Supplementary information

A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl (CH3CC, X2A1) – Propylene (CH3CHCH2, X1A′) System and the Formation of 1,3-dimethylvinylacetylene (CH3CCCHCHCH3, X1A′) under Single Collision Conditions

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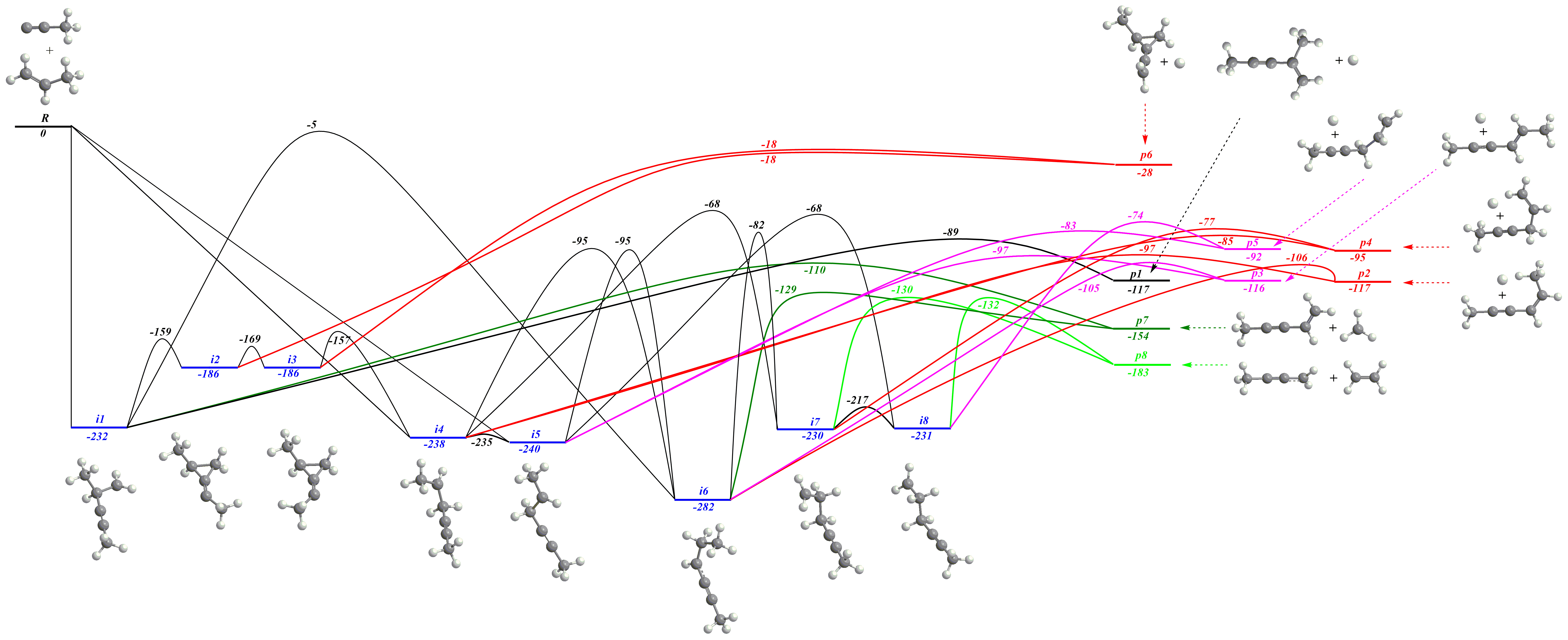


Figure S1. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with Propylene (CH3CHCH2, X1A′) calculated at the CCSD(T)-F12/cc-pVTZ-F12//ωB97X-D/6-311G(d,p) level of theory. Relative energies of various species are shown in kJ mol–1. Part I.

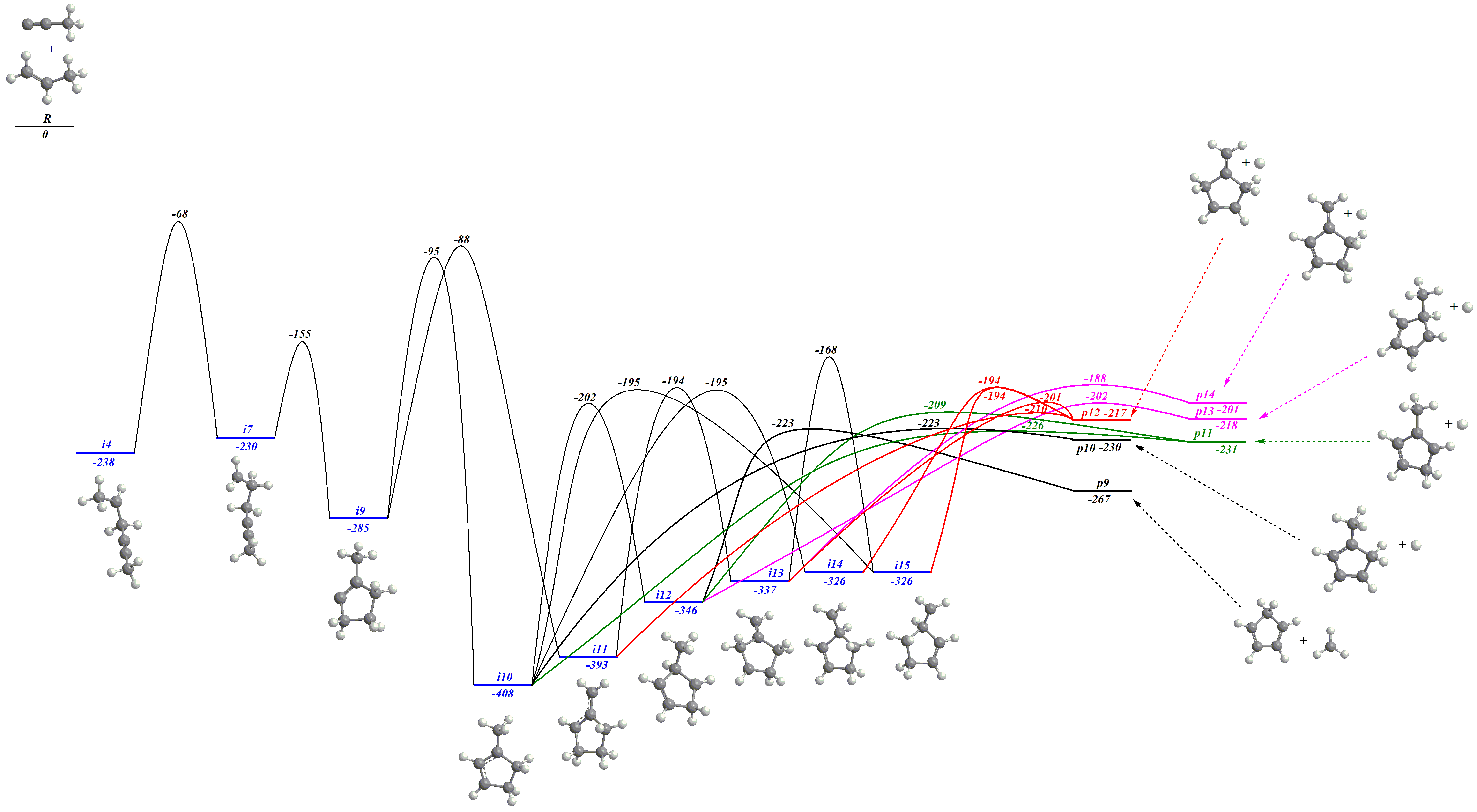


Figure S2. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with Propylene (CH3CHCH2, X1A′) calculated at the CCSD(T)-F12/cc-pVTZ-F12//ωB97X-D/6-311G(d,p) level of theory. Relative energies of various species are shown in kJ mol–1. Part II.

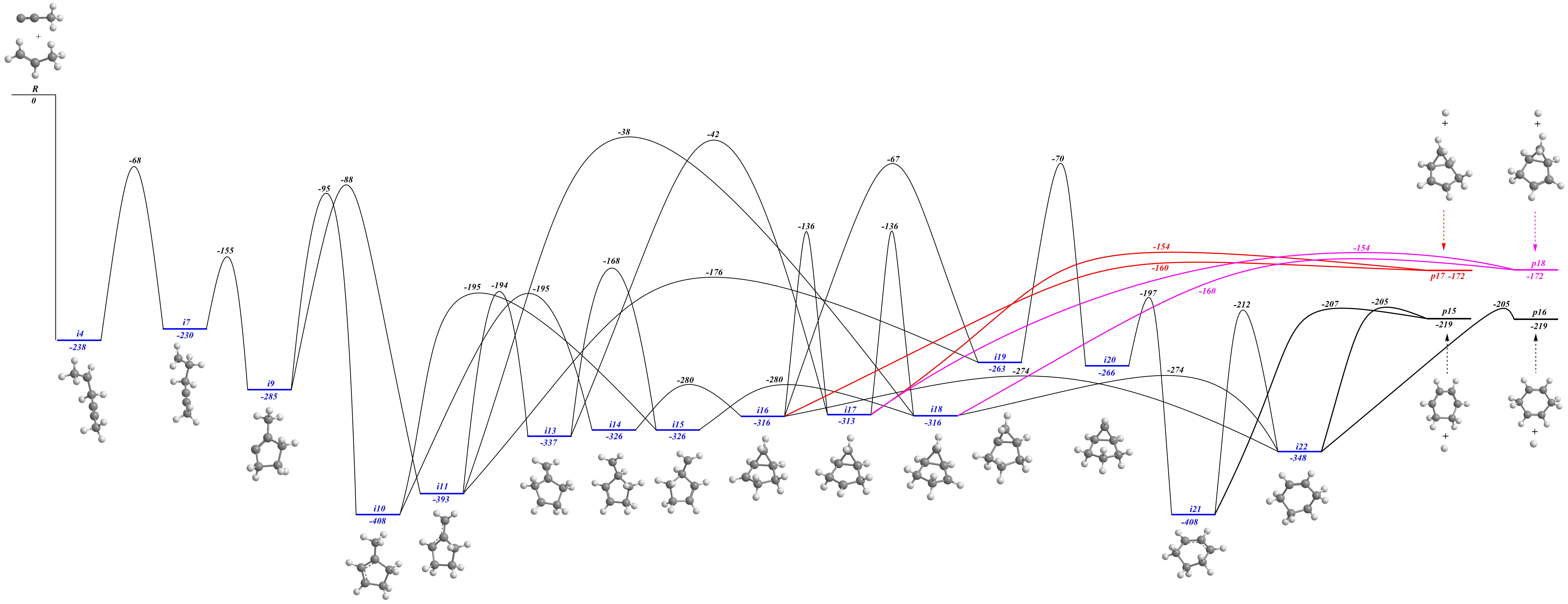


Figure S3. Potential energy surface for the bimolecular reaction of the 1-propynyl (CH3CC; X2A1) radical with Propylene (CH3CHCH2, X1A′) calculated at the CCSD(T)-F12/cc-pVTZ-F12//ωB97X-D/6-311G(d,p) level of theory. Relative energies of various species are shown in kJ mol–1. Part III.

Table S1. Statistical branching ratios (%) for the reaction of 1-propynyl + propene with ***i1*** and ***i4/i5*** as initial intermediates at different collision energies (*EC,* kJ mol–1)

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | ***i1*** | | ***i4/i5*** | |
| *EC* | **0** | **37** | **0** | **37** |
| ***p1*** | 0.4 | 0.6 | 0.4 | 0.5 |
| ***p2*** | 4.3 | 4.6 | 5.4 | 7.7 |
| ***p3*** | 6.0 | 6.5 | 7.6 | 11.0 |
| ***p4*** | 0.9 | 1.4 | 1.2 | 2.4 |
| ***p5*** | 2.1 | 3.5 | 2.7 | 5.8 |
| ***p6*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p7*** | 86.1 | 83.1 | 82.5 | 72.1 |
| ***p8*** | 0.2 | 0.3 | 0.2 | 0.5 |
| ***p9*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p10*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p11*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p12*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p14*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p14*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p15*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p16*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p17*** | 0.0 | 0.0 | 0.0 | 0.0 |
| ***p18*** | 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 (*EC,* kJ mol–1)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| ***EC*** | 0 | | 37 | | ***EC*** | 0 | | 37 | |
| **Reaction step** | *k(E)* | *E* | *k(E)* | *E* | **Reaction step** | *k(E)* | *E* | *k(E)* | *E* |
| ***i4 – i3*** | 2.63E+09 | 238 | 5.67E+09 | 275 | ***i14 – i10*** | 3.96E+08 | 326 | 8.99E+08 | 363 |
| ***i3 – i4*** | 2.83E+12 | 186 | 4.10E+12 | 223 | ***i13 – p12*** | 3.79E+09 | 337 | 9.33E+09 | 374 |
| ***i1 – i2*** | 1.49E+08 | 232 | 2.91E+08 | 269 | ***i13 – p14*** | 1.39E+09 | 337 | 3.85E+09 | 374 |
| ***i2 – i1*** | 3.22E+12 | 186 | 4.56E+12 | 223 | ***i12 – p9*** | 1.01E+10 | 346 | 2.12E+10 | 383 |
| ***i5 – p3*** | 5.90E+06 | 240 | 4.11E+07 | 277 | ***i12 – p11*** | 1.09E+09 | 346 | 2.59E+09 | 383 |
| ***i5 – p5*** | 2.13E+06 | 240 | 2.22E+07 | 277 | ***i12 – p13*** | 1.52E+09 | 346 | 3.87E+09 | 383 |
| ***i5 – i6*** | 6.06E+06 | 240 | 3.62E+07 | 277 | ***i4 – i6*** | 8.61E+06 | 238 | 5.05E+07 | 275 |
| ***i6 – i5*** | 1.26E+05 | 282 | 9.90E+05 | 319 | ***i6 – i4*** | 5.14E+04 | 282 | 4.00E+05 | 319 |
| ***i6 – p7*** | 3.57E+07 | 282 | 1.79E+08 | 319 | ***i5 – i4*** | 2.27E+12 | 240 | 2.34E+12 | 277 |
| ***i6 – p3*** | 4.70E+05 | 282 | 3.68E+06 | 319 | ***i4 – i5*** | 7.89E+12 | 238 | 8.08E+12 | 275 |
| ***i5 – i8*** | 8.58E+04 | 240 | 1.02E+06 | 277 | ***i20 – i19*** | 6.55E+04 | 266 | 6.62E+05 | 303 |
| ***i8 – i5*** | 3.08E+05 | 231 | 3.45E+06 | 268 | ***i19 – i20*** | 1.12E+05 | 263 | 1.12E+06 | 300 |
| ***i8 – p5*** | 7.23E+05 | 231 | 9.01E+06 | 268 | ***i13 – i17*** | 4.18E+00 | 337 | 2.20E+02 | 374 |
| ***i4 – i7*** | 3.05E+05 | 238 | 3.54E+06 | 275 | ***i17 – i13*** | 1.33E+02 | 313 | 6.40E+03 | 350 |
| ***i7 – i4*** | 9.27E+05 | 230 | 1.02E+07 | 267 | ***i13 – i15*** | 2.20E+07 | 337 | 6.92E+07 | 374 |
| ***i4 – p4*** | 3.26E+06 | 238 | 3.12E+07 | 275 | ***i15 – i13*** | 2.28E+07 | 326 | 6.79E+07 | 363 |
| ***i4 – p2*** | 1.45E+07 | 238 | 9.92E+07 | 275 | ***i7 – p8*** | 9.04E+09 | 230 | 2.92E+10 | 267 |
| ***i9 – i10*** | 2.57E+06 | 285 | 1.95E+07 | 322 | ***i14 – i16*** | 7.59E+10 | 326 | 9.50E+10 | 363 |
| ***i10 – i9*** | 1.59E+02 | 408 | 1.96E+03 | 445 | ***i16 – i14*** | 1.30E+12 | 316 | 1.59E+12 | 353 |
| ***i7 – i9*** | 1.21E+09 | 230 | 2.41E+09 | 267 | ***i14 – p12*** | 4.47E+08 | 326 | 1.10E+09 | 363 |
| ***i9 – i7*** | 2.50E+09 | 285 | 7.60E+09 | 322 | ***i15 – p12*** | 4.52E+08 | 326 | 1.11E+09 | 363 |
| ***i9 – i11*** | 5.67E+05 | 285 | 4.19E+06 | 322 | ***i15 – i18*** | 7.66E+10 | 326 | 9.59E+10 | 363 |
| ***i11 – i9*** | 3.94E+02 | 393 | 4.52E+03 | 430 | ***i18 – i15*** | 1.30E+12 | 316 | 1.59E+12 | 353 |
| ***i11 – p12*** | 1.09E+09 | 393 | 3.09E+09 | 430 | ***i10 – i15*** | 5.79E+06 | 408 | 1.80E+07 | 445 |
| ***i10 – p10*** | 2.66E+08 | 408 | 7.22E+08 | 445 | ***i15 – i10*** | 4.00E+08 | 326 | 9.07E+08 | 363 |
| ***i10 – p11*** | 3.75E+08 | 408 | 9.96E+08 | 445 | ***i22 – p15*** | 2.34E+09 | 348 | 5.75E+09 | 385 |
| ***i3 – i2*** | 4.71E+12 | 186 | 5.81E+12 | 223 | ***i22 – p16*** | 3.02E+09 | 348 | 7.38E+09 | 385 |
| ***i2 – i3*** | 6.19E+12 | 186 | 7.66E+12 | 223 | ***i16 – i22*** | 9.41E+11 | 316 | 1.17E+12 | 353 |
| ***i3 – p6*** | 5.44E+02 | 186 | 1.49E+05 | 223 | ***i22 – i16*** | 6.48E+10 | 348 | 9.29E+10 | 385 |
| ***i8 – i7*** | 9.03E+11 | 231 | 1.01E+12 | 268 | ***i16 – i19*** | 1.15E+03 | 316 | 1.58E+04 | 353 |
| ***i7 – i8*** | 2.66E+12 | 230 | 2.97E+12 | 267 | ***i19 – i16*** | 1.29E+05 | 263 | 1.39E+06 | 300 |
| ***i11 – i18*** | 1.61E-01 | 393 | 1.41E+01 | 430 | ***i18 – i17*** | 8.67E+06 | 313 | 3.45E+07 | 350 |
| ***i18 – i11*** | 3.36E+01 | 316 | 2.21E+03 | 353 | ***i17 – i18*** | 1.57E+07 | 313 | 6.16E+07 | 350 |
| ***i2 – p6*** | 9.20E+02 | 186 | 2.44E+05 | 223 | ***i17 – i16*** | 1.57E+07 | 313 | 6.16E+07 | 350 |
| ***i1 – p7*** | 1.63E+07 | 232 | 8.05E+07 | 269 | ***i16 – i17*** | 8.68E+06 | 316 | 3.45E+07 | 353 |
| ***i1 – p1*** | 8.39E+04 | 232 | 6.44E+05 | 269 | ***i16 – p17*** | 1.81E+08 | 316 | 6.03E+08 | 353 |
| ***i1 – i6*** | 2.06E-03 | 232 | 2.31E+00 | 269 | ***i20 – i21*** | 6.67E+10 | 266 | 1.09E+11 | 303 |
| ***i6 – i1*** | 1.90E-04 | 282 | 3.01E-01 | 319 | ***i21 – i20*** | 5.36E+06 | 408 | 1.60E+07 | 445 |
| ***i8 – p1*** | 1.77E+09 | 231 | 5.55E+09 | 268 | ***i11 – i19*** | 1.99E+06 | 393 | 6.97E+06 | 430 |
| ***i11 – i13*** | 3.32E+07 | 393 | 9.88E+07 | 430 | ***i19 – i11*** | 4.69E+10 | 263 | 9.56E+10 | 300 |
| ***i13 – i11*** | 3.94E+08 | 337 | 9.47E+08 | 374 | ***i18 – p18*** | 1.80E+08 | 316 | 6.02E+08 | 353 |
| ***i10 – i12*** | 3.59E+06 | 408 | 1.05E+07 | 445 | ***i17 – p18*** | 1.85E+08 | 313 | 6.48E+08 | 350 |
| ***i12 – i10*** | 2.93E+08 | 346 | 6.85E+08 | 383 | ***i17 – p17*** | 1.85E+08 | 313 | 6.49E+08 | 350 |
| ***i7 – p4*** | 1.93E+06 | 230 | 2.08E+07 | 267 | ***i21 – p15*** | 4.00E+08 | 408 | 1.20E+09 | 445 |
| ***i18 – i22*** | 4.70E+11 | 316 | 5.87E+11 | 353 | ***i21 – i22*** | 1.68E+08 | 408 | 4.50E+08 | 445 |
| ***i22 – i18*** | 3.24E+10 | 348 | 4.65E+10 | 385 | ***i22 – i21*** | 1.09E+09 | 348 | 2.34E+09 | 385 |
| ***i6 – p2*** | 4.90E+05 | 282 | 3.66E+06 | 319 | ***i6 – i7*** | 5.67E+03 | 282 | 5.54E+04 | 319 |
| ***i10 – i14*** | 5.79E+06 | 408 | 1.80E+07 | 445 | ***i7 – i6*** | 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)*, s–1 |
| ***i1-p1*** | 2.80E+05 – 1.47E+06 |
| ***i4-p2*** | 4.42E+07 – 2.21E+08 |
| ***i6-p2*** | 1.71E+06 – 7.77E+06 |
| ***i5-p3*** | 1.83E+07 – 9.16E+07 |
| ***i6-p3*** | 1.71E+06 – 7.83E+06 |
| ***i4-p4*** | 1.35E+07 – 7.14E+07 |
| ***i7-p4*** | 8.82E+06 – 4.87E+07 |
| ***i5-p5*** | 9.54E+06 – 5.10E+07 |
| ***i8-p5*** | 3.77E+06 – 2.14E+07 |
| ***i2-p6*** | 7.66E+04 – 7.50E+05 |
| ***i3-p6*** | 4.68E+04 – 4.62E+05 |

## Table S4. Total rates of formation for products p2 and p3 from i6 (Ecol = 37 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

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

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

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

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

**Frequencies**

102.7242 103.9810 166.3498

230.7671 262.1611 375.3720

424.7671 496.1699 673.1810

787.7788 860.6261 904.8513

948.6809 1038.8483 1047.4609

1052.9777 1071.4325 1086.7954

1125.5009 1178.8839 1199.7254

1367.9962 1397.5528 1421.4529

1466.2992 1467.6031 1480.1392

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

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

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

**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

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

***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

C 0.011888 1.261825 0.167811

H 0.120611 1.722064 1.163269

H -2.236550 1.459064 -0.176350

H -2.309618 -1.144432 0.259816

H -1.551142 -0.951643 -1.313238

H -0.189115 -1.367002 1.374463

H 0.259646 -2.097004 -0.170937

H 2.720273 0.810478 -0.377029

H 2.636430 -1.037895 -0.286166

H 0.349216 2.018860 -0.551342

**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**

119.7845 132.0009 292.7179

336.4880 458.6359 536.9615

585.7098 735.6350 766.3563

852.7636 870.9209 910.9852

950.3286 977.4537 1005.9040

1029.8507 1106.4345 1116.3103

1148.1663 1195.2313 1228.6932

1284.8842 1288.1170 1325.1715

1341.0723 1390.7056 1464.5697

1484.5154 1505.2048 1712.1427

2912.0116 3035.2865 3062.7404

3094.7661 3126.2291 3152.1371

3197.6399 3223.8278 3260.2217

***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

**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

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

***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

***i6 – 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

***i6 – 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

**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

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

***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

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

**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

***i1 – p1***

**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

***i1 – 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

**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

***i11 – i13***

**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

1481.8451 1500.3666 1693.4450

2197.1841 2998.7812 3039.2988

3097.7711 3130.0129 3159.4922

3221.1922 3238.4506 3248.6532

***i10 – i12***

**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

**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

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

***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

***i12 – 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

***i12 – 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

***i12 – 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

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

**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

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

***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

H -1.082211 1.442793 -1.213842

H 2.811503 -1.571723 0.517284

H 3.622116 -0.013344 0.716524

H 3.399106 -0.695610 -0.901359

C -2.120986 -0.111639 0.556311

C -2.227089 -1.171091 -0.296070

H -2.900259 0.643905 0.571573

H -1.543285 -0.210620 1.468715

H -2.928639 -1.161592 -1.122796

H -1.545359 -2.011269 -0.233675

**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**

-644.4294 183.2529 355.3790

372.0551 546.7042 633.9784

668.5600 696.6698 782.3048

807.7675 868.3288 879.2344

923.9567 958.6695 972.4201

1015.5546 1084.7042 1111.4222

1119.6653 1196.7575 1211.1387

1253.1452 1305.5708 1316.9224

1360.3530 1374.0708 1453.8998

1468.6383 1484.0585 1499.5343

3012.5148 3068.7076 3083.3692

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

***i16 – i19***

**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

***i17 – i18***

**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

***i16 – i17***

**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

**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

***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

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

***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

**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

***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**

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

**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**

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

***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**

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

***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

**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

C 0.833865 0.009483 0.013629

C -0.014130 1.204423 0.036263

H -2.126002 1.593468 -0.001406

H -2.194331 -0.955538 0.728257

H -1.996045 -0.884366 -1.012931

H 0.023051 -1.706703 1.023443

H 0.132029 -1.911422 -0.719935

H 2.741347 0.902495 -0.070367

H 2.714129 -0.950038 -0.070753

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

736.7955 791.4135 816.0065

881.5165 955.4149 975.4720

975.4978 1002.5103 1026.9264

1087.5171 1098.2208 1110.3170

1150.8865 1269.5459 1290.7110

1326.3120 1404.1776 1418.3285

1498.0551 1499.1851 1596.2573

1675.6847 3018.6302 3046.3084

3123.9025 3128.6960 3207.3103

3217.3584 3236.8499 3243.8601

***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

C 1.252440 0.724947 0.110077

C 1.252054 -0.725525 -0.110153

C 0.111386 -1.417977 -0.063013

H -2.033738 -1.268215 -0.177023

H -1.331280 -0.735534 1.341474

H -1.330785 0.736194 -1.341538

H -2.033093 1.269205 0.176952

H 0.113021 2.495490 0.191786

H 2.198123 1.224752 0.290846

H 2.197374 -1.226031 -0.290856

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

547.7452 582.6579 630.7131

728.5501 869.6169 904.7520

962.0939 967.4598 979.3249

990.4649 1015.3736 1033.7863

1057.5572 1197.1774 1237.9043

1237.9407 1242.3994 1375.6437

1401.1077 1427.0936 1449.4048

1471.3891 1473.6879 1741.5939

1787.9959 3016.8388 3018.0292

3035.0505 3036.1626 3166.7591

3167.1991 3190.1750 3192.7673

***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

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

**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

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