.204472	-0.203060
C	2.154899	-0.059294	0.124878
C	0.841103	-0.007547	-0.043517
C	-0.000749	1.258902	-0.064881
H	-2.276586	1.387377	0.026229
H	-1.639414	-0.909516	1.964235
H	-2.365195	-1.185925	-0.097349
H	0.139856	-1.994814	0.518201
H	0.012786	-1.645215	-1.203677
H	2.745059	0.842894	0.247915
H	2.685786	-1.005176	0.147863
H	0.229172	1.916612	0.780671
H	0.177380	1.845004	-0.975529

Frequencies

-648.0890	72.2793	245.6887
367.4161	385.0565	431.3502
440.6575	632.5160	694.1611
733.1824	798.5524	830.0601
922.9578	928.5976	944.9228
984.3161	988.3469	991.0462
1009.9032	1121.1407	1167.3349
1197.0685	1260.2544	1305.5825

1306.5032	1377.3437	1449.7628
1462.0777	1481.1170	1635.3148
1763.7299	3033.7686	3035.2971
3070.2838	3101.0316	3154.0352
3207.9375	3229.4085	3239.5686

iI2 – p9

Cartesian coordinates

C	-1.267550	0.870622	0.293997
C	-1.439964	-0.617165	0.427835
C	-0.298882	-1.159774	-0.378239
C	2.234027	-0.011284	0.616140
C	0.490770	-0.124303	-0.810074
C	-0.176201	1.137883	-0.431244
H	-1.935274	1.596017	0.739403
H	-1.398818	-0.935620	1.479701
H	-2.411103	-0.956642	0.044978
H	-0.124923	-2.212188	-0.554243
H	1.705461	0.097856	1.555741
H	2.745672	0.872821	0.249616
H	2.732685	-0.959347	0.449159
H	1.229966	-0.200004	-1.596468
H	0.203130	2.121228	-0.678369

Frequencies

-540.8740	126.6432	155.5673
166.4051	348.5669	498.7850
533.3891	559.3213	683.7832
707.7505	795.6325	816.4661
857.9299	919.8027	938.3958
962.0495	969.0578	976.8106
1012.2870	1102.4662	1125.8732
1130.5470	1278.2673	1322.1457
1400.8856	1425.6235	1428.8110
1429.5305	1483.6173	1655.1082
3018.9928	3056.0864	3093.2292
3213.5027	3221.5112	3239.1257
3246.3446	3252.8208	3262.5329

iI2 – p11

Cartesian coordinates

C	1.448962	0.806322	-0.057128
C	1.552247	-0.691449	-0.039684
C	0.121274	-1.126915	-0.025448
C	-2.182343	-0.003224	-0.136454
C	-0.694026	-0.037762	0.060747

C	0.162839	1.167068	-0.002362
H	2.303106	1.469440	-0.084674
H	2.096742	-1.083975	-0.907430
H	2.093272	-1.044130	0.849931
H	-0.203417	-2.158817	-0.040836
H	-2.407879	0.235237	-1.181132
H	-2.651516	0.757944	0.489818
H	-2.634128	-0.968144	0.099057
H	-0.826350	-0.070243	1.955540
H	-0.223553	2.178454	0.021698

Frequencies

-842.0574	188.8416	224.1117
307.0692	367.4766	414.5516
498.3520	587.6574	637.2973
718.8780	733.4442	817.5908
915.1100	925.2682	948.2190
969.4046	983.2415	1027.4513
1061.7258	1104.7025	1132.5670
1220.8693	1262.0598	1314.3059
1389.2045	1421.3110	1425.8834
1489.9278	1496.4048	1579.0271
1665.5352	3031.0036	3046.7851
3070.6991	3118.6877	3148.6776
3217.2434	3229.7443	3243.2447

iI2 – p13

Cartesian coordinates

C	-1.369567	0.796646	0.131412
C	-1.417295	-0.675370	0.059082
C	-0.201631	-1.125983	-0.341097
C	1.982526	-0.068435	0.426522
C	0.747573	0.029297	-0.481771
C	-0.134022	1.210150	-0.170324
H	-2.208276	1.420709	0.410298
H	-1.368324	-1.043937	1.986077
H	-2.323696	-1.263622	0.116188
H	0.075232	-2.157493	-0.513435
H	1.677131	-0.135241	1.473490
H	2.620728	0.810670	0.308164
H	2.575408	-0.953589	0.183277
H	1.086741	0.091560	-1.526486
H	0.219555	2.233110	-0.180514

Frequencies

-772.7152	145.6313	238.7675
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278.7215	338.8860	356.2599
541.6933	587.1350	725.0393
741.7455	797.1969	813.4884
878.0630	950.4630	973.9720
990.1586	994.4150	1024.3783
1084.5107	1094.9932	1109.8436
1140.9771	1274.8780	1281.9432
1325.1464	1396.4875	1411.7694
1495.5632	1501.2216	1542.5106
1656.6288	3022.2267	3049.3927
3127.0183	3134.2071	3214.8220
3222.8996	3239.2055	3246.6667

i4 – i6

Cartesian coordinates

C	-2.051055	-0.255428	-0.008374
C	-0.831720	-1.121780	0.021782
C	2.947336	0.412426	-0.007677
C	1.596520	-0.134362	0.013086
C	0.479021	-0.592816	0.031735
C	-1.939159	1.232578	0.016659
H	-2.975659	-0.742630	0.276046
H	-1.482766	-0.914245	-1.042374
H	-0.974245	-2.153406	0.323640
H	2.953672	1.404690	-0.466592
H	3.620060	-0.227287	-0.585349
H	3.355508	0.508206	1.002601
H	-1.701433	1.593181	1.027629
H	-2.868462	1.707359	-0.304158
H	-1.132329	1.580423	-0.634707

Frequencies

-1913.3970	91.7999	96.3075
117.1614	166.3838	255.4597
260.4278	393.3923	406.1658
570.4821	599.7752	747.8926
813.5021	917.4739	1021.1160
1051.4064	1057.1769	1081.0261
1142.6166	1232.1085	1265.1672
1369.3960	1397.9035	1423.2371
1426.8141	1479.5685	1486.1679
1489.3805	1493.8595	2213.3001
2323.6025	3005.5999	3043.2086
3085.9436	3109.0939	3119.0220
3132.7726	3190.4603	3212.3806

i4 – i5

Cartesian coordinates

C	-0.733338	0.911660	-0.051852
C	3.162966	-0.447923	-0.030499
C	1.787711	0.038680	-0.043577
C	0.656744	0.442125	-0.056680
H	-0.777522	1.856657	0.509866
H	-1.032616	1.156756	-1.077234
H	3.219407	-1.443188	0.417627
H	3.807538	0.218716	0.547962
H	3.565409	-0.511595	-1.044651
C	-1.686009	-0.090107	0.530775
C	-2.838852	-0.606799	-0.251832
H	-1.435783	-0.526233	1.490962
H	-3.500345	-1.223102	0.359908
H	-2.506039	-1.222922	-1.101659
H	-3.435374	0.209090	-0.680786

Frequencies

-62.7667	76.7078	82.2458
131.6227	188.8059	293.1093
348.2702	388.2090	404.2656
511.3922	758.8853	868.8120
920.8188	987.4931	1055.8703
1062.4030	1115.3505	1147.8234
1170.5454	1233.4679	1299.7783
1397.7594	1421.3943	1429.1056
1465.3217	1479.1226	1486.7810
1486.7976	1490.7613	2392.5767
2983.1280	2997.2443	3039.9297
3049.8503	3064.9195	3120.8094
3122.0304	3122.2311	3207.6781

i19 – i20

Cartesian coordinates

C	0.490677	1.277747	-0.094057
C	1.348855	0.092619	0.406701
C	0.777204	-1.180934	-0.266897
C	-1.474004	-0.169349	0.646487
C	-0.664057	-0.783540	-0.428070
C	-0.887153	0.696474	-0.406460
H	0.907313	1.684686	-1.021173
H	0.460598	2.093115	0.633466
H	2.409238	0.234732	0.191016
H	1.246139	-0.005232	1.490378
H	1.241396	-1.359718	-1.240864

H	0.918490	-2.072954	0.347069
H	-1.361659	-0.260683	1.719207
H	-1.862212	-1.134265	-0.140550
H	-1.508433	1.222212	-1.124773

1232.5922	1259.7404	1292.8252
1327.4421	1360.3689	1436.3633
1468.5429	1478.3252	1517.9346
2399.4604	2923.5726	2983.3318
2996.7510	3069.5373	3166.8320
3227.0698	3232.6317	3268.5560

Frequencies

-1882.4416	231.2670	297.8836
360.8579	586.9865	647.9698
709.3446	786.8741	838.5461
882.4561	891.0854	903.7327
924.2764	980.8556	1014.6590
1020.4449	1074.3640	1118.2929
1153.3660	1177.1867	1202.3365
1257.3051	1308.0535	1329.6727
1335.4316	1365.6813	1430.2999
1495.2163	1499.7027	1516.0620
2309.3520	3057.7307	3064.7499
3073.5777	3104.9220	3118.0511
3133.1368	3162.0459	3206.3490

i13 – i17

Cartesian coordinates

C	-1.398342	0.804856	0.102004
C	-1.565751	-0.674590	-0.057003
C	-0.156951	-1.187044	-0.061357
C	2.224346	-0.102655	-0.069017
C	0.816996	-0.083241	0.080561
C	0.023709	1.216957	-0.077819
H	-2.227393	1.499874	0.128648
H	-2.205469	-1.116138	0.721195
H	-2.065221	-0.919430	-1.012970
H	0.595801	-0.468837	1.174768
H	0.124483	-2.230598	-0.014324
H	2.779834	0.819411	0.043154
H	2.774420	-1.035559	-0.080419
H	0.349712	1.991650	0.624084
H	0.209793	1.613929	-1.088344

Frequencies

-1520.1886	159.8692	186.9873
337.1839	402.0475	435.7235
451.4442	515.9654	604.9973
620.9361	737.6800	834.5489
887.9613	911.9620	923.6552
938.4334	1008.8557	1042.9364
1059.2718	1108.3497	1192.0070

i13 – i15

Cartesian coordinates

C	-1.388053	0.837936	-0.140256
C	-1.526336	-0.643518	0.097483
C	-0.092524	-1.186230	-0.095799
C	2.207894	-0.027893	-0.033101
C	0.834016	0.016132	0.049235
C	-0.060378	1.201984	-0.025573
H	-2.216489	1.532181	-0.141515
H	-1.872656	-0.826984	1.126153
H	-2.246689	-1.128749	-0.565682
H	0.158786	-2.002901	0.582302
H	0.035803	-1.551580	-1.119775
H	2.801745	0.877953	-0.051144
H	2.724884	-0.977765	0.003777
H	0.427198	0.681528	1.157195
H	0.339703	2.205852	-0.103244

Frequencies

-1884.9746	138.3129	316.9564
357.9093	489.2895	535.9324
607.8050	633.1433	684.4639
747.1002	821.8395	870.9197
912.5230	918.5089	950.7997
1008.0696	1013.3016	1089.9173
1129.3895	1173.5592	1227.7942
1263.0126	1310.8470	1318.8282
1332.6176	1429.7791	1471.3807
1491.1723	1501.6506	1561.5657
1662.7234	2993.9413	3065.3238
3094.4882	3131.0323	3163.9047
3215.2223	3243.3352	3262.8992

i7 – p8

Cartesian coordinates

C	-0.662836	1.305693	-0.223384
C	2.933940	-0.576348	0.080607
C	1.651345	0.105653	-0.030777
C	0.599756	0.693276	-0.133869

H	-0.877751	2.104197	0.480667	-644.4294	183.2529	355.3790
H	-1.082211	1.442793	-1.213842	372.0551	546.7042	633.9784
H	2.811503	-1.571723	0.517284	668.5600	696.6698	782.3048
H	3.622116	-0.013344	0.716524	807.7675	868.3288	879.2344
H	3.399106	-0.695610	-0.901359	923.9567	958.6695	972.4201
C	-2.120986	-0.111639	0.556311	1015.5546	1084.7042	1111.4222
C	-2.227089	-1.171091	-0.296070	1119.6653	1196.7575	1211.1387
H	-2.900259	0.643905	0.571573	1253.1452	1305.5708	1316.9224
H	-1.543285	-0.210620	1.468715	1360.3530	1374.0708	1453.8998
H	-2.928639	-1.161592	-1.122796	1468.6383	1484.0585	1499.5343
H	-1.545359	-2.011269	-0.233675	3012.5148	3068.7076	3083.3692

Frequencies

-627.7280	43.4746	49.1687
91.6485	202.5707	219.4951
281.8284	394.1210	402.1589
476.5270	608.1057	747.0512
808.1239	824.9598	854.0527
1002.2835	1023.3399	1049.3785
1055.0635	1073.7342	1223.2949
1244.5786	1288.5577	1419.0757
1461.6521	1465.5106	1482.8724
1484.3827	1568.8452	2296.4089
3041.1028	3109.3535	3117.2805
3133.0716	3137.7598	3153.6979
3222.1803	3222.7946	3251.7672

i14 – i16

Cartesian coordinates

C	1.450663	-0.114756	-0.375492
C	0.793791	1.175165	0.035871
C	-0.484564	0.948592	0.493272
C	-1.556884	-0.109248	-0.725233
C	-0.805858	-0.517915	0.480308
C	0.543526	-1.202753	0.248796
H	2.486679	-0.197719	-0.034052
H	1.481084	-0.202663	-1.470593
H	1.228114	2.151739	-0.133459
H	-1.147725	1.692824	0.911608
H	-1.096439	-0.161734	-1.702747
H	-2.602396	0.160133	-0.657981
H	-1.399855	-0.913476	1.301874
H	0.456403	-2.094373	-0.376245
H	0.950089	-1.509242	1.216453

Frequencies

3121.7324	3138.2775	3171.6636
3215.6248	3240.5599	3285.1914

i14 – p12

Cartesian coordinates

C	1.530989	-0.613105	0.085161
C	1.334784	0.872941	-0.065769
C	0.044645	1.207813	-0.061018
C	-2.161043	-0.009782	-0.059401
C	-0.809845	0.010773	0.028593
C	0.119015	-1.181630	-0.156147
H	1.881353	-0.836846	1.100782
H	2.274827	-1.016927	-0.606513
H	2.158948	1.574313	-0.116253
H	-0.354065	2.213779	-0.102462
H	-2.708042	-0.945054	-0.082376
H	-2.734253	0.909885	-0.039023
H	-0.765300	-0.081611	1.915758
H	0.028071	-1.520762	-1.192957
H	-0.132812	-2.018834	0.494535

Frequencies

-896.4310	121.9678	333.3256
344.3037	458.4715	494.8062
530.2397	630.1056	630.8499
753.6644	794.1585	828.1933
870.9977	879.4475	928.6436
963.0552	983.9850	1019.2062
1036.2553	1122.4994	1178.6683
1238.2025	1274.0775	1304.4387
1341.8950	1364.5779	1449.0354
1468.5624	1492.8181	1619.9910
1685.8637	3039.7325	3067.5070
3095.6891	3139.3814	3158.6019
3210.9370	3235.7217	3254.2556

i15 – p12

Cartesian coordinates

C	-1.334787	0.872934	-0.065757
C	-1.530967	-0.613112	0.085214
C	-0.119012	-1.181619	-0.156220
C	2.161046	-0.009778	-0.059336
C	0.809844	0.010778	0.028576
C	-0.044648	1.207811	-0.061065
H	-2.158959	1.574299	-0.116219
H	-1.881233	-0.836849	1.100871
H	-2.274861	-1.016954	-0.606388
H	0.132863	-2.018890	0.494356
H	-0.028123	-1.520637	-1.193074
H	2.734255	0.909889	-0.038929
H	2.708050	-0.945049	-0.082277
H	0.765091	-0.081664	1.915724
H	0.354061	2.213777	-0.102534

Frequencies

-896.4440	122.0109	333.3425
344.3024	458.4894	494.8316
530.2280	630.1062	630.8488
753.6585	794.1589	828.1924
870.9970	879.4578	928.6458
963.0558	983.9859	1019.2021
1036.2512	1122.4965	1178.6633
1238.1974	1274.0776	1304.4383
1341.8958	1364.5767	1449.0371
1468.5571	1492.8075	1619.9948
1685.8563	3039.7224	3067.4946
3095.6983	3139.3749	3158.6012
3210.9376	3235.7215	3254.2537

i15 – i18

Cartesian coordinates

C	-0.793776	1.175175	0.035826
C	-1.450722	-0.114738	-0.375440
C	-0.543533	-1.202767	0.248738
C	1.556953	-0.109247	-0.725189
C	0.805850	-0.517920	0.480306
C	0.484564	0.948587	0.493249
H	-1.228101	2.151755	-0.133466
H	-2.486693	-0.197664	-0.033853
H	-1.481316	-0.202666	-1.470530
H	-0.950073	-1.509366	1.216368

H	-0.456391	-2.094328	-0.376385
H	2.602454	0.160158	-0.657856
H	1.096590	-0.161756	-1.702739
H	1.399794	-0.913481	1.301911
H	1.147717	1.692814	0.911606

Frequencies

-644.4333	183.1286	355.3666
372.0227	546.7024	633.9842
668.5539	696.6675	782.3024
807.7416	868.3251	879.2160
923.9504	958.6614	972.4148
1015.5494	1084.7047	1111.4223
1119.6696	1196.7521	1211.1341
1253.1466	1305.5698	1316.9124
1360.3487	1374.0693	1453.9028
1468.6273	1484.0563	1499.5313
3012.5384	3068.7079	3083.3577
3121.7355	3138.2735	3171.6665
3215.6248	3240.5613	3285.1962

i10 – i15

Cartesian coordinates

C	-1.388182	0.861888	-0.062478
C	-1.559830	-0.631421	0.076907
C	-0.124877	-1.176461	-0.105382
C	2.232342	-0.010199	-0.046849
C	0.760652	0.038241	0.094295
C	-0.087390	1.205939	-0.025264
H	-2.217307	1.555252	-0.119636
H	-1.955167	-0.876400	1.071216
H	-2.259547	-1.050876	-0.651153
H	0.111204	-2.002407	0.569847
H	0.019386	-1.544272	-1.130084
H	2.789072	0.902103	-0.214073
H	2.715224	-0.970552	-0.161001
H	1.505908	0.039776	1.111474
H	0.294940	2.219452	-0.063962

Frequencies

-1952.2115	139.5367	290.6863
317.6759	387.7784	489.2662
588.0892	629.7099	714.8650
754.4174	833.3457	870.8108
919.2006	940.7387	955.4663
1006.5577	1025.8301	1110.3751

1136.9009	1196.9184	1227.0151
1272.4661	1287.2240	1319.5842
1332.6591	1428.9783	1449.9467
1479.2900	1503.0565	1609.3260
2207.4124	3022.5656	3030.4825
3083.7767	3102.4265	3168.6878
3206.2126	3233.1664	3291.1618

i22 – p15

Cartesian coordinates

C	-1.457022	0.114192	-0.180147
C	-0.763988	-1.176928	0.266757
C	0.669142	-1.216126	-0.183702
C	1.395632	-0.078185	-0.212040
C	0.746224	1.218983	0.033856
C	-0.583781	1.319865	0.053670
H	-2.412026	0.224685	0.339781
H	-1.693958	0.058641	-1.252644
H	-0.777794	-1.235661	1.365876
H	-1.310610	-2.049780	-0.097735
H	1.134415	-2.171679	-0.399150
H	2.290419	-0.209112	1.584669
H	2.418191	-0.086982	-0.573038
H	1.372716	2.092764	0.173328
H	-1.058602	2.286320	0.188562

Frequencies

-680.1191	186.9630	257.2373
312.8601	369.6337	486.0862
547.6198	570.8009	702.5703
770.5131	782.5525	867.2065
945.3941	966.5695	994.1041
1001.2207	1012.8523	1046.1757
1080.8031	1179.7708	1192.3594
1205.9326	1277.0196	1355.9430
1367.2581	1409.4661	1443.9208
1471.4703	1488.5453	1618.3180
1720.2751	3000.4148	3014.3212
3097.7663	3104.0919	3180.1917
3189.3127	3206.6883	3216.2334

i22 – p16

Cartesian coordinates

C	-1.401057	0.464464	-0.123286
C	-0.975896	-0.979071	-0.057685
C	0.311158	-1.361943	-0.106181

C	1.458062	-0.402721	-0.025348
C	1.020975	1.031381	0.065431
C	-0.248763	1.415927	0.021483
H	-2.156149	0.670717	0.642944
H	-1.905011	0.641428	-1.083678
H	-1.233364	-1.227924	1.898837
H	-1.755464	-1.726577	-0.167540
H	0.549729	-2.420614	-0.142798
H	2.083536	-0.656602	0.842071
H	2.116129	-0.537860	-0.894837
H	1.804160	1.776486	0.170481
H	-0.490444	2.472726	0.088034

Frequencies

-677.1536	106.4907	242.6501
391.5076	434.8349	458.3347
547.2628	583.6489	652.6285
746.3249	866.7775	904.9525
955.6877	958.8868	979.1844
989.2158	1017.7993	1031.3666
1058.8661	1192.7072	1226.2678
1234.3387	1236.6587	1371.6235
1394.8880	1425.2651	1448.5702
1462.8255	1486.2049	1671.1541
1769.3446	3013.5129	3021.3127
3033.6987	3063.0998	3165.5679
3169.9159	3189.3653	3191.5206

i16 – i22

Cartesian coordinates

C	-1.376535	0.227022	0.397258
C	-0.491941	1.290163	-0.180263
C	0.841628	0.932698	-0.257220
C	1.385263	-0.176552	0.593889
C	0.633565	-0.979063	-0.396291
C	-0.846774	-1.115449	-0.196743
H	-2.431514	0.382593	0.165249
H	-1.299342	0.191565	1.491605
H	-0.890149	2.102239	-0.775310
H	1.531197	1.461060	-0.906474
H	1.032043	-0.212436	1.626180
H	2.466218	-0.276886	0.544437
H	1.145314	-1.456990	-1.220296
H	-1.090972	-1.954100	0.467368
H	-1.334032	-1.309956	-1.156543

Frequencies		
-647.1415	234.6904	345.1524
430.6781	575.5386	580.3890
602.1000	669.9235	830.5937
882.3546	896.5378	926.7036
934.8100	999.8778	1013.7684
1085.9705	1099.1704	1156.9502
1184.5337	1198.2824	1209.0613
1234.7392	1300.7653	1337.6541
1375.6714	1394.4403	1477.9624
1483.2911	1493.5885	1509.1805
3022.6346	3036.3537	3078.8946
3087.8078	3118.6214	3169.8229
3197.7139	3221.7516	3227.0241

iI6 – iI9

Cartesian coordinates

C	0.634590	1.194162	0.155726
C	1.587557	-0.029848	0.054339
C	0.639602	-1.221239	0.056220
C	-1.717239	-0.030786	0.423146
C	-0.684683	-0.773144	-0.362394
C	-0.686116	0.700218	-0.448937
H	1.022862	2.065523	-0.375583
H	0.499770	1.487860	1.201840
H	2.177467	0.020262	-0.867125
H	2.301209	-0.085718	0.881110
H	0.011715	-1.621854	-1.062200
H	0.770533	-2.091735	0.690411
H	-1.594876	-0.005742	1.503886
H	-2.745093	-0.017843	0.077009
H	-1.085854	1.213072	-1.317952

Frequencies

-2049.7012	147.1339	302.4691
381.0599	590.2294	637.7086
704.5298	760.3010	826.5975
881.4969	894.3596	925.8107
953.7309	977.7849	998.4497
1013.1717	1045.2680	1100.3022
1113.6103	1168.7937	1187.6578
1229.7863	1248.6423	1307.6486
1326.8546	1351.3564	1385.0100
1473.3563	1484.3334	1501.5351
2156.8936	3049.5430	3061.7939
3099.0393	3113.4789	3121.6883

3170.2734	3195.4079	3211.6047
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iI7 – iI8

Cartesian coordinates

C	-1.481069	-0.038885	0.260493
C	-0.703094	1.218606	-0.070909
C	0.705071	0.749245	-0.413925
C	1.472920	-0.000801	0.635658
C	0.715389	-0.772891	-0.423799
C	-0.659655	-1.238682	-0.087451
H	-2.563262	-0.082378	0.260683
H	-1.149073	1.697179	-0.952834
H	-0.712132	1.961921	0.733744
H	1.267665	1.313215	-1.148497
H	2.554292	0.014443	0.564459
H	1.087740	-0.021491	1.651386
H	1.286993	-1.333548	-1.152734
H	-1.087961	-2.152575	-0.479121
H	-0.981638	-0.896312	1.122511

Frequencies

-1963.2025	232.9551	302.4619
445.5962	598.4122	652.7889
671.3781	771.1396	789.0766
818.1333	883.6174	916.1615
957.2455	978.1522	982.8408
1041.8596	1052.9792	1090.4123
1096.1488	1100.6474	1186.5527
1218.1445	1262.1243	1286.7368
1311.7485	1333.2664	1368.0931
1389.1520	1489.4986	1499.1790
2195.5531	3023.5854	3066.0492
3127.6137	3188.1993	3195.0061
3204.2925	3214.2833	3223.8348

iI6 – iI7

Cartesian coordinates

C	1.481050	-0.038860	0.260521
C	0.659678	-1.238683	-0.087459
C	-0.715376	-0.772907	-0.423783
C	-1.472899	-0.000807	0.635672
C	-0.705088	0.749231	-0.413942
C	0.703068	1.218614	-0.070932
H	2.563243	-0.082342	0.260768
H	1.088014	-2.152502	-0.479267
H	0.981657	-0.896332	1.122512

H	-1.286996	-1.333594	-1.152681
H	-2.554272	0.014398	0.564495
H	-1.087698	-0.021456	1.651394
H	-1.267695	1.313186	-1.148517
H	1.149055	1.697160	-0.952869
H	0.712096	1.961953	0.733699

1001.7553	1023.9073	1054.9559
1074.5598	1096.4362	1108.2621
1128.9209	1194.3078	1215.3734
1308.7327	1333.5605	1386.4555
1397.8284	1482.4166	1491.5143
1619.0902	3054.7075	3100.8011
3133.9088	3194.2893	3201.2604
3211.0180	3230.5833	3233.7836

Frequencies

-1963.2074	232.9811	302.4754
445.5989	598.4226	652.8281
671.3725	771.1467	789.0829
818.1423	883.6171	916.1613
957.2426	978.1529	982.8381
1041.8624	1052.9817	1090.4123
1096.1481	1100.6489	1186.5507
1218.1452	1262.1181	1286.7303
1311.7589	1333.2567	1368.0970
1389.1517	1489.4988	1499.1799
2195.5499	3023.5781	3066.0534
3127.6144	3188.2025	3195.0143
3204.3028	3214.2934	3223.8369

i20 – i21

Cartesian coordinates

C	-0.940648	-1.094805	-0.140111
C	-1.318294	0.292570	0.407568
C	-0.386804	1.301688	-0.246626
C	1.413184	-0.297542	0.569368
C	1.038909	0.817249	-0.159818
C	0.544949	-1.137754	-0.281544
H	-1.417899	-1.270099	-1.110256
H	-1.303055	-1.876840	0.542315
H	-2.369798	0.528791	0.232023
H	-1.147709	0.305546	1.487769
H	-0.660332	1.472804	-1.295080
H	-0.445060	2.278989	0.249223
H	2.455362	-0.535564	0.743258
H	1.782991	1.471691	-0.625836
H	0.997723	-1.663758	-1.116436

i16 – p17

Cartesian coordinates

C	-1.437264	0.151984	0.094938
C	-0.628865	1.190782	-0.182183
C	0.760699	0.745522	-0.454361
C	1.429494	0.003650	0.687703
C	0.713767	-0.771733	-0.377361
C	-0.735246	-1.172008	-0.124932
H	-2.499189	0.228139	0.290833
H	-1.366817	0.225630	2.152580
H	-0.925517	2.232201	-0.159349
H	1.377459	1.276607	-1.168921
H	0.974633	0.089773	1.668999
H	2.512280	-0.040242	0.680744
H	1.310287	-1.371115	-1.053361
H	-0.841397	-1.851138	0.725569
H	-1.157248	-1.679034	-0.999915

Frequencies

-562.9842	275.2946	323.1055
378.0864	390.4872	491.6493
680.2474	771.8338	780.9368
788.0786	820.2631	894.4767
933.9494	948.8634	971.4818

Frequencies

-901.1801	235.1955	298.1205
436.0423	545.0326	615.1535
627.1874	753.6830	831.2873
856.8359	895.7856	916.1143
959.4953	985.7653	1039.7326
1082.4851	1133.1829	1146.6760
1180.5614	1218.8207	1252.3417
1319.1235	1327.4301	1361.6626
1369.1015	1381.9421	1471.8163
1485.8802	1497.8864	1511.3069
3002.0596	3032.5517	3061.6397
3066.7218	3072.9655	3078.0657
3124.8321	3170.3014	3204.4243

i11 – i19

Cartesian coordinates

C	1.070884	-1.059237	-0.053871
C	1.401586	0.403657	-0.414149

C	0.338650	1.253325	0.331396
C	-1.911821	0.107269	-0.445177
C	-0.821363	0.307144	0.522981
C	-0.383247	-0.992846	0.347742
H	1.654581	-1.413399	0.806702
H	1.257739	-1.760597	-0.870639
H	2.426436	0.681451	-0.159960
H	1.283272	0.541953	-1.492853
H	0.718537	1.568070	1.309717
H	0.064223	2.158314	-0.214930
H	-1.753992	0.359060	-1.489619
H	-2.842770	-0.373516	-0.170940
H	-0.976157	-1.877203	0.548993

Frequencies

-817.3991	150.7969	296.1058
329.3242	511.6522	575.5617
607.0599	737.4605	773.1841
826.3143	857.4363	901.3139
914.7684	943.8330	993.5084
1025.3361	1040.9724	1130.4463
1173.2708	1223.5545	1242.5087
1285.6595	1311.0060	1334.7787
1364.1154	1427.2827	1471.5492
1480.4974	1491.3423	1511.3831
3029.9740	3049.5149	3063.7510
3102.6374	3109.9222	3123.3190
3137.5461	3209.3231	3250.0883

i18 - p18

Cartesian coordinates

C	1.437259	0.151986	0.094977
C	0.735250	-1.172006	-0.124934
C	-0.713763	-0.771734	-0.377364
C	-1.429491	0.003642	0.687702
C	-0.760698	0.745523	-0.454361
C	0.628860	1.190786	-0.182178
H	2.499189	0.228145	0.290841
H	1.366790	0.225611	2.152377
H	1.157261	-1.678996	-0.999934
H	0.841401	-1.851163	0.725543
H	-1.310280	-1.371115	-1.053367
H	-2.512278	-0.040248	0.680741
H	-0.974631	0.089765	1.668998
H	-1.377461	1.276611	-1.168914
H	0.925512	2.232204	-0.159349

Frequencies

-563.7727	275.3583	323.2362
378.2298	390.5695	491.6599
680.2455	771.8504	780.9357
788.0892	820.2650	894.4779
933.9468	948.8660	971.5002
1001.7502	1023.9096	1054.9570
1074.5603	1096.4370	1108.2629
1128.9162	1194.3095	1215.3762
1308.7330	1333.5634	1386.4549
1397.8297	1482.4232	1491.5213
1619.0455	3054.7114	3100.8143
3133.9120	3194.2910	3201.2624
3211.0225	3230.5864	3233.7877

i17 - p18

Cartesian coordinates

C	1.475736	0.059936	0.116422
C	0.706049	-1.234651	0.061978
C	-0.702793	-0.809066	-0.337288
C	-1.471012	0.073993	0.600439
C	-0.689080	0.699759	-0.529150
C	0.706045	1.122541	-0.198448
H	2.517953	0.116441	0.405991
H	1.142651	-1.910886	-0.682095
H	0.725170	-1.767200	1.020070
H	-1.264937	-1.441247	-1.013012
H	-2.551032	0.061661	0.510844
H	-1.092624	0.227314	1.605941
H	-1.221053	1.187302	-1.336774
H	1.080325	2.120186	-0.390175
H	0.513879	1.931357	1.595486

Frequencies

-754.3205	254.4004	323.6337
387.0174	404.7679	550.9457
682.4575	740.7679	773.5025
781.9574	817.0191	895.7135
929.6143	951.0447	982.8639
1003.5075	1027.2611	1054.2777
1073.4465	1098.3074	1107.4854
1126.6249	1188.4130	1214.3039
1307.0009	1329.0775	1386.3476
1393.8468	1479.6142	1489.5599
1602.1369	3040.7947	3074.0137

3133.1247 3186.7531 3198.9870
 3210.1203 3228.9133 3231.3043

i17 – p17

Cartesian coordinates

C -1.475816 0.059843 0.116298
 C -0.706147 1.122512 -0.198403
 C 0.689014 0.699841 -0.529089
 C 1.471128 0.074025 0.600363
 C 0.702839 -0.808997 -0.337331
 C -0.705966 -1.234667 0.062038
 H -2.518076 0.116244 0.405741
 H -1.080464 2.120160 -0.390048
 H -0.514181 1.931013 1.595975
 H 1.220932 1.187405 -1.336740
 H 2.551134 0.061795 0.510589
 H 1.092923 0.227248 1.605952
 H 1.264909 -1.441109 -1.013185
 H -1.142512 -1.911149 -0.681834
 H -0.724977 -1.766944 1.020289

Frequencies

-753.4360 254.3489 323.5790
 386.8924 404.3747 550.8592
 682.4630 740.8068 773.4988
 781.9411 817.0065 895.7154
 929.6121 951.0314 982.8415
 1003.5065 1027.2667 1054.3042
 1073.4743 1098.3138 1107.4900
 1126.6260 1188.4206 1214.3041
 1307.0080 1329.0713 1386.3589
 1393.8406 1479.6219 1489.5679
 1602.1599 3040.7887 3074.0033
 3133.1293 3186.7242 3198.9747
 3210.0933 3228.9057 3231.2875

i21 – p15

Cartesian coordinates

C -1.352434 -0.215696 0.178580
 C -0.393227 -1.328823 -0.182059
 C 1.043505 -0.986878 0.223021
 C 0.461475 1.389149 -0.113369
 C 1.397586 0.433353 -0.132356
 C -0.918460 1.061124 0.224277
 H -2.354728 -0.467105 0.506398
 H -2.390557 -0.054238 -1.612033

H -0.704638 -2.264863 0.287460
 H -0.437629 -1.492897 -1.265587
 H 1.166235 -1.108969 1.309321
 H 1.738837 -1.688239 -0.244612
 H 0.719427 2.423323 -0.314105
 H 2.434101 0.677727 -0.340368
 H -1.601710 1.861884 0.484965

Frequencies

-607.3534 181.6977 231.9274
 355.3693 376.4794 494.1986
 528.4704 572.8834 707.4698
 763.7739 820.2542 864.8459
 942.4170 979.5974 993.4689
 1003.4981 1016.2208 1050.8622
 1085.7959 1184.1049 1204.5547
 1206.7331 1277.7535 1355.1985
 1373.5666 1410.3282 1446.9604
 1477.1261 1491.9946 1608.0698
 1709.1879 3006.1025 3041.1361
 3098.6745 3107.0153 3179.7061
 3192.9300 3203.1942 3215.3694

i21 – i22

Cartesian coordinates

C -0.216707 -1.423244 0.071620
 C 1.123265 -0.853898 -0.275791
 C 1.293245 0.585098 0.244827
 C -1.142664 0.914652 -0.122660
 C 0.096244 1.442535 -0.057852
 C -1.378695 -0.497704 0.063597
 H -0.901779 -0.923769 1.149582
 H -0.415699 -2.483810 -0.012609
 H 1.929973 -1.490472 0.097535
 H 1.216194 -0.831649 -1.372728
 H 1.452812 0.549037 1.332123
 H 2.199861 1.025317 -0.180658
 H -2.003081 1.554738 -0.285517
 H 0.240580 2.510472 -0.178698
 H -2.366989 -0.914497 -0.091472

Frequencies

-1892.0762 209.1620 253.1101
 478.2811 504.3077 519.1432
 611.7858 699.7744 756.7935
 846.2815 859.2315 905.2159

959.4806	964.5417	1011.7301
1032.3622	1074.9776	1139.8587
1177.4718	1181.6113	1259.5234
1268.3697	1336.9250	1340.2023
1389.3353	1399.0770	1453.3942
1484.2727	1494.1054	1631.1853
2186.9140	2986.8082	3013.0474
3085.2480	3091.3500	3183.9091
3192.3700	3209.5087	3220.1365

C	-2.076678	0.000015	0.001646
C	1.968065	0.000011	0.001022
C	0.513473	-0.000036	-0.005379
C	-0.707263	-0.000021	-0.001234
H	-2.630457	-0.930765	0.002598
H	-2.630382	0.930838	0.002621
H	2.361711	-0.887174	-0.501886
H	2.351878	0.002288	1.026138
H	2.361667	0.884995	-0.505801

i6 – i7

Cartesian coordinates

C	0.817041	0.674415	0.362220
C	1.836349	0.231654	-0.699449
C	2.481674	-0.773553	0.244420
C	-3.119863	-0.316321	-0.102300
C	-1.719120	0.052701	0.058777
C	-0.563298	0.371670	0.190415
H	1.043062	1.616929	0.857545
H	1.365524	-0.217100	-1.573706
H	2.499180	1.033132	-1.026519
H	2.265419	-1.826421	0.085476
H	1.453648	-0.256725	1.115239
H	3.462248	-0.547732	0.655515
H	-3.765350	0.563754	-0.039132
H	-3.432267	-1.019948	0.674244
H	-3.288157	-0.789286	-1.073167

Frequencies

-2137.6487	74.2984	103.9476
134.6442	197.1814	310.5559
349.7699	461.3063	528.1471
600.1264	733.7170	803.1322
900.1682	931.7819	980.3946
1029.1477	1051.0992	1061.0888
1105.2982	1203.8242	1230.4605
1267.4445	1322.1560	1364.7700
1420.2690	1434.9946	1487.3763
1489.2930	1500.9811	1792.8987
2338.3823	3045.3493	3097.8625
3115.6302	3117.9594	3122.9296
3144.9359	3159.0636	3232.0066

Products

p8+ethylene

Cartesian coordinates

Frequencies

24.1554	186.6524	207.4785
394.8964	423.6534	666.8736
777.9809	1034.4319	1034.6080
1055.0215	1259.9190	1417.2372
1468.5806	1478.8501	1479.6621
2166.3237	3036.9405	3103.5750
3118.1095	3157.2073	3254.3195

p7+methyl

Cartesian coordinates

C	1.470976	-0.481949	0.000040
C	2.400683	0.472376	-0.000002
C	-2.564865	0.160195	-0.000132
C	-1.124742	-0.060669	-0.000101
C	0.065458	-0.236081	0.000035
H	1.772148	-1.526432	0.000010
H	2.133433	1.522977	0.000021
H	3.454690	0.220975	-0.000109
H	-2.891166	0.593027	0.949058
H	-3.101405	-0.780156	-0.147452
H	-2.852762	0.846381	-0.800569

Frequencies

62.2203	144.1056	175.7482
333.9529	382.9890	546.2987
701.5039	727.1909	953.0699
1014.4842	1051.7153	1054.9339
1063.0179	1200.1488	1323.8088
1419.4363	1449.4851	1484.5871
1487.1699	1707.5821	2378.7205
3052.4247	3123.0037	3128.8760
3156.9526	3167.8921	3255.8417

p1+H

Cartesian coordinates

C	-1.799390	1.273345	0.000019
C	-1.132296	0.117268	-0.000004
C	-1.818521	-1.225098	0.000014
C	2.958577	-0.044539	0.000012
C	1.502871	0.020444	-0.000083
C	0.301881	0.089704	-0.000047
H	-2.883777	1.288817	0.000042
H	-1.280356	2.224030	0.000013
H	-1.525684	-1.803706	-0.880515
H	-2.903779	-1.109999	0.000122
H	-1.525506	-1.803763	0.880446
H	3.367494	0.420282	0.900801
H	3.370302	0.478687	-0.866794
H	3.302581	-1.081086	-0.033583

Frequencies

8.7783	106.2884	118.7892
193.6163	278.1005	294.8696
393.5194	470.2445	517.1423
811.8176	825.8995	950.7315
997.8539	1054.9896	1057.9118
1073.1499	1133.8392	1207.6818
1322.2932	1337.6456	1417.4390
1420.9627	1482.3680	1484.0205
1484.7807	1495.4878	1739.4319
2379.6002	3033.3082	3043.3356
3092.9851	3114.1356	3118.1969
3123.0354	3148.5866	3166.9497

Frequencies

32.5100	115.5770	150.4823
187.0151	311.8288	362.1859
382.3357	551.7947	579.3082
664.3232	751.0505	938.0799
941.0601	1033.4445	1054.7238
1058.9928	1075.3225	1096.5341
1331.2636	1414.4198	1420.8557
1442.9417	1481.5879	1484.1234
1484.4506	1499.7290	1716.8907
2376.6073	3045.7299	3046.8104
3113.6989	3118.6806	3122.0681
3139.3336	3158.4242	3253.2032

p2+H

Cartesian coordinates

C	0.874227	-1.078398	0.000070
C	1.990408	-0.343307	0.000763
C	2.054984	1.149241	-0.000191
C	-2.936314	0.401962	0.000738
C	-1.575332	-0.119210	-0.001399
C	-0.449518	-0.544881	-0.001124
H	0.954207	-2.161511	0.000848
H	2.940218	-0.871830	0.002111
H	2.597666	1.511698	0.878894
H	1.058454	1.593503	-0.000331
H	2.597345	1.510502	-0.879980
H	-3.168089	0.878966	0.956639
H	-3.660870	-0.399594	-0.162334
H	-3.069665	1.145830	-0.788987

p3+H

Cartesian coordinates

C	0.719777	0.538998	0.000000
C	1.669194	-0.399127	0.000000
C	3.137071	-0.116410	0.000000
C	-3.298861	-0.203560	0.000000
C	-1.864884	0.056097	0.000000
C	-0.679463	0.262419	0.000000
H	1.004837	1.589196	0.000000
H	1.367715	-1.443851	0.000001
H	3.618476	-0.556977	0.879114
H	3.339258	0.957021	0.000003
H	3.618474	-0.556972	-0.879119
H	-3.863067	0.732300	0.000125
H	-3.591333	-0.775716	0.884329
H	-3.591371	-0.775503	-0.884456

Frequencies

84.4528	99.6158	101.4742
172.1500	264.6448	349.3442
414.2680	506.4172	606.6963
747.9298	792.4629	939.6487
994.7440	1055.3214	1060.9335
1068.5644	1104.1387	1179.7344
1276.9418	1398.6045	1420.0341
1444.2900	1482.7977	1483.6562
1486.9609	1491.7952	1726.8988
2375.5028	3043.2504	3048.6736
3100.2555	3119.2248	3123.5520
3144.2591	3168.9830	3189.9496

p5+H

Cartesian coordinates

C	0.819526	0.885875	-0.020313
C	1.775641	-0.207893	-0.425935
C	2.821042	-0.589269	0.293117
C	-3.089745	-0.423615	0.061371
C	-1.708476	0.044493	0.033614
C	-0.572221	0.431149	0.015133
H	0.898253	1.716031	-0.733000
H	1.104216	1.283766	0.958804
H	1.563273	-0.690413	-1.376829
H	3.486713	-1.373932	-0.048097
H	3.048080	-0.130858	1.251324
H	-3.751146	0.279560	-0.450873
H	-3.443335	-0.534462	1.089467
H	-3.180652	-1.394126	-0.432720

Frequencies

34.3562	74.7163	129.5401
204.0587	299.4692	397.7260
411.5196	488.9522	621.4057
798.1488	920.9544	944.5617
968.2193	1046.3428	1053.5903
1061.7062	1136.4715	1172.8460
1252.9540	1322.4014	1341.8008
1418.8581	1458.2373	1471.5895
1482.2145	1492.6037	1740.0986
2398.0456	3040.0941	3052.3726
3088.3526	3123.0952	3126.0686
3150.4889	3173.8349	3241.8593

p4+H**Cartesian coordinates**

C	-0.971884	-1.097343	0.000234
C	-2.059877	-0.050512	0.000316
C	-1.876814	1.261064	-0.000154
C	2.870796	0.387995	0.000590
C	1.510119	-0.138041	-0.000976
C	0.391998	-0.574827	-0.000816
H	-1.109664	-1.747980	-0.871997
H	-1.108493	-1.746759	0.873577
H	-3.069771	-0.454345	0.000939
H	-2.719228	1.943225	0.000022
H	-0.880367	1.690946	-0.000574
H	3.000803	1.133553	-0.787778
H	3.597438	-0.410909	-0.166603
H	3.103262	0.862246	0.957254

Frequencies

94.8602	106.0664	108.7344
204.3396	283.2157	391.3560
427.2512	565.7741	579.1319
774.4927	924.1401	948.4296
968.7201	1033.2157	1059.7159
1062.1799	1080.1128	1175.6459
1240.3235	1334.0865	1366.6070
1421.9722	1447.8136	1463.0789
1485.0771	1494.1451	1742.0048
2398.3944	3038.5794	3050.5564
3066.4233	3121.4125	3125.1322
3156.4640	3174.3382	3251.1409

p6+H**Cartesian coordinates**

C	0.813659	1.320923	-0.275810
C	1.149695	0.052323	0.498168
C	1.920368	-1.065811	-0.162716
C	-2.711277	-0.402583	-0.046071
C	-1.463764	-0.024158	0.015448
C	-0.235460	0.344609	0.079631
H	0.829175	2.267811	0.254026
H	1.119983	1.372656	-1.316638
H	1.356564	0.197620	1.555772
H	1.693975	-2.025369	0.308669
H	2.997525	-0.892703	-0.085839
H	1.658879	-1.142223	-1.221256
H	-3.422969	-0.118610	0.722116
H	-3.072461	-1.010998	-0.868750

Frequencies

114.5576	168.3578	232.0578
318.8692	353.3476	427.1496
559.8137	611.1567	664.0948
816.8952	866.6736	895.7588
968.8673	980.5619	1027.1045
1050.4154	1084.7405	1126.8690
1140.9489	1181.0818	1336.8395
1401.8999	1426.6432	1466.6710
1493.5565	1506.3712	1558.9026
2141.4012	3048.2073	3122.4442
3125.2357	3127.3272	3149.3203
3151.1396	3214.6816	3231.3549

p9+methyl

Cartesian coordinates

C	-1.169070	-0.303021	0.000004
C	0.023791	-1.212423	0.000008
C	1.180323	-0.257347	-0.000041
C	0.714096	1.000478	-0.000005
C	-0.752798	0.972089	0.000007
H	-2.193362	-0.650027	-0.000084
H	0.036137	-1.869687	0.878658
H	0.036063	-1.869951	-0.878450
H	2.217752	-0.562788	-0.000014
H	1.310954	1.903469	0.000076
H	-1.385597	1.850329	-0.000031

Frequencies

334.4510	530.6072	680.0477
718.7326	818.2709	819.8509
921.1516	934.6993	972.1620
974.9127	981.6375	1020.9599
1109.3169	1129.5792	1138.8857
1276.7760	1323.8013	1400.6223
1416.6582	1590.1458	1671.2482
3044.0381	3078.2653	3209.6559
3219.9733	3240.0396	3247.0414

p10+H

Cartesian coordinates

C	-1.511265	0.739943	-0.000013
C	-1.581743	-0.598903	-0.000055
C	-0.189759	-1.159537	0.000028
C	2.178360	0.004947	-0.000029
C	0.686418	0.065367	0.000036
C	-0.103784	1.152066	0.000031
H	-2.350630	1.423815	0.000013
H	-2.479490	-1.201788	-0.000080
H	0.000225	-1.788729	0.879041
H	0.000381	-1.788973	-0.878768
H	2.554357	-0.526943	0.880390
H	2.613254	1.006460	-0.000245
H	2.554206	-0.527223	-0.880346
H	0.238334	2.180093	0.000002

Frequencies

118.9289	224.6416	324.1392
357.3420	530.2449	623.0746
700.6152	826.6114	854.7542

892.7581	913.8943	961.6803
975.3673	1003.0898	1029.6012
1054.8464	1125.1530	1149.2161
1195.7828	1263.7610	1338.9287
1390.6110	1413.6708	1422.7750
1480.9634	1496.4859	1621.5608
1701.4480	3037.7802	3043.7829
3077.9287	3094.3752	3133.6518
3210.1504	3220.5251	3242.5806

p11+H

Cartesian coordinates

C	1.435256	0.804076	-0.000004
C	1.531520	-0.693179	-0.000005
C	0.094929	-1.122956	0.000011
C	-2.199308	-0.003879	-0.000008
C	-0.704536	-0.043622	0.000016
C	0.143704	1.160443	0.000006
H	2.290026	1.466947	-0.000019
H	2.073261	-1.065413	-0.878843
H	2.073284	-1.065418	0.878814
H	-0.228033	-2.156097	-0.000001
H	-2.623431	-1.009681	-0.000014
H	-2.576345	0.525494	-0.880796
H	-2.576389	0.525511	0.880750
H	-0.241757	2.173355	0.000014

Frequencies

134.0049	230.5913	325.7138
365.0139	579.0625	624.0601
717.3706	752.9477	826.3008
918.4687	929.8578	948.8845
966.9954	984.6045	1025.5842
1069.3647	1103.3583	1131.3969
1224.5052	1260.5079	1310.9459
1398.1239	1421.8577	1428.1615
1482.2892	1498.8394	1613.6091
1714.2317	3045.1175	3045.3193
3078.3457	3104.3281	3138.1374
3210.3421	3223.3858	3240.3404

p12+H

Cartesian coordinates

C	-1.307972	0.882651	0.001900
C	-1.524600	-0.606575	-0.063655
C	-0.098242	-1.190920	0.067164

C	2.164330	-0.015502	-0.045268	736.7955	791.4135	816.0065
C	0.833865	0.009483	0.013629	881.5165	955.4149	975.4720
C	-0.014130	1.204423	0.036263	975.4978	1002.5103	1026.9264
H	-2.126002	1.593468	-0.001406	1087.5171	1098.2208	1110.3170
H	-2.194331	-0.955538	0.728257	1150.8865	1269.5459	1290.7110
H	-1.996045	-0.884366	-1.012931	1326.3120	1404.1776	1418.3285
H	0.023051	-1.706703	1.023443	1498.0551	1499.1851	1596.2573
H	0.132029	-1.911422	-0.719935	1675.6847	3018.6302	3046.3084
H	2.741347	0.902495	-0.070367	3123.9025	3128.6960	3207.3103
H	2.714129	-0.950038	-0.070753	3217.3584	3236.8499	3243.8601
H	0.386322	2.210743	0.063492			

Frequencies

80.1020	295.1949	361.8882
520.3069	637.3301	682.8119
775.3298	805.7151	848.0347
868.5634	903.6773	926.2378
966.2778	990.8236	1023.7847
1040.6534	1125.4181	1180.9280
1248.5519	1277.2910	1292.1506
1342.1352	1377.5927	1456.4281
1480.1631	1506.4256	1680.8906
1745.3104	3051.8353	3074.7644
3087.1075	3123.9757	3153.6708
3208.2941	3232.8064	3241.0541

p13+H

Cartesian coordinates

C	-1.423399	-0.734327	-0.174445
C	-1.423427	0.734288	-0.174455
C	-0.208676	1.172483	0.184145
C	1.980278	0.000005	-0.380794
C	0.694236	0.000019	0.455081
C	-0.208637	-1.172471	0.184175
H	-2.277801	-1.349236	-0.427347
H	-2.277884	1.349136	-0.427315
H	0.108730	2.203357	0.273836
H	1.738920	-0.000289	-1.446610
H	2.584866	-0.884450	-0.164641
H	2.584588	0.884757	-0.165075
H	0.967471	0.000067	1.521067
H	0.108860	-2.203321	0.273846

Frequencies

168.1150	237.3471	297.6431
546.1185	566.5988	721.3589

p14+H

Cartesian coordinates

C	1.474123	0.664036	-0.029535
C	1.474122	-0.664036	-0.029538
C	0.082213	-1.236522	0.036058
C	-2.129448	0.000000	-0.035748
C	-0.804377	0.000000	0.013908
C	0.082213	1.236521	0.036057
H	2.361706	1.284802	-0.062267
H	2.361706	-1.284801	-0.062274
H	-0.133337	-1.905266	-0.804509
H	-0.069752	-1.822329	0.950602
H	-2.695153	0.925800	-0.057417
H	-2.695153	-0.925800	-0.057419
H	-0.133333	1.905255	-0.804519
H	-0.069757	1.822339	0.950593

Frequencies

38.6151	367.1051	374.3601
435.8276	626.1713	698.1519
701.7746	797.7001	826.3721
922.9503	929.7765	945.9881
988.6374	988.8271	998.5234
1007.1779	1126.8781	1171.6057
1196.9855	1259.2491	1303.4046
1306.8842	1377.0903	1449.8336
1467.1880	1473.5736	1715.1671
1763.2751	3040.4855	3042.5151
3073.8634	3073.9765	3147.4558
3195.5562	3221.0341	3232.5380

p15+H

Cartesian coordinates

C	-1.188484	-0.723196	0.250560
C	-1.188101	0.723773	-0.250621

C	0.112106	1.417928	0.063127	547.7452	582.6579	630.7131
C	1.252440	0.724947	0.110077	728.5501	869.6169	904.7520
C	1.252054	-0.725525	-0.110153	962.0939	967.4598	979.3249
C	0.111386	-1.417977	-0.063013	990.4649	1015.3736	1033.7863
H	-2.033738	-1.268215	-0.177023	1057.5572	1197.1774	1237.9043
H	-1.331280	-0.735534	1.341474	1237.9407	1242.3994	1375.6437
H	-1.330785	0.736194	-1.341538	1401.1077	1427.0936	1449.4048
H	-2.033093	1.269205	0.176952	1471.3891	1473.6879	1741.5939
H	0.113021	2.495490	0.191786	1787.9959	3016.8388	3018.0292
H	2.198123	1.224752	0.290846	3035.0505	3036.1626	3166.7591
H	2.197374	-1.226031	-0.290856	3167.1991	3190.1750	3192.7673
H	0.111969	-2.495561	-0.191510			

Frequencies

197.1717	306.1000	482.2071
529.6251	574.5856	689.4616
764.8536	794.0711	867.1909
945.0995	972.2335	994.9021
1009.9445	1020.5106	1053.5992
1084.8341	1182.0964	1194.9929
1208.2698	1275.9947	1355.9404
1369.4236	1411.4225	1446.2853
1476.7467	1489.1535	1682.1519
1737.2803	3003.9400	3013.4173
3098.9693	3099.5757	3177.7293
3184.2256	3200.4921	3210.1197

p16+H

Cartesian coordinates

C	-1.494599	0.000055	-0.000006
C	-0.663703	1.251311	0.000001
C	0.663802	1.251275	0.000002
C	1.494599	-0.000054	-0.000001
C	0.663704	-1.251311	0.000002
C	-0.663802	-1.251274	0.000002
H	-2.164642	0.000087	-0.870624
H	-2.164618	0.000088	0.870635
H	-1.199095	2.196650	0.000007
H	1.199264	2.196571	0.000007
H	2.164607	-0.000087	-0.870650
H	2.164651	-0.000088	0.870610
H	1.199094	-2.196651	0.000004
H	-1.199265	-2.196570	0.000007

Frequencies

115.9479	391.8013	401.3328
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p17+H

Cartesian coordinates

C	-1.461653	0.178611	0.204084
C	-0.652539	1.203498	-0.055562
C	0.712288	0.745431	-0.441352
C	1.450745	-0.019286	0.635388
C	0.645355	-0.769796	-0.387076
C	-0.787271	-1.153778	-0.035175
H	-2.480016	0.264368	0.564377
H	-0.919321	2.249615	0.036889
H	1.279178	1.275486	-1.197244
H	1.070935	0.054770	1.649194
H	2.529395	-0.085828	0.551314
H	1.184226	-1.367114	-1.111651
H	-0.838238	-1.805431	0.844284
H	-1.267709	-1.693942	-0.859002

Frequencies

285.0100	359.3661	487.1619
684.3881	731.1266	780.4651
786.0365	816.1657	896.0815
933.5528	949.0481	964.4280
1010.7151	1028.2668	1056.5958
1075.8637	1095.0570	1105.0721
1138.3332	1193.0954	1213.5786
1310.3644	1333.3834	1387.8800
1395.8132	1479.4064	1488.7078
1696.2170	3040.0384	3074.8708
3133.2958	3189.8529	3202.7781
3204.6859	3227.4341	3230.3036

p18+H

Cartesian coordinates

C	1.461653	0.178611	0.204084
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C	0.787271	-1.153778	-0.035175
C	-0.645355	-0.769796	-0.387076
C	-1.450745	-0.019286	0.635388
C	-0.712288	0.745431	-0.441352
C	0.652539	1.203498	-0.055562
H	2.480016	0.264368	0.564377
H	1.267709	-1.693942	-0.859002
H	0.838238	-1.805432	0.844284
H	-1.184226	-1.367114	-1.111651
H	-2.529395	-0.085828	0.551314
H	-1.070935	0.054770	1.649194
H	-1.279178	1.275486	-1.197244
H	0.919321	2.249615	0.036889

H	1.230928	-0.924159	0.000106
H	1.231231	0.924011	-0.000084

Frequencies

840.1622	983.0978	991.7761
1072.6034	1241.8730	1388.1884
1471.0756	1715.5501	3141.5279
3161.6164	3223.3876	3249.8270

Frequencies

285.0100	359.3662	487.1620
684.3881	731.1266	780.4651
786.0365	816.1657	896.0815
933.5528	949.0481	964.4280
1010.7151	1028.2668	1056.5958
1075.8637	1095.0570	1105.0721
1138.3332	1193.0954	1213.5786
1310.3644	1333.3834	1387.8800
1395.8132	1479.4064	1488.7078
1696.2169	3040.0384	3074.8708
3133.2958	3189.8529	3202.7781
3204.6859	3227.4341	3230.3036

Fragments

methyl

Cartesian coordinates

C	-0.000147	0.000018	0.0
H	0.598306	-0.900124	-0.0
H	0.481424	0.967479	-0.0
H	-1.078846	-0.067462	-0.0

Frequencies

470.9451	1399.8856	1409.5749
3117.6199	3301.0861	3304.8947

ethylene

Cartesian coordinates

C	-0.662232	0.000081	0.000063
C	0.662191	0.000019	-0.000024
H	-1.231178	0.923815	-0.000033
H	-1.230737	-0.924266	-0.000223