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Computational study of a new Heck reaction mechanism catalyzed by palladium(II/IV) species

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Table S1: absolute energies (hartree) for all species enumerated in the paper All energies obtained with the pruned (99,590) grid (except for B3LYP/B\_large, where the pruned (75,302) grid was used) at the geometries given elsewhere in the same supplementary material collection

|                                | <b>E</b><br><b>(B3LYP/lanl2dz)</b> | <b>E (B3LYP/lanl2dz+p//</b><br><b>B3LYP/lanl2dz)</b> | <b>E (B3LYP/B_large)//</b><br><b>B3LYP/lanl2dz</b> | <b>E (mPW1PW91/lanl2dz+p//</b><br><b>B3LYP/lanl2dz)</b> | <b>H<sub>298</sub></b><br><b>(B3LYP/lanl2dz)</b> | <b>G<sub>298</sub></b><br><b>(B3LYP/lanl2dz)</b> |
|--------------------------------|------------------------------------|--|--|---|--|--|
| <b>1<sub>(0-II)</sub></b>      | <b>-220.7296935</b>                | <b>-220.8181172</b>                                  | <b>-891.7803813</b>                                | <b>-220.8492143</b>                                     | <b>-220.628242</b>                               | <b>-220.669891</b>                               |
| <b>2<sub>(0-II)</sub></b>      | <b>-299.3485844</b>                | <b>-299.4459432</b>                                  | <b>-970.4424745</b>                                | <b>-299.4598343</b>                                     | <b>-299.189879</b>                               | <b>-299.239399</b>                               |
| <b>3<sub>(0-II)</sub></b>      | <b>-463.7365533</b>                | <b>-463.8754319</b>                                  | <b>-1134.9393400</b>                               | <b>-463.8747059</b>                                     | <b>-463.536524</b>                               | <b>-463.600036</b>                               |
| <b>TS-3-4<sub>(0-II)</sub></b> | <b>-463.7328098</b>                | <b>-463.8704802</b>                                  | <b>-1134.9333679</b>                               | <b>-463.8684852</b>                                     | <b>-463.533596</b>                               | <b>-463.596324</b>                               |
| <b>4<sub>(0-II)</sub></b>      | <b>-463.7778479</b>                | <b>-463.9118486</b>                                  | <b>-1134.9813699</b>                               | <b>-463.9095566</b>                                     | <b>-463.576175</b>                               | <b>-463.639558</b>                               |
| <b>5<sub>(0-II)</sub></b>      | <b>-530.7297985</b>                | <b>-530.8729956</b>                                  | <b>-1201.9354130</b>                               | <b>-530.8356268</b>                                     | <b>-530.472122</b>                               | <b>-530.536494</b>                               |
| <b>TS-5-6<sub>(0-II)</sub></b> | <b>-530.7191911</b>                | <b>-530.8600271</b>                                  | <b>-1201.9209874</b>                               | <b>-530.8244881</b>                                     | <b>-530.462737</b>                               | <b>-530.523870</b>                               |
| <b>6<sub>(0-II)</sub></b>      | <b>-530.7597606</b>                | <b>-530.9023041</b>                                  | <b>-1201.9590413</b>                               | <b>-530.8700689</b>                                     | <b>-530.500504</b>                               | <b>-530.561392</b>                               |
| <b>TS-6-7<sub>(0-II)</sub></b> | <b>-530.7435937</b>                | <b>-530.8876377</b>                                  | <b>-1201.9434161</b>                               | <b>-530.8517097</b>                                     | <b>-530.486459</b>                               | <b>-530.548014</b>                               |
| <b>7<sub>(0-II)</sub></b>      | <b>-530.7494864</b>                | <b>-530.8948572</b>                                  | <b>-1201.9535466</b>                               | <b>-530.8599307</b>                                     | <b>-530.492247</b>                               | <b>-530.554066</b>                               |

|                            | E<br>(B3LYP/lanl2dz) | E<br>(B3LYP/lanl2dz) | E (B3LYP/lanl2dz+p//<br>B3LYP/lanl2dz) | E (B3LYP/B_large//<br>B3LYP/lanl2dz) | E (mPW1PW91/lanl2dz+p//<br>B3LYP/lanl2dz) | H <sub>298</sub> (B3LYP/lanl2dz) | G <sub>298</sub><br>(B3LYP/lanl2dz) |
|----------------------------|----------------------|----------------------|--|--------------------------------------|---|----------------------------------|-------------------------------------|
| TS-7-8 <sub>(0-II)</sub>   | -530.7415042         | -530.8884950         | -1201.9477033                          | -530.8523598                         | -530.487579                               | -530.548742                      |                                     |
| 8 <sub>(0-II)</sub>        | -530.7463441         | -530.8920663         | -1201.9511173                          | -530.8530802                         | -530.490360                               | -530.553345                      |                                     |
| 1 <sub>(II-IV)</sub>       | -231.9257223         | -232.0154486         | -903.0193789                           | -232.0642763                         | -231.819091                               | -231.867254                      |                                     |
| 2 <sub>(II-IV)</sub>       | -310.5456947         | -310.6442517         | -981.6753579                           | -310.6752108                         | -310.381333                               | -310.437239                      |                                     |
| 3 <sub>(II-IV)</sub>       | -474.9356575         | -475.0900147         | -1146.1928135                          | -475.1059370                         | -474.730588                               | -474.797773                      |                                     |
| 3a <sub>(II-IV)</sub>      | -553.5239478         | -553.6764802         | -1224.8070052                          | -553.6698081                         | -553.260594                               | -553.341478                      |                                     |
| TS-3-4 <sub>(II-IV)</sub>  | -474.9001401         | -475.0353897         | -1146.1393876                          | -475.0488534                         | -474.695923                               | -474.761723                      |                                     |
| 4a <sub>(II-IV)</sub>      | -474.9075687         | -475.0423982         | -1146.1484538                          | -475.0561989                         | -474.702409                               | -474.770103                      |                                     |
| 4c <sub>(II-IV)</sub>      | -474.9016690         | -475.0353468         | -1146.1392513                          | -475.0481676                         | -474.696804                               | -474.766710                      |                                     |
| 4d <sub>(II-IV)</sub>      | -474.8990921         | -475.0382573         | -1146.1445313                          | -475.0536799                         | -474.693531                               | -474.760629                      |                                     |
| TS-3a-5 <sub>(II-IV)</sub> | -553.4763955         | -553.6266724         | -1224.7568015                          | -553.6221188                         | -553.214363                               | -553.289068                      |                                     |
| 5a <sub>(II-IV)</sub>      | -553.4930218         | -553.6409854         | -1224.7751451                          | -553.6358948                         | -553.229802                               | -553.305478                      |                                     |
| 5b <sub>(II-IV)</sub>      | -553.4920408         | -553.6432295         | -1224.7793381                          | -553.6433448                         | -553.227767                               | -553.300364                      |                                     |
| 5c <sub>(II-IV)</sub>      | -553.4906752         | -553.6375453         | -1224.7704004                          | -553.6344561                         | -553.227249                               | -553.301238                      |                                     |
| 5d <sub>(II-IV)</sub>      | -553.5054739         | -553.6543422         | -1224.7884302                          | -553.6539650                         | -553.241243                               | -553.314261                      |                                     |
| TS-5-6 <sub>(II-IV)</sub>  | -553.4967701         | -553.6423207         | -1224.7751689                          | -553.6432969                         | -553.233594                               | -553.304470                      |                                     |
| 6 <sub>(II-IV)</sub>       | -553.5427242         | -553.6908068         | -1224.8197297                          | -553.6946039                         | -553.277165                               | -553.347673                      |                                     |
| TS-6-7 <sub>(II-IV)</sub>  | -553.5260343         | -553.6770101         | -1224.8079659                          | -553.6768063                         | -553.333276                               | -553.262393                      |                                     |

|                                 |                     |                     |                      |                     |                    |                    |
|---------------------------------|---------------------|---------------------|----------------------|---------------------|--------------------|--------------------|
| <b>7<sub>(II-IV)</sub></b>      | <b>-553.5331444</b> | <b>-553.6833556</b> | <b>-1224.8155828</b> | <b>-553.6840634</b> | <b>-553.269351</b> | <b>-553.342659</b> |
| <b>TS-7-8<sub>(II-IV)</sub></b> | <b>-553.5276163</b> | <b>-553.6784385</b> | <b>-1224.8104279</b> | <b>-553.6789309</b> | <b>-553.267517</b> | <b>-553.338936</b> |
| <b>8<sub>(II-IV)</sub></b>      | <b>-553.5364906</b> | <b>-553.6863454</b> | <b>-1224.8179018</b> | <b>-553.6828770</b> | <b>-553.274222</b> | <b>-553.347992</b> |

=== 1\_0-IIfrq.txt ===

Total energy (Hartree)= -220.7296935  
94.1(B,0.5562);158.5(A,0.1700E-02);204.6(A,0.7420E-01);222.3(B,1.693);  
250.3(A,0.4210E-01);282.4(B,8.756);302.5(A,2.378);378.2(B,10.73);  
582.5(A,3.235);602.5(B,2.272);725.2(B,28.26);735.2(A,0.5160);  
799.6(A,58.01);820.4(B,34.84);902.3(B,80.83);993.8(A,49.90);1050.4(A,0.8814);  
1107.5(B,89.35);1115.2(A,6.545);1165.4(B,2.560);1202.6(A,10.56);  
1313.0(B,2.132);1329.2(A,1.056);1486.9(B,14.19);1488.7(A,4.786);  
2219.1(B,470.2);2228.0(A,47.50);2255.5(A,17.89);2255.6(B,155.9);  
3060.4(B,17.51);3067.5(A,35.94);3123.2(A,15.00);3134.6(B,16.99);  
--- Zero-point energy (kcal/mol): 58.12 ---  
Total number of freqs. 33

=== 2\_0-IIfrq.txt ===

Total energy (Hartree)= -299.3485844  
46.4(B,0.4105);93.6(B,2.829);103.7(A,0.6200E-02);106.4(B,1.223);  
159.5(A,1.881);194.5(A,0.2820E-01);203.0(B,0.4690);259.6(A,0.4760E-01);  
297.7(A,1.168);299.0(B,0.6391);349.7(A,28.82);381.4(B,0.2689);  
407.4(B,0.9082);575.7(B,2.987);594.9(A,8.380);609.9(B,0.6093);  
731.7(B,9.124);736.6(A,1.547);787.0(A,111.9);820.7(B,22.64);825.4(B,1.155);  
903.1(B,62.74);925.3(A,0.0000E+00);930.0(A,0.7069);942.2(B,9.511);  
999.7(A,70.02);1048.5(A,1.661);1113.8(B,71.00);1118.7(A,15.64);  
1159.0(B,2.719);1194.9(A,14.30);1229.7(A,0.9800E-02);1253.0(A,60.16);  
1308.6(B,0.9266);1327.4(A,0.9326);1472.9(B,10.13);1488.3(B,13.60);  
1491.7(A,6.025);1545.8(A,15.40);2267.2(B,299.3);2273.1(A,72.30);  
2287.6(A,0.1335);2288.2(B,113.1);3066.9(B,17.43);3071.0(A,29.14);  
3126.0(B,24.63);3130.7(A,15.97);3141.4(B,15.04);3145.2(A,5.203);  
3219.5(A,0.2600E-02);3249.5(B,35.83);  
--- Zero-point energy (kcal/mol): 91.93 ---  
Total number of freqs. 51

=== 3\_0-IIfrq.txt ===

Total energy (Hartree)= -463.7365533  
25.5(a,0.2542);27.2(a,1.054);47.4(a,0.6939);74.4(a,0.8274);92.1(a,0.6652);  
108.6(a,0.6582);120.0(a,0.3326);150.7(a,1.445);184.3(a,0.4776);  
195.7(a,0.6350);223.7(a,6.460);233.1(a,0.7921);245.6(a,25.18);  
249.9(a,15.96);285.8(a,12.61);293.8(a,2.686);382.3(a,3.178);429.5(a,8.465);  
460.4(a,36.35);597.4(a,7.717);612.7(a,0.9803);613.5(a,2.012);  
628.0(a,25.64);696.0(a,7.361);727.0(a,12.91);735.8(a,3.986);748.3(a,230.9);  
781.7(a,135.2);819.5(a,18.29);835.4(a,7.542);895.5(a,14.42);904.7(a,53.11);  
962.1(a,23.98);984.6(a,17.69);995.5(a,23.59);999.2(a,80.86);1013.8(a,0.5830E-01);  
1032.0(a,1.081);1050.2(a,2.656);1079.6(a,5.370);1110.9(a,59.57);  
1115.2(a,26.62);1163.2(a,2.294);1198.9(a,2.583);1199.5(a,17.55);  
1207.5(a,1.039);1311.5(a,3.600);1312.7(a,0.6419);1328.9(a,1.503);

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1368.9(a,4.872);1436.8(a,9.169);1466.3(a,24.36);1489.8(a,14.17);
1492.6(a,6.312);1558.1(a,16.63);1610.2(a,8.207);2262.7(a,241.2);
2272.3(a,166.5);2287.9(a,35.43);2291.5(a,59.58);3067.3(a,16.55);
3070.9(a,31.39);3130.7(a,16.48);3140.8(a,12.94);3183.0(a,0.8635);
3192.8(a,14.14);3210.1(a,18.70);3218.9(a,23.72);3229.5(a,25.67);
--- Zero-point energy (kcal/mol): 115.04 ---
Total number of freqs. 69
=== TS-3-4_0-IIfrq.txt ===
Total energy (Hartree)= -463.7328098
-62.1(a,14.13);20.1(a,0.3750);40.0(a,3.580);54.3(a,0.9726);83.1(a,0.5790);
86.5(a,1.185);98.4(a,0.9487);117.9(a,9.069);145.4(a,31.58);165.5(a,4.681);
196.6(a,0.6160E-01);201.6(a,1.218);215.8(a,0.9722);245.7(a,3.620);
265.1(a,8.334);316.8(a,0.8975);379.2(a,3.338);426.2(a,0.1900);
452.3(a,40.97);597.3(a,6.237);612.6(a,1.594);616.1(a,2.531);628.4(a,35.62);
702.1(a,0.9870E-01);726.0(a,15.07);737.2(a,27.58);750.9(a,251.1);
783.0(a,103.1);820.4(a,17.83);840.2(a,0.8446);907.6(a,57.42);
909.5(a,17.30);979.1(a,44.48);990.5(a,21.39);997.6(a,3.697);998.7(a,86.45);
1021.2(a,0.1752);1041.5(a,0.6881);1053.4(a,2.668);1088.9(a,7.562);
1111.5(a,53.78);1119.3(a,44.08);1165.2(a,2.045);1199.4(a,0.1546);
1202.3(a,19.53);1208.4(a,0.9020);1314.6(a,1.114);1323.9(a,2.690);
1329.5(a,1.880);1365.1(a,0.5410);1446.6(a,7.005);1471.0(a,46.75);
1490.5(a,13.99);1492.8(a,7.159);1581.9(a,23.17);1603.3(a,20.30);
2240.5(a,232.0);2268.2(a,57.71);2277.9(a,189.3);2299.0(a,59.18);
3066.9(a,16.10);3070.6(a,32.86);3130.0(a,18.47);3139.7(a,12.72);
3185.4(a,1.686);3195.1(a,18.67);3216.1(a,34.14);3229.1(a,17.74);
3237.1(a,8.772);
--- Zero-point energy (kcal/mol): 114.79 ---
Total number of freqs. 69
=== 4_0-IIfrq.txt ===
Total energy (Hartree)= -463.7777852
29.4(a,0.1340E-01);37.0(a,0.5466);42.2(a,0.1026);49.0(a,1.946);
65.2(a,2.046);97.2(a,1.808);147.2(a,5.342);157.5(a,3.441);185.9(a,0.7390E-01);
186.8(a,0.3223);199.1(a,0.1335);248.0(a,0.1700);261.6(a,6.448);
293.1(a,2.345);336.0(a,0.2692);355.4(a,0.6100E-02);407.1(a,0.1500E-01);
421.0(a,0.3300);487.4(a,0.8880);606.0(a,4.079);618.3(a,1.155);
626.0(a,0.2753);670.1(a,16.27);716.3(a,19.01);723.2(a,2.480);
729.2(a,15.89);763.4(a,98.81);784.8(a,150.7);804.9(a,14.83);865.9(a,0.1933);
899.1(a,51.50);935.6(a,3.017);993.6(a,92.89);1004.2(a,0.5487);
1006.8(a,5.542);1027.0(a,1.705);1033.8(a,35.00);1041.9(a,4.372);
1082.7(a,14.58);1088.5(a,7.448);1107.2(a,45.38);1109.9(a,14.46);
1163.2(a,2.383);1198.8(a,0.3544);1199.1(a,17.33);1211.2(a,0.8040E-01);
1314.1(a,2.212);1329.6(a,1.695);1331.0(a,2.331);1354.5(a,0.1726);
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1454.5(a,7.071);1490.0(a,29.19);1490.1(a,28.65);1493.1(a,4.348);
1608.8(a,69.98);1613.0(a,2.911);2329.9(a,104.5);2334.0(a,57.55);
2359.7(a,31.22);2360.3(a,13.96);3075.2(a,11.50);3078.9(a,20.91);
3138.0(a,8.610);3149.4(a,8.731);3176.0(a,3.962);3183.1(a,5.284);
3198.8(a,13.27);3206.0(a,46.85);3221.2(a,46.54);
--- Zero-point energy (kcal/mol): 116.23 ---
Total number of freqs. 69
=== 5_0-IIfrq.txt ===
Total energy (Hartree)= -530.7297985
12.0(a,0.3210E-01);43.4(a,0.3287);58.5(a,0.1838);65.2(a,1.390);
67.2(a,0.1557);109.9(a,3.528);128.5(a,9.199);162.0(a,0.5302);
185.9(a,0.4415);190.4(a,0.5724);202.7(a,0.1126);216.6(a,1.448);
238.7(a,2.682);259.6(a,0.7788);297.2(a,0.7686);308.7(a,2.072);
340.4(a,1.925);378.7(a,0.1308);409.0(a,0.3900E-02);443.3(a,1.308);
482.1(a,1.444);548.1(a,0.4225);611.7(a,0.5536);622.4(a,0.1520E-01);
628.1(a,1.456);661.6(a,22.25);715.7(a,8.028);730.3(a,4.395);736.5(a,4.311);
769.4(a,104.8);792.9(a,145.3);806.5(a,8.999);852.4(a,4.537);871.2(a,0.2006);
898.0(a,45.98);951.2(a,4.893);995.5(a,92.04);1006.1(a,11.78);
1016.9(a,0.6360E-01);1024.5(a,33.29);1028.8(a,23.00);1029.6(a,4.040);
1044.1(a,19.45);1048.2(a,4.244);1050.1(a,43.16);1073.9(a,10.08);
1090.3(a,19.24);1093.5(a,7.518);1100.1(a,19.61);1173.3(a,1.355);
1208.7(a,0.4220E-01);1212.8(a,11.40);1214.8(a,0.4652);1248.2(a,0.1466);
1323.8(a,3.129);1333.3(a,0.9436);1341.0(a,3.743);1342.3(a,1.351);
1351.7(a,1.736);1459.1(a,10.41);1487.5(a,0.9160E-01);1490.5(a,18.37);
1490.9(a,57.74);1493.7(a,8.069);1598.5(a,13.74);1602.9(a,46.60);
1615.3(a,5.596);2349.1(a,45.40);2375.1(a,9.219);2384.1(a,11.76);
2412.9(a,2.194);3085.7(a,4.106);3089.3(a,4.338);3150.3(a,0.1246);
3158.8(a,2.832);3162.0(a,2.195);3187.6(a,0.3873);3189.2(a,2.361);
3190.8(a,2.090);3209.2(a,0.8970E-01);3217.6(a,18.94);3238.0(a,17.41);
3264.0(a,1.175);3304.8(a,1.223);
--- Zero-point energy (kcal/mol): 150.61 ---
Total number of freqs. 84
=== TS-5-6_0-IIfrq.txt ===
Total energy (Hartree)= -530.7191911
-284.8(a,32.40);24.4(a,0.6200E-02);44.6(a,0.9443);62.6(a,1.102);
86.7(a,0.5901);106.7(a,0.7440E-01);133.0(a,3.177);140.8(a,7.425);
172.2(a,0.2550E-01);192.9(a,2.194);209.3(a,6.393);219.7(a,0.2740E-01);
243.9(a,1.888);271.3(a,3.603);314.5(a,1.417);335.7(a,0.3938);
361.6(a,0.3307);411.5(a,5.992);414.4(a,0.2341);431.6(a,0.7282);
476.7(a,7.589);611.2(a,0.2885);621.3(a,0.2000E-02);626.8(a,0.9955);
644.5(a,7.646);682.5(a,0.6609);715.4(a,1.833);725.1(a,8.380);
729.2(a,1.950);761.1(a,118.4);783.8(a,122.5);805.5(a,11.86);875.8(a,0.6121);
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```
880.8(a,1.123);899.2(a,41.05);952.4(a,1.844);981.0(a,0.7297);
993.2(a,40.16);998.8(a,34.48);1006.8(a,10.52);1012.1(a,30.10);
1020.2(a,0.1008);1046.9(a,3.351);1047.5(a,0.8380E-01);1054.2(a,2.632);
1096.6(a,9.883);1096.9(a,14.62);1101.0(a,21.02);1104.9(a,1.210);
1173.0(a,1.303);1209.9(a,0.1270E-01);1213.3(a,12.10);1216.5(a,0.7840E-01);
1230.6(a,6.367);1257.8(a,0.2702);1324.7(a,1.883);1338.7(a,3.896);
1340.4(a,0.8083);1357.2(a,2.761);1461.6(a,12.05);1482.4(a,1.632);
1488.7(a,26.97);1492.5(a,21.43);1494.3(a,6.225);1539.2(a,0.5555);
1601.6(a,9.512);1611.0(a,3.472);2356.3(a,34.02);2358.3(a,27.40);
2383.1(a,8.587);2384.8(a,7.124);3086.4(a,5.755);3088.2(a,5.313);
3138.9(a,4.666);3151.0(a,0.3281);3161.5(a,2.621);3187.7(a,2.987);
3193.6(a,1.850);3194.2(a,1.455);3211.8(a,0.4778);3221.4(a,14.87);
3239.3(a,15.57);3243.1(a,1.647);3300.3(a,0.3043);
--- Zero-point energy (kcal/mol): 150.48 ---
Total number of freqs. 84
=== 6_0-IIfrq.txt ===
Total energy (Hartree)= -530.7597606
37.1(a,0.6405);43.5(a,0.6534);58.0(a,0.5230);70.4(a,0.6934);83.9(a,0.2505);
111.5(a,1.346);124.1(a,2.255);165.1(a,0.7265);195.4(a,0.6150);
223.6(a,5.087);236.9(a,2.109);280.2(a,6.197);309.3(a,1.865);324.3(a,1.922);
340.9(a,0.5458);369.5(a,0.5890);420.3(a,0.1055);436.3(a,0.2975);
485.3(a,17.80);520.9(a,1.800);609.8(a,0.3150E-01);620.0(a,17.99);
628.0(a,0.7492);631.2(a,0.2600);696.7(a,3.309);724.4(a,36.82);
730.9(a,1.778);735.4(a,3.250);776.7(a,74.49);784.2(a,104.8);803.3(a,28.85);
806.3(a,10.26);890.3(a,2.425);897.6(a,1.351);902.4(a,44.86);976.9(a,0.3300E-01);
996.6(a,77.32);1007.6(a,1.679);1026.2(a,3.716);1030.4(a,0.2544);
1046.7(a,2.882);1048.4(a,3.609);1058.3(a,0.1210E-01);1072.8(a,3.573);
1092.8(a,25.20);1103.8(a,33.65);1113.1(a,8.109);1134.7(a,3.282);
1175.0(a,1.563);1203.8(a,3.442);1213.4(a,0.1361);1215.3(a,10.57);
1224.0(a,1.425);1253.0(a,5.036);1322.9(a,4.335);1326.1(a,2.467);
1339.8(a,3.811);1375.8(a,1.899);1380.9(a,2.671);1473.0(a,14.06);
1482.4(a,7.709);1491.2(a,16.92);1494.7(a,10.79);1506.7(a,9.383);
1522.8(a,3.610);1607.9(a,3.278);1633.0(a,4.869);2346.4(a,35.34);
2364.8(a,27.95);2372.2(a,10.07);2390.8(a,7.121);3067.1(a,25.04);
3085.5(a,5.707);3087.3(a,5.688);3093.6(a,20.34);3136.8(a,5.454);
3149.9(a,0.4101);3160.3(a,2.770);3184.3(a,12.58);3199.8(a,1.016);
3204.4(a,0.9390);3215.3(a,2.443);3226.9(a,10.77);3240.9(a,8.928);
--- Zero-point energy (kcal/mol): 152.32 ---
Total number of freqs. 84
=== TS-6-7_0-IIfrq.txt ===
Total energy (Hartree)= -530.7435937
-71.3(a,0.2888);6.6(a,0.4526);32.8(a,1.013);49.8(a,0.4745);64.5(a,1.629);
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97.4(a,0.9073);150.8(a,1.696);154.5(a,3.346);188.7(a,0.5937);  
197.6(a,1.075);237.1(a,0.3494);304.7(a,4.248);318.6(a,1.317);  
326.2(a,0.7210);344.1(a,3.640);370.0(a,0.8663);416.2(a,0.3023);  
435.3(a,0.4248);495.4(a,10.14);509.6(a,4.375);571.6(a,10.10);  
607.2(a,0.1225);625.7(a,0.6280);637.8(a,0.3460E-01);722.3(a,7.570);  
726.2(a,62.03);730.4(a,0.5458);747.7(a,8.621);775.2(a,27.93);  
785.7(a,148.5);807.0(a,20.72);813.7(a,10.41);836.5(a,8.266);876.9(a,6.219);  
901.3(a,47.42);948.5(a,4.673);985.2(a,52.26);995.9(a,50.83);1012.7(a,2.759);  
1019.7(a,0.6940E-01);1048.9(a,1.321);1049.1(a,2.854);1049.7(a,3.061);  
1064.1(a,1.634);1092.9(a,34.33);1104.2(a,27.48);1110.5(a,13.57);  
1123.0(a,27.44);1178.5(a,2.116);1195.8(a,60.41);1210.2(a,2.663);  
1216.8(a,4.321);1221.0(a,3.994);1238.5(a,3.842);1327.4(a,1.649);  
1343.1(a,4.615);1345.4(a,7.003);1365.7(a,2.827);1376.2(a,0.9730E-01);  
1477.9(a,6.784);1478.9(a,14.06);1481.4(a,42.76);1491.7(a,19.35);  
1493.5(a,10.13);1525.0(a,11.74);1630.7(a,5.465);1648.4(a,7.857);  
2350.5(a,37.75);2369.6(a,19.56);2375.9(a,11.13);2397.5(a,5.606);  
2899.8(a,32.84);3034.6(a,4.050);3086.1(a,4.149);3088.8(a,5.636);  
3094.9(a,25.03);3103.8(a,47.56);3150.6(a,0.6470E-01);3161.4(a,2.190);  
3188.9(a,11.50);3196.2(a,4.022);3208.9(a,1.355);3221.2(a,16.57);  
3239.4(a,13.94);

--- Zero-point energy (kcal/mol): 151.37 ---

Total number of freqs. 84

=== 7\_0-IIfrq.txt ===

Total energy (Hartree)= -530.7494864

22.1(a,1.196);28.4(a,0.7331);43.0(a,0.4235);59.8(a,0.3508);106.5(a,2.196);  
111.9(a,1.679);163.4(a,1.811);172.0(a,1.827);192.9(a,0.1996);  
217.5(a,0.4823);248.3(a,0.3462);300.8(a,6.775);321.4(a,0.4427);  
340.4(a,1.918);366.1(a,0.4279);417.9(a,0.1955);424.3(a,1.389);  
449.2(a,1.372);475.4(a,12.32);517.3(a,10.94);570.2(a,9.379);607.3(a,0.1145);  
626.2(a,0.7959);636.5(a,0.6160E-01);715.1(a,7.244);726.6(a,34.78);  
729.6(a,3.834);743.9(a,4.544);775.5(a,55.78);786.3(a,137.8);798.6(a,12.29);  
808.3(a,10.08);834.6(a,42.94);880.9(a,1.178);899.6(a,44.66);960.3(a,6.073);  
994.4(a,94.29);1009.2(a,12.44);1019.1(a,2.849);1020.6(a,1.224);  
1048.0(a,10.64);1048.6(a,6.468);1049.4(a,0.1731);1059.9(a,0.3859);  
1091.5(a,3.126);1097.9(a,31.13);1103.0(a,10.93);1125.4(a,17.49);  
1176.3(a,1.852);1203.1(a,2.000);1211.0(a,0.2300E-01);1216.0(a,10.67);  
1222.9(a,0.8528);1239.9(a,5.188);1326.0(a,1.244);1330.4(a,4.975);  
1340.9(a,3.750);1377.2(a,1.245);1386.8(a,6.096);1479.4(a,11.80);  
1489.6(a,14.60);1491.4(a,13.97);1493.7(a,13.52);1512.1(a,25.97);  
1524.0(a,21.92);1634.3(a,1.167);1649.5(a,4.158);2160.0(a,92.53);  
2359.2(a,33.94);2371.6(a,19.42);2384.3(a,8.956);2397.8(a,5.298);  
3086.4(a,4.639);3088.8(a,5.229);3109.6(a,2.703);3128.9(a,8.582);

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3151.3(a,0.1232);3161.5(a,37.72);3161.8(a,2.524);3195.4(a,6.094);
3210.4(a,2.350);3222.6(a,19.02);3232.3(a,3.081);3240.3(a,13.30);
--- Zero-point energy (kcal/mol): 151.12 ---
Total number of freqs. 84
=== TS-7-8_0-IIfrq.txt ===
Total energy (Hartree)= -530.7415042
-574.0(a,53.86);25.3(a,1.023);35.2(a,0.2765);44.2(a,0.4383);62.1(a,0.4458);
108.0(a,5.043);113.5(a,4.053);157.4(a,0.8378);191.4(a,1.844);
204.8(a,2.788);232.2(a,1.837);271.3(a,3.033);284.7(a,4.005);333.2(a,2.811);
360.4(a,0.9690);371.4(a,12.54);416.3(a,0.2177);428.4(a,1.198);
443.5(a,6.207);477.1(a,63.61);510.0(a,25.30);564.6(a,25.87);608.6(a,0.3038);
624.9(a,0.7834);634.5(a,0.1139);675.4(a,1.177);717.5(a,24.05);
732.3(a,6.304);737.3(a,23.12);766.5(a,38.39);787.9(a,27.61);790.1(a,79.74);
809.6(a,14.96);824.7(a,25.16);883.2(a,0.9044);900.7(a,42.66);
974.3(a,0.8639);992.5(a,4.154);997.5(a,126.5);1015.8(a,0.3466);
1027.7(a,0.1210);1042.7(a,8.061);1048.6(a,2.975);1055.0(a,0.5990E-01);
1064.4(a,3.704);1099.8(a,28.08);1101.3(a,14.31);1115.4(a,8.246);
1165.0(a,28.24);1175.5(a,1.829);1205.8(a,29.26);1215.5(a,8.856);
1216.0(a,1.604);1228.6(a,2.202);1272.4(a,17.38);1325.8(a,1.408);
1340.0(a,4.129);1362.7(a,28.96);1385.1(a,4.066);1434.2(a,39.31);
1485.8(a,8.508);1491.5(a,20.79);1493.5(a,6.726);1520.8(a,20.50);
1541.3(a,28.45);1630.8(a,2.775);1647.8(a,21.82);1853.5(a,149.6);
2360.4(a,32.81);2369.8(a,25.27);2386.1(a,8.858);2395.9(a,6.705);
3086.3(a,5.371);3088.3(a,5.386);3151.0(a,0.3014);3152.1(a,0.4762);
3161.6(a,2.547);3168.5(a,5.356);3192.4(a,6.083);3199.7(a,8.220);
3215.2(a,2.852);3227.5(a,17.63);3243.1(a,12.43);3260.4(a,1.215);
--- Zero-point energy (kcal/mol): 149.12 ---
Total number of freqs. 84
=== 8_0-IIfrq.txt ===
Total energy (Hartree)= -530.7463441
12.9(a,0.3630);30.7(a,0.5617);47.3(a,0.2341);56.3(a,1.903);95.8(a,5.430);
103.7(a,2.579);144.6(a,1.884);179.1(a,1.160);193.5(a,0.1431);
232.8(a,1.271);238.9(a,0.2028);280.0(a,1.129);306.1(a,1.514);
310.1(a,4.259);359.0(a,7.215);371.0(a,15.10);418.5(a,0.1311);
430.0(a,1.595);447.7(a,10.83);506.3(a,28.97);548.6(a,10.42);567.7(a,11.47);
609.4(a,0.1441);624.7(a,0.6726);634.3(a,0.2485);709.2(a,20.11);
718.0(a,30.02);736.5(a,1.481);755.4(a,23.65);783.8(a,131.4);789.4(a,45.91);
798.0(a,28.55);812.5(a,18.32);830.4(a,35.82);887.8(a,0.9344);
900.9(a,38.79);978.5(a,0.5796);994.8(a,79.97);1004.1(a,102.0);
1013.6(a,0.6251);1023.2(a,19.17);1032.5(a,2.533);1047.1(a,1.509);
1049.9(a,1.700);1057.4(a,0.9570E-01);1080.3(a,5.495);1096.0(a,21.10);
1103.4(a,9.790);1122.9(a,5.780);1176.0(a,2.269);1213.7(a,10.63);
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1214.0(a,2.229);1226.3(a,14.39);1237.4(a,17.93);1315.1(a,13.78);  
1324.9(a,2.525);1341.8(a,3.736);1370.9(a,35.56);1387.0(a,5.908);  
1461.4(a,46.09);1490.4(a,3.579);1491.3(a,20.10);1493.2(a,8.821);  
1525.0(a,4.186);1592.4(a,110.9);1626.1(a,16.59);1646.1(a,40.37);  
2043.5(a,90.96);2352.6(a,24.55);2377.2(a,9.139);2382.0(a,22.33);  
2408.4(a,3.636);3086.0(a,4.919);3088.6(a,4.813);3150.4(a,0.1818);  
3161.3(a,2.200);3170.5(a,6.758);3189.7(a,0.5716);3197.5(a,4.140);  
3199.3(a,4.240);3215.5(a,1.775);3227.1(a,15.73);3242.6(a,12.37);  
3276.5(a,1.705);

--- Zero-point energy (kcal/mol): 150.07 ---

Total number of freqs. 84

=== 1\_II-IVfreq.txt ===

Total energy (Hartree)= -231.9257223

54.2(a,0.1696);73.8(a,2.526);96.0(a,2.114);163.1(a,11.16);197.1(a,0.3910E-01);  
224.6(a,2.044);284.4(a,5.510);337.7(a,6.136);362.0(a,3.028);401.6(a,0.6233);  
463.7(a,0.6441);610.8(a,0.5377);629.1(a,0.4473);725.0(a,7.265);  
731.8(a,4.528);789.7(a,172.8);796.8(a,27.91);889.9(a,69.16);995.5(a,65.10);  
1049.5(a,2.523);1071.4(a,6.268);1091.3(a,25.84);1178.6(a,3.092);  
1218.0(a,8.665);1328.2(a,5.701);1347.7(a,3.585);1487.0(a,19.81);  
1491.7(a,11.68);2374.0(a,12.07);2403.8(a,1.571);2406.0(a,0.1486);  
2440.3(a,0.5374);3085.6(a,1.202);3093.3(a,0.9746);3151.5(a,1.970);  
3165.5(a,1.550);

--- Zero-point energy (kcal/mol): 60.34 ---

Total number of freqs. 36

=== 2\_II-IVfreq.txt ===

Total energy (Hartree)= -310.5456946

53.0(a,0.8770);59.1(a,0.8575);89.8(a,2.928);96.0(a,0.2820E-01);  
108.3(a,5.202);137.5(a,6.735);162.0(a,4.181);194.0(a,0.1837);  
215.4(a,0.8742);250.4(a,0.7271);273.3(a,4.339);281.1(a,4.019);  
305.9(a,2.248);352.0(a,1.208);387.8(a,0.2839);450.0(a,1.293);  
502.7(a,6.810);612.0(a,0.1484);628.0(a,1.309);728.6(a,6.535);  
731.3(a,1.920);787.5(a,154.2);799.8(a,13.12);850.1(a,1.624);891.3(a,64.98);  
996.3(a,73.91);1006.7(a,0.2114);1045.3(a,6.599);1048.5(a,4.176);  
1061.6(a,101.5);1077.7(a,5.273);1092.4(a,24.66);1173.5(a,3.309);  
1213.6(a,11.24);1241.8(a,0.6700E-02);1324.3(a,8.085);1337.9(a,17.57);

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1343.0(a,2.275);1489.5(a,27.99);1489.8(a,18.38);1492.8(a,6.807);
1594.9(a,4.628);2362.0(a,23.50);2390.3(a,3.602);2399.6(a,2.478);
2433.1(a,0.1870E-01);3087.5(a,2.395);3091.3(a,1.128);3151.9(a,0.7499);
3162.1(a,0.9810E-01);3164.6(a,1.695);3175.9(a,1.732);3269.7(a,1.642);
3296.3(a,1.131);
--- Zero-point energy (kcal/mol):    94.30 ---
Total number of freqs.              54
=== 3_II-IVfreq.txt ===
Total energy (Hartree)= -474.9460564
22.5(a,1.854);27.6(a,1.462);40.0(a,0.8295);57.5(a,0.7980E-01);
74.0(a,1.592);84.3(a,0.8210E-01);99.9(a,5.489);101.6(a,2.376);
143.9(a,0.6083);160.7(a,6.370);193.7(a,1.674);206.5(a,10.80);
230.6(a,0.4708);232.1(a,11.46);263.8(a,2.305);283.8(a,5.013);
321.5(a,1.593);361.0(a,1.397);400.0(a,1.345);419.1(a,4.789);458.1(a,1.690);
488.1(a,13.08);615.2(a,0.7707);622.0(a,1.044);630.0(a,1.335);
659.3(a,16.25);706.7(a,3.438);729.8(a,5.965);732.8(a,5.143);785.5(a,104.2);
793.8(a,176.1);799.7(a,22.73);889.9(a,63.13);909.6(a,23.92);952.3(a,26.44);
994.6(a,31.97);996.9(a,47.63);1011.4(a,6.737);1028.4(a,37.95);
1047.6(a,3.146);1050.2(a,6.618);1075.6(a,23.27);1078.0(a,4.380);
1084.5(a,2.728);1089.0(a,23.97);1172.7(a,3.010);1212.1(a,13.04);
1213.1(a,2.017);1219.7(a,3.140);1324.2(a,10.01);1338.8(a,4.578);
1343.0(a,3.723);1365.4(a,8.290);1450.6(a,11.50);1483.0(a,82.44);
1489.1(a,20.40);1492.7(a,6.835);1587.2(a,34.57);1602.6(a,22.84);
2369.0(a,12.64);2400.0(a,4.975);2402.9(a,2.698);2433.8(a,0.2220E-01);
3086.2(a,2.513);3090.2(a,1.918);3150.3(a,0.3924);3163.0(a,1.747);
3212.3(a,0.1223);3214.5(a,4.017);3227.4(a,1.220);3235.1(a,0.6103);
3246.5(a,4.384);
--- Zero-point energy (kcal/mol):    117.91 ---
Total number of freqs.              72
=== TS-3-4_II-IVfreq.txt ===
Total energy (Hartree)= -474.9001401
-35.3(a,0.5641);32.9(a,2.498);49.3(a,0.2882);61.4(a,0.7085);69.4(a,3.146);
76.0(a,0.7597);92.1(a,1.641);100.2(a,3.140);135.8(a,2.629);151.6(a,3.989);
168.8(a,0.2056);184.7(a,3.006);195.7(a,0.2179);207.9(a,0.5297);
243.3(a,0.3047);260.6(a,1.913);287.0(a,3.456);346.8(a,0.4216);
374.7(a,1.795);408.3(a,1.643);440.1(a,0.4368);460.8(a,1.708);
609.2(a,0.3700);611.7(a,0.1968);626.4(a,1.482);647.9(a,33.77);
687.3(a,22.50);723.6(a,4.270);728.1(a,5.391);765.9(a,72.16);778.9(a,196.0);
798.5(a,9.653);834.6(a,1.417);888.4(a,60.07);954.9(a,0.2146);
978.9(a,23.52);993.3(a,92.45);1009.0(a,23.85);1014.1(a,0.9131);
1042.9(a,3.348);1049.1(a,2.966);1058.3(a,8.512);1084.4(a,18.37);
1085.4(a,13.31);1104.4(a,9.830);1170.4(a,3.403);1209.8(a,22.00);
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1210.9(a,0.3185);1226.0(a,12.46);1320.4(a,9.972);1339.3(a,1.365);
1341.4(a,5.636);1351.7(a,14.16);1453.5(a,13.83);1471.0(a,16.03);
1489.9(a,19.64);1492.9(a,8.758);1570.2(a,6.771);1592.1(a,4.902);
2372.3(a,12.65);2376.5(a,12.38);2404.5(a,1.632);2413.8(a,0.9467);
3085.2(a,2.404);3089.3(a,1.220);3149.1(a,1.350);3161.7(a,1.663);
3207.8(a,0.4506);3216.2(a,0.8684);3229.1(a,5.109);3241.1(a,11.94);
3265.1(a,5.870);
--- Zero-point energy (kcal/mol): 117.04 ---
Total number of freqs. 72
=== 3a_II-IVfrq.txt ===
Total energy (Hartree)= -553.5239478
11.4(a,0.6497);18.7(a,0.5543);26.5(a,0.1075);33.6(a,0.3140);37.7(a,0.8433);
43.5(a,2.886);61.0(a,1.672);71.0(a,0.7358);84.8(a,1.099);95.5(a,2.346);
131.3(a,1.307);141.2(a,1.409);152.7(a,7.535);158.4(a,4.599);167.0(a,12.19);
173.2(a,1.161);204.9(a,2.821);218.9(a,0.2143);221.1(a,0.4916);
247.9(a,0.9514);259.8(a,0.7180E-01);277.0(a,0.8468);309.5(a,2.611);
374.0(a,0.3959);414.8(a,0.1825);449.2(a,5.950);467.7(a,13.93);
541.4(a,7.247);605.1(a,0.4466);616.2(a,2.576);622.2(a,0.7000E-02);
652.3(a,32.56);703.4(a,18.14);733.4(a,5.290);741.4(a,6.451);775.6(a,92.02);
786.6(a,105.7);812.6(a,20.28);849.7(a,1.479);867.9(a,0.2923);
910.8(a,46.49);960.9(a,1.055);987.1(a,76.45);995.5(a,8.203);998.6(a,46.04);
1020.6(a,1.556);1020.8(a,0.2830);1038.4(a,14.70);1052.8(a,0.2047);
1056.4(a,60.56);1058.6(a,2.358);1072.3(a,0.2466);1093.1(a,17.54);
1104.1(a,6.048);1109.3(a,29.18);1179.8(a,0.6481);1214.5(a,0.3590E-01);
1220.1(a,15.59);1223.3(a,4.415);1242.1(a,0.1566);1325.4(a,12.25);
1329.1(a,3.113);1343.4(a,5.221);1348.3(a,0.8548);1362.3(a,6.505);
1468.6(a,15.78);1489.4(a,7.712);1490.3(a,21.90);1492.7(a,33.17);
1495.6(a,26.89);1586.4(a,3.365);1606.0(a,12.31);1624.9(a,3.729);
2290.7(a,101.8);2335.9(a,27.27);2368.0(a,25.05);2412.4(a,2.249);
3079.5(a,3.907);3092.2(a,6.967);3144.5(a,1.259);3159.6(a,2.211);
3168.1(a,0.3083);3180.2(a,1.132);3212.9(a,0.9570E-01);3219.3(a,0.7582);
3230.5(a,2.097);3237.7(a,6.814);3248.2(a,8.588);3275.0(a,0.3043);
3300.4(a,0.6779);
--- Zero-point energy (kcal/mol): 151.02 ---
Total number of freqs. 90
=== TS-3a-5_II-IVfrq.txt ===
Total energy (Hartree)= -553.4763955
-189.5(a,45.19);33.1(a,3.269);39.2(a,3.319);50.8(a,1.770);54.2(a,2.926);
70.4(a,3.519);80.1(a,4.646);86.1(a,1.731);106.2(a,0.2739);112.6(a,0.9282);
116.1(a,3.006);138.5(a,1.171);147.8(a,16.57);157.8(a,2.220);172.0(a,8.467);
180.9(a,0.4636);189.9(a,0.3774);197.9(a,1.161);215.3(a,0.8361);
220.3(a,0.4244);237.4(a,2.894);268.0(a,1.690);299.4(a,1.131);
```

393.1(a,1.629);419.5(a,0.3442);421.9(a,8.191);476.6(a,11.67);  
516.5(a,1.360);609.7(a,1.704);612.6(a,2.817);616.3(a,63.91);626.6(a,2.377);  
686.2(a,3.629);722.1(a,46.17);734.3(a,9.082);753.5(a,161.8);790.2(a,90.27);  
821.1(a,61.37);829.7(a,0.3374);851.3(a,1.107);903.0(a,69.68);  
937.5(a,1.229);962.0(a,105.8);991.1(a,77.19);1006.4(a,0.7309);  
1007.9(a,3.796);1013.4(a,2.704);1037.6(a,23.74);1040.3(a,4.022);  
1057.0(a,17.56);1059.3(a,9.136);1061.9(a,77.14);1081.0(a,13.21);  
1096.6(a,43.21);1105.8(a,12.26);1182.7(a,1.817);1211.4(a,0.9760E-01);  
1218.0(a,20.11);1222.3(a,3.003);1244.6(a,0.4790E-01);1327.3(a,7.497);  
1340.4(a,3.394);1344.4(a,0.4586);1347.8(a,35.88);1349.0(a,2.870);  
1460.7(a,10.96);1472.8(a,79.20);1486.3(a,8.851);1493.0(a,26.27);  
1498.2(a,9.944);1581.1(a,52.44);1601.5(a,6.602);1616.7(a,6.653);  
2303.5(a,91.17);2339.7(a,17.05);2369.2(a,15.24);2415.9(a,0.7500E-02);  
3078.9(a,1.623);3094.9(a,3.708);3144.9(a,1.550);3164.6(a,0.9511);  
3186.8(a,0.8340E-01);3198.5(a,0.4699);3210.5(a,0.7732);3217.3(a,2.259);  
3238.7(a,4.425);3250.0(a,5.814);3261.5(a,4.215);3288.0(a,0.9195);  
3316.8(a,1.169);

--- Zero-point energy (kcal/mol): 150.81 ---

Total number of freqs. 90

=== 4a\_II-IVfrq.txt ===

Total energy (Hartree)= -474.9075687

28.8(a,0.3340E-01);47.6(a,2.037);58.7(a,0.4856);66.4(a,0.8671);  
73.0(a,0.7932);79.4(a,4.178);92.9(a,0.2434);121.9(a,2.606);139.1(a,0.4117);  
151.8(a,3.176);163.4(a,3.033);171.1(a,2.907);196.1(a,0.1010);  
227.8(a,1.411);233.3(a,3.278);279.5(a,5.558);298.2(a,4.839);361.0(a,1.040);  
385.0(a,0.3340E-01);417.0(a,0.2197);442.7(a,2.054);465.4(a,1.538);  
600.3(a,0.7980E-01);606.7(a,0.2690);620.3(a,0.9372);645.9(a,74.05);  
673.1(a,6.318);707.7(a,5.350);724.2(a,6.154);755.3(a,75.60);770.4(a,151.4);  
788.7(a,17.68);813.5(a,10.09);877.8(a,71.35);941.6(a,1.335);978.7(a,162.3);  
989.1(a,88.01);1008.4(a,0.6052);1018.4(a,4.331);1040.2(a,0.2330E-01);  
1042.1(a,1.598);1065.7(a,3.946);1074.8(a,13.69);1082.1(a,13.65);  
1099.8(a,12.25);1171.0(a,5.419);1209.0(a,3.692);1209.6(a,13.82);  
1220.7(a,0.9436);1320.4(a,12.62);1333.2(a,11.07);1341.1(a,4.698);  
1343.2(a,2.033);1457.2(a,15.25);1473.7(a,106.3);1489.0(a,18.46);  
1495.4(a,13.43);1573.2(a,98.06);1616.8(a,11.41);2382.3(a,8.996);  
2384.1(a,3.661);2419.8(a,0.4481);2420.3(a,0.4004);3085.0(a,2.252);  
3091.4(a,1.616);3147.5(a,1.436);3161.1(a,3.153);3207.9(a,0.3246);  
3218.5(a,1.092);3234.9(a,8.175);3244.6(a,4.800);3287.3(a,2.060);

--- Zero-point energy (kcal/mol): 117.17 ---

Total number of freqs. 72

=== 4c\_II-IVfrq.txt ===

Total energy (Hartree)= -474.9016690

11.7(a,0.2625);41.5(a,1.782);45.2(a,0.5751);49.3(a,0.4138);60.2(a,0.5636);  
65.3(a,3.055);83.3(a,0.4803);107.6(a,3.421);145.0(a,1.757);146.3(a,4.114);  
152.4(a,1.012);183.8(a,2.260);197.3(a,0.2399);218.1(a,1.577);  
243.8(a,0.6284);256.3(a,7.170);289.4(a,5.795);325.3(a,2.310);  
371.4(a,1.142);404.2(a,2.041);439.0(a,3.482);473.7(a,1.963);608.1(a,0.5418);  
609.2(a,0.1126);625.3(a,0.8331);659.4(a,42.56);672.6(a,26.79);  
718.1(a,11.80);719.2(a,9.933);761.6(a,77.12);773.2(a,168.7);795.7(a,12.59);  
818.8(a,7.144);893.0(a,58.95);944.8(a,1.536);986.4(a,138.8);992.5(a,48.70);  
1011.9(a,0.2443);1016.4(a,1.995);1041.1(a,7.292);1046.9(a,3.536);  
1059.5(a,1.122);1079.5(a,22.27);1091.1(a,14.02);1100.1(a,10.64);  
1174.6(a,3.430);1208.4(a,0.3686);1213.3(a,17.62);1217.6(a,3.511);  
1324.2(a,4.335);1339.2(a,2.334);1341.6(a,4.287);1344.1(a,10.21);  
1455.4(a,14.88);1478.4(a,70.39);1489.8(a,20.27);1493.9(a,10.94);  
1571.1(a,54.18);1610.2(a,8.785);2362.0(a,27.30);2362.7(a,11.31);  
2392.6(a,3.401);2415.8(a,1.405);3085.9(a,4.499);3088.9(a,1.383);  
3149.7(a,0.4689);3161.2(a,1.522);3167.7(a,0.8467);3209.9(a,0.2637);  
3219.8(a,5.596);3238.1(a,6.594);3258.9(a,6.791);

--- Zero-point energy (kcal/mol): 116.81 ---

Total number of freqs. 72

=== 4d\_II-IVfrq.txt ===

Total energy (Hartree)= -474.8990921

23.6(a,3.296);43.3(a,1.947);55.0(a,1.156);65.5(a,2.765);86.7(a,1.477);  
91.0(a,0.1711);104.1(a,2.585);123.1(a,0.6850);138.6(a,6.049);  
152.8(a,2.457);167.3(a,6.549);202.6(a,2.863);207.2(a,0.8286);  
234.3(a,3.655);244.0(a,3.597);259.9(a,6.471);346.1(a,12.48);381.7(a,4.598);  
408.9(a,0.9208);424.1(a,0.3220E-01);471.3(a,5.224);497.4(a,17.01);  
601.9(a,2.611);609.7(a,0.1305);629.1(a,5.123);656.9(a,42.28);  
677.7(a,18.33);713.1(a,9.707);724.5(a,22.20);766.0(a,92.14);776.4(a,105.4);  
786.1(a,54.54);824.2(a,6.135);890.1(a,59.73);948.7(a,4.818);981.6(a,100.3);  
991.4(a,9.819);1010.7(a,8.143);1013.8(a,6.844);1042.7(a,3.896);  
1043.0(a,4.548);1059.7(a,5.798);1067.0(a,13.02);1085.2(a,25.32);  
1105.1(a,8.899);1190.5(a,1.521);1211.7(a,0.4500E-02);1220.0(a,12.33);  
1225.4(a,7.752);1332.0(a,3.360);1341.0(a,0.4204);1351.1(a,6.801);  
1351.7(a,10.16);1454.7(a,14.35);1474.9(a,27.29);1477.4(a,17.27);  
1488.2(a,20.39);1568.1(a,3.859);1597.6(a,6.224);2365.3(a,28.01);  
2400.7(a,1.040);2406.5(a,0.2776);2449.6(a,3.144);3083.0(a,1.355);  
3093.9(a,1.517);3153.9(a,0.8366);3166.6(a,0.6811);3207.7(a,0.3578);  
3214.9(a,0.6573);3226.7(a,4.576);3238.7(a,4.815);3248.9(a,10.90);

--- Zero-point energy (kcal/mol): 117.62 ---

Total number of freqs. 72

=== 5a\_II-IVfrq.txt ===

Total energy (Hartree)= -553.4930218

42.0(a,0.3753);43.3(a,2.088);60.2(a,3.132);62.0(a,0.2081);69.9(a,3.980);  
78.9(a,2.857);82.3(a,1.368);92.4(a,1.309);97.6(a,0.5440);102.7(a,3.209);  
113.8(a,0.3947);145.6(a,2.350);152.2(a,4.452);161.3(a,1.856);  
165.4(a,2.440);177.5(a,1.137);187.3(a,0.7850E-01);198.4(a,0.2968);  
234.1(a,0.2887);236.5(a,0.3366);281.8(a,5.430);303.3(a,3.750);  
340.2(a,1.315);378.8(a,1.144);409.8(a,0.7635);419.8(a,0.8800E-02);  
453.3(a,1.898);475.8(a,0.8380);596.1(a,0.1940);613.3(a,0.2995);  
621.3(a,0.7657);646.0(a,60.30);687.7(a,6.912);715.0(a,2.620);  
722.2(a,6.725);758.3(a,77.88);775.4(a,150.5);790.7(a,17.05);828.6(a,8.168);  
850.7(a,2.279);872.5(a,72.89);944.1(a,1.006);984.5(a,117.8);989.8(a,154.8);  
1005.3(a,70.55);1010.9(a,0.3895);1020.0(a,3.654);1040.2(a,0.4605);  
1042.3(a,0.9900E-02);1045.7(a,2.175);1056.0(a,146.2);1069.5(a,0.8182);  
1078.4(a,16.42);1086.0(a,13.37);1103.9(a,12.64);1173.9(a,5.864);  
1210.2(a,0.2074);1211.3(a,13.62);1226.9(a,0.5419);1252.6(a,0.7380E-01);  
1321.4(a,14.12);1339.9(a,1.885);1340.0(a,9.532);1348.8(a,2.625);  
1375.7(a,25.09);1458.1(a,9.099);1482.3(a,86.16);1485.8(a,11.27);  
1488.6(a,23.02);1497.9(a,14.00);1584.3(a,93.82);1617.6(a,11.02);  
1638.9(a,27.08);2384.2(a,13.86);2384.8(a,5.395);2420.7(a,1.085);  
2421.2(a,2.858);3088.9(a,3.340);3095.7(a,0.6363);3146.2(a,3.544);  
3149.6(a,2.363);3165.1(a,4.277);3180.9(a,2.289);3205.0(a,0.6696);  
3217.0(a,1.894);3234.2(a,10.68);3243.8(a,7.489);3254.0(a,3.424);  
3284.2(a,2.746);3295.7(a,2.931);  
--- Zero-point energy (kcal/mol): 151.17 ---  
Total number of freqs. 90  
=== 5b\_II-IVfrq.txt ===  
Total energy (Hartree)= -553.4920408  
33.4(a,0.6299);49.6(a,1.865);58.2(a,1.429);73.8(a,0.9320);79.4(a,0.2900E-01);  
93.1(a,2.990);103.0(a,2.053);124.0(a,2.673);128.4(a,6.541);133.0(a,3.153);  
134.4(a,0.4881);154.0(a,5.970);170.7(a,6.926);186.9(a,1.312);  
199.8(a,4.725);213.7(a,1.194);221.4(a,1.973);232.5(a,1.124);234.2(a,0.8897);  
280.4(a,4.161);282.9(a,3.860);326.3(a,3.096);390.8(a,1.519);418.3(a,0.1905);  
448.6(a,0.2632);475.6(a,1.525);489.6(a,12.10);547.5(a,6.463);  
615.2(a,0.2779);622.4(a,0.3876);632.8(a,5.092);639.3(a,26.53);  
706.2(a,5.163);727.5(a,2.424);738.5(a,14.19);768.8(a,53.66);783.3(a,112.1);  
802.7(a,111.1);849.0(a,2.075);862.1(a,2.692);891.6(a,72.11);959.1(a,1.202);  
990.2(a,94.72);998.9(a,87.90);1007.7(a,0.8513);1016.2(a,2.636);  
1020.5(a,1.542);1044.6(a,8.306);1048.9(a,5.529);1051.1(a,16.67);  
1055.9(a,5.415);1066.3(a,73.31);1070.7(a,50.47);1077.4(a,27.50);  
1106.1(a,7.212);1184.9(a,3.965);1211.5(a,0.6860E-01);1213.8(a,11.11);  
1231.5(a,1.196);1246.6(a,0.4028);1327.9(a,15.41);1335.0(a,0.2553);  
1338.8(a,32.06);1353.4(a,0.9407);1355.5(a,5.962);1456.0(a,8.423);  
1485.2(a,33.36);1487.6(a,13.45);1489.2(a,18.81);1491.7(a,45.63);

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1589.1(a,28.15);1595.4(a,73.99);1614.1(a,8.249);2353.0(a,36.79);
2399.8(a,6.342);2411.4(a,1.429);2442.6(a,1.285);3086.6(a,1.027);
3099.1(a,0.2571);3154.1(a,1.950);3175.8(a,0.8389);3182.8(a,0.2004);
3194.7(a,1.193);3201.7(a,0.4228);3208.8(a,1.141);3223.5(a,7.473);
3230.8(a,6.343);3242.3(a,19.54);3291.0(a,0.7492);3318.0(a,0.4916);
--- Zero-point energy (kcal/mol): 152.48 ---
Total number of freqs. 90
=== 5c_II-IVfreq.txt ===
Total energy (Hartree)= -553.4906752
38.9(a,0.6337);52.9(a,0.8753);58.0(a,0.5429);70.5(a,1.011);76.7(a,0.6592);
86.1(a,2.602);99.4(a,0.5312);100.2(a,0.8186);108.7(a,0.9545);
131.7(a,1.490);139.6(a,2.228);151.4(a,0.6495);158.7(a,4.475);
164.3(a,0.6933);169.0(a,6.902);194.7(a,2.601);207.2(a,1.577);
217.0(a,1.826);235.5(a,0.8854);249.6(a,4.745);254.3(a,1.745);
281.7(a,5.622);362.2(a,0.6545);393.5(a,1.864);414.2(a,0.1729);
447.4(a,2.485);480.2(a,0.7274);496.4(a,4.204);608.8(a,0.2738);
618.2(a,0.1132);629.2(a,0.9158);645.3(a,42.75);698.2(a,11.53);
723.3(a,12.57);727.6(a,13.77);765.1(a,81.56);776.3(a,174.9);799.6(a,23.36);
847.3(a,4.270);853.7(a,2.004);890.6(a,78.93);951.0(a,0.5815);
989.5(a,168.4);996.6(a,37.71);1013.7(a,0.9439);1018.4(a,3.499);
1021.7(a,2.252);1031.8(a,47.24);1043.1(a,3.112);1048.7(a,3.418);
1063.4(a,101.4);1073.2(a,21.91);1079.9(a,30.51);1085.6(a,12.36);
1105.2(a,11.90);1176.5(a,4.935);1210.0(a,0.3870E-01);1213.6(a,16.55);
1229.0(a,0.4499);1252.8(a,0.4386);1324.2(a,9.240);1339.4(a,3.219);
1344.1(a,2.535);1352.8(a,6.332);1355.1(a,34.34);1457.8(a,8.082);
1485.1(a,19.21);1488.3(a,26.51);1488.5(a,67.08);1493.8(a,11.14);
1589.8(a,83.27);1604.7(a,29.57);1615.3(a,9.500);2335.6(a,34.55);
2356.8(a,30.54);2403.4(a,1.308);2410.3(a,1.033);3084.6(a,5.006);
3092.1(a,0.7077);3149.3(a,1.317);3164.4(a,2.310);3165.1(a,1.393);
3194.5(a,1.131);3195.9(a,4.108);3209.9(a,0.3432);3217.9(a,14.50);
3237.7(a,8.221);3259.5(a,8.371);3276.8(a,1.031);3314.2(a,0.8030);
--- Zero-point energy (kcal/mol): 151.58 ---
Total number of freqs. 90
=== 5d_II-IVfreq.txt ===
Total energy (Hartree)= -553.5054739
30.6(a,0.6639);51.0(a,3.692);67.5(a,1.698);71.8(a,0.9603);86.4(a,3.803);
90.2(a,0.3972);103.3(a,1.023);114.5(a,1.173);118.2(a,0.3987);
129.0(a,2.215);136.2(a,1.933);153.7(a,12.80);161.4(a,2.931);171.0(a,1.551);
183.2(a,1.647);207.0(a,1.996);212.9(a,0.2575);238.4(a,2.049);
247.9(a,0.4027);251.3(a,4.998);283.4(a,2.303);330.5(a,3.206);
385.3(a,1.778);413.9(a,0.1253);431.0(a,0.4376);474.2(a,2.512);
490.3(a,6.460);549.5(a,9.957);609.5(a,0.4839);618.8(a,0.2130);
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630.6(a,2.562);638.7(a,45.64);697.4(a,5.288);724.2(a,14.06);730.2(a,13.63);  
772.6(a,59.99);786.0(a,184.6);792.0(a,19.77);860.0(a,0.5704);  
861.7(a,1.763);890.7(a,74.45);966.4(a,2.654);985.0(a,159.5);995.7(a,22.74);  
1014.7(a,0.4765);1017.0(a,0.3199);1025.1(a,0.7248);1046.1(a,2.254);  
1049.3(a,10.76);1052.5(a,16.78);1064.6(a,37.54);1069.3(a,3.701);  
1074.2(a,99.34);1086.4(a,22.31);1106.2(a,11.80);1186.1(a,2.271);  
1210.9(a,0.7000E-02);1216.0(a,12.70);1232.2(a,4.306);1256.6(a,0.1305);  
1328.3(a,11.52);1337.6(a,1.346);1343.5(a,20.62);1352.0(a,2.872);  
1356.4(a,7.621);1457.6(a,8.849);1483.0(a,19.10);1483.3(a,0.4237);  
1487.8(a,106.6);1489.0(a,10.58);1589.1(a,57.49);1591.3(a,40.35);  
1614.2(a,10.68);2358.2(a,32.94);2391.8(a,1.669);2401.7(a,5.057);  
2440.3(a,0.2180);3086.7(a,0.7180);3095.8(a,1.127);3154.4(a,0.7520);  
3168.6(a,0.8169);3170.9(a,0.4610E-01);3190.7(a,0.2244);3205.5(a,0.2490E-01);  
3213.3(a,5.772);3234.9(a,2.818);3248.6(a,4.136);3253.6(a,20.58);  
3282.7(a,0.1330E-01);3314.3(a,0.4470E-01);  
--- Zero-point energy (kcal/mol): 152.36 ---  
Total number of freqs. 90  
=== TS-5-6\_II-IVfreq.txt ===  
Total energy (Hartree)= -553.4967701  
-254.3(a,28.25);35.3(a,0.2900E-02);48.1(a,3.929);64.9(a,1.496);  
76.3(a,0.2224);88.1(a,4.152);90.2(a,2.420);109.4(a,1.783);116.5(a,0.4150E-01);  
120.5(a,0.2450E-01);145.9(a,6.063);153.4(a,5.759);168.2(a,10.83);  
179.1(a,0.8268);197.1(a,5.756);198.2(a,0.7605);210.2(a,0.6481);  
245.1(a,0.5685);245.9(a,0.7449);284.7(a,4.490);305.9(a,0.5193);  
382.1(a,1.390);402.3(a,10.96);417.3(a,0.3386);438.3(a,0.6882);  
458.5(a,6.361);471.4(a,7.216);609.8(a,0.4178);618.8(a,0.8640E-01);  
625.3(a,11.18);632.3(a,1.847);691.8(a,3.211);702.1(a,2.976);716.0(a,14.80);  
720.0(a,10.48);769.7(a,104.8);776.4(a,174.9);787.2(a,8.189);872.1(a,0.2112);  
889.2(a,8.739);890.6(a,58.35);953.1(a,2.939);974.7(a,0.1124);  
977.2(a,8.017);991.9(a,83.48);1010.9(a,19.11);1029.5(a,0.6170);  
1046.4(a,11.11);1049.3(a,3.855);1051.6(a,32.19);1059.3(a,14.87);  
1080.6(a,21.88);1083.6(a,21.12);1098.7(a,3.124);1108.2(a,9.829);  
1188.1(a,0.9648);1211.5(a,0.1487);1217.8(a,14.50);1230.9(a,17.15);  
1237.7(a,5.439);1261.9(a,0.5800E-01);1331.4(a,3.763);1346.6(a,0.6970E-01);  
1351.2(a,2.452);1360.7(a,10.74);1459.6(a,11.56);1478.9(a,5.288);  
1485.2(a,36.01);1487.2(a,23.51);1488.6(a,9.110);1537.6(a,3.506);  
1589.7(a,4.857);1605.1(a,5.499);2373.5(a,24.36);2374.2(a,11.13);  
2407.8(a,0.5590);2410.0(a,0.7163);3090.5(a,1.204);3095.8(a,1.547);  
3155.9(a,0.2486);3165.5(a,0.7461);3168.9(a,0.4563);3194.9(a,2.201);  
3208.2(a,0.1540E-01);3216.6(a,4.937);3235.0(a,2.136);3246.7(a,0.7828);  
3251.2(a,27.15);3277.5(a,0.1590E-01);3317.6(a,0.3438);  
--- Zero-point energy (kcal/mol): 152.29 ---

```
Total number of freqs.          90
=== 6_II-IVfrq.txt ===
Total energy (Hartree)= -553.5427242
47.3(a,3.199);56.4(a,2.365);62.2(a,1.055);66.6(a,0.6349);73.9(a,1.012);
90.1(a,1.447);101.5(a,0.1247);106.1(a,5.508);118.3(a,0.7848);
127.1(a,5.073);144.1(a,9.444);164.0(a,1.625);184.3(a,10.94);200.4(a,3.560);
217.1(a,5.538);228.3(a,1.582);237.6(a,4.982);295.2(a,23.02);317.5(a,4.453);
359.9(a,1.637);363.9(a,0.6510);401.6(a,0.6629);421.7(a,9.386);
451.0(a,6.936);485.2(a,11.56);501.9(a,9.925);583.4(a,20.40);609.9(a,0.5103);
630.4(a,3.587);632.1(a,1.717);721.4(a,3.893);722.6(a,20.10);727.0(a,9.703);
749.7(a,8.463);777.7(a,36.07);780.0(a,242.2);794.3(a,3.828);809.8(a,29.01);
888.6(a,131.5);897.5(a,30.66);922.7(a,9.692);948.2(a,93.76);991.1(a,96.65);
1002.9(a,3.710);1020.0(a,8.454);1035.0(a,10.62);1044.2(a,0.4180);
1050.2(a,2.893);1057.8(a,2.689);1071.3(a,16.62);1078.7(a,9.147);
1090.2(a,29.90);1118.2(a,27.63);1135.0(a,6.053);1186.8(a,2.776);
1213.2(a,9.873);1217.5(a,20.94);1218.9(a,5.375);1231.4(a,28.87);
1241.9(a,31.97);1330.1(a,6.313);1350.9(a,2.304);1352.5(a,5.657);
1369.4(a,6.144);1404.9(a,17.41);1470.6(a,12.17);1477.7(a,4.960);
1484.0(a,13.62);1491.4(a,18.80);1505.2(a,17.23);1519.6(a,14.38);
1593.0(a,23.91);1634.0(a,113.6);2346.9(a,36.27);2380.4(a,4.631);
2388.0(a,11.36);2423.3(a,0.5710E-01);3055.9(a,4.850);3086.4(a,0.8433);
3095.3(a,2.477);3119.6(a,7.992);3125.4(a,5.455);3154.3(a,0.4499);
3167.3(a,0.9260);3176.3(a,5.915);3210.3(a,1.104);3215.1(a,0.8233);
3224.4(a,2.934);3228.2(a,6.432);3244.5(a,11.47);
--- Zero-point energy (kcal/mol): 153.89 ---
Total number of freqs.          90
=== TS-6-7_II-IVfrq.txt ===
Total energy (Hartree)= -553.5260343
-41.4(a,0.1254);32.1(a,1.155);39.9(a,2.588);42.8(a,1.178);60.9(a,1.835);
70.0(a,1.977);84.2(a,0.2912);96.3(a,0.1716);102.7(a,1.189);121.9(a,0.2492);
136.1(a,10.00);142.5(a,0.5703);177.2(a,0.7037);198.6(a,10.96);
204.5(a,2.879);228.2(a,2.446);238.3(a,2.265);297.4(a,1.823);332.0(a,7.155);
360.2(a,1.510);372.1(a,2.141);404.9(a,0.9703);416.4(a,0.6707);
433.0(a,19.16);487.1(a,21.63);492.2(a,15.89);559.1(a,2.281);599.8(a,1.919);
627.9(a,6.063);635.2(a,0.9444);709.9(a,29.60);713.7(a,7.314);
724.8(a,48.98);746.6(a,12.80);763.6(a,38.23);775.0(a,208.0);786.7(a,9.499);
815.6(a,7.359);834.9(a,48.21);888.4(a,1.141);890.9(a,67.53);963.3(a,4.790);
983.3(a,137.4);993.4(a,10.99);1017.9(a,5.607);1024.0(a,0.1171);
1043.3(a,2.599);1049.9(a,0.7803);1050.7(a,3.214);1068.6(a,3.716);
1073.2(a,13.41);1086.8(a,31.63);1114.2(a,15.59);1127.2(a,11.23);
1192.7(a,4.778);1196.0(a,82.05);1210.8(a,0.7789);1221.5(a,32.62);
1223.1(a,1.214);1243.0(a,30.43);1332.9(a,6.143);1347.0(a,7.116);
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1352.1(a,3.174);1379.3(a,2.330);1385.6(a,3.599);1461.2(a,42.50);
1478.1(a,8.671);1478.9(a,4.900);1485.8(a,17.37);1488.8(a,22.36);
1527.6(a,4.748);1628.5(a,5.541);1645.8(a,56.04);2358.2(a,33.04);
2393.3(a,1.891);2399.8(a,4.629);2435.7(a,1.349);2938.8(a,59.38);
3069.2(a,5.427);3083.8(a,1.079);3094.5(a,1.958);3119.7(a,15.37);
3153.6(a,0.7685);3166.4(a,0.8646);3178.9(a,6.505);3182.2(a,5.536);
3208.4(a,0.8742);3219.7(a,16.07);3220.1(a,4.761);3237.8(a,29.71);
--- Zero-point energy (kcal/mol): 305.93 ---
Total number of freqs. 90
=== 7_II-IVfreq.txt ===
Total energy (Hartree)= -553.5331444
19.2(a,1.228);26.2(a,0.5352);34.3(a,2.315);59.2(a,2.077);64.6(a,1.216);
72.5(a,0.8995);97.9(a,0.2960);105.7(a,0.4499);123.2(a,0.2373);
127.7(a,4.387);141.2(a,11.65);149.7(a,0.9579);184.1(a,4.262);
207.5(a,2.228);211.4(a,5.603);232.2(a,0.4163);244.0(a,2.090);
310.5(a,3.634);325.7(a,15.24);375.9(a,3.243);407.0(a,2.606);415.1(a,1.370);
419.9(a,0.4185);452.8(a,25.15);477.1(a,19.44);483.1(a,17.44);
580.8(a,4.107);604.7(a,1.067);630.0(a,4.526);633.4(a,0.2660E-01);
708.5(a,19.78);713.1(a,27.37);717.1(a,5.784);736.0(a,36.45);767.1(a,159.7);
774.1(a,120.6);788.6(a,11.25);803.4(a,1.495);839.6(a,18.54);880.8(a,3.209);
891.3(a,69.36);963.6(a,0.5060E-01);987.1(a,106.1);1012.2(a,16.80);
1023.4(a,0.1600);1030.0(a,2.899);1044.9(a,4.183);1050.5(a,3.588);
1052.1(a,1.143);1072.1(a,11.28);1078.2(a,11.08);1085.2(a,23.08);
1093.3(a,1.727);1124.7(a,17.36);1191.0(a,2.815);1205.2(a,32.13);
1213.5(a,0.8221);1221.5(a,21.68);1228.5(a,14.01);1234.6(a,4.260);
1321.2(a,55.00);1333.1(a,4.332);1351.1(a,3.346);1367.5(a,3.594);
1381.4(a,2.115);1449.9(a,26.01);1482.5(a,12.45);1484.6(a,3.382);
1488.5(a,21.10);1496.5(a,8.366);1521.8(a,3.073);1621.7(a,4.668);
1641.6(a,83.51);2366.1(a,27.30);2392.9(a,10.59);2401.1(a,1.484);
2429.3(a,0.2395);2450.3(a,128.4);3065.1(a,4.444);3087.1(a,0.8223);
3094.9(a,1.902);3150.2(a,4.612);3154.8(a,0.5782);3167.3(a,0.8349);
3186.4(a,5.293);3196.0(a,3.199);3213.1(a,0.8541);3224.7(a,16.19);
3241.1(a,26.11);3259.4(a,0.1410);
--- Zero-point energy (kcal/mol): 305.21 ---
Total number of freqs. 90
=== TS-7-8_II-IVfreq.txt ===
Total energy (Hartree)= -553.5276163
-682.0(a,428.1);30.5(a,0.9834);37.0(a,4.068);55.1(a,1.394);58.1(a,1.288);
63.2(a,1.401);78.7(a,0.3066);105.3(a,1.233);107.9(a,1.016);123.3(a,0.6360E-01);
125.8(a,2.560);144.5(a,12.38);162.3(a,0.7224);203.0(a,1.324);
212.7(a,2.381);219.1(a,2.875);256.9(a,0.5871);265.3(a,5.751);
295.3(a,5.318);365.2(a,6.829);375.8(a,1.119);412.9(a,2.439);430.5(a,7.665);
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433.3(a,2.230);458.0(a,7.051);474.6(a,19.27);526.0(a,34.07);571.3(a,43.28);  
609.6(a,0.1314);630.4(a,0.6641);631.5(a,1.511);702.9(a,18.35);  
718.0(a,31.61);721.1(a,3.864);731.9(a,39.00);772.2(a,117.0);778.3(a,79.00);  
792.7(a,5.030);796.5(a,7.404);836.4(a,24.97);879.1(a,2.299);894.0(a,61.54);  
982.7(a,0.5396);990.3(a,93.88);1013.3(a,32.74);1021.1(a,76.22);  
1031.6(a,1.832);1041.4(a,1.963);1047.8(a,3.224);1058.9(a,0.2416);  
1065.5(a,2.872);1080.8(a,26.40);1083.2(a,31.65);1116.7(a,6.230);  
1177.0(a,47.49);1187.5(a,1.841);1197.0(a,48.85);1217.6(a,1.009);  
1219.5(a,16.04);1232.2(a,34.51);1274.1(a,97.18);1331.1(a,2.499);  
1349.6(a,3.903);1368.3(a,70.57);1394.8(a,21.77);1434.4(a,81.55);  
1484.8(a,6.201);1488.5(a,20.97);1488.9(a,11.54);1514.4(a,13.10);  
1534.3(a,70.83);1614.9(a,1.325);1638.1(a,258.8);1727.9(a,176.7);  
2373.3(a,26.32);2378.2(a,18.18);2407.1(a,1.221);2414.4(a,0.8071);  
3089.5(a,1.332);3094.2(a,2.334);3154.9(a,0.1108);3157.7(a,3.874);  
3166.9(a,0.5098);3170.0(a,0.8027);3195.2(a,2.097);3214.8(a,0.2100);  
3226.5(a,4.324);3238.0(a,12.06);3248.1(a,12.38);3283.9(a,0.6263);  
--- Zero-point energy (kcal/mol): 150.54 ---  
Total number of freqs. 90  
=== 8\_II-IVfrq.txt ===  
Total energy (Hartree)= -553.5364906  
21.1(a,1.911);31.7(a,3.852);42.7(a,1.578);48.6(a,3.686);61.2(a,0.8470E-01);  
76.5(a,1.703);90.9(a,0.2278);93.0(a,1.605);115.2(a,2.812);124.0(a,0.2095);  
130.2(a,1.537);136.8(a,8.540);187.6(a,2.131);205.1(a,0.7752);  
214.7(a,9.186);239.7(a,2.347);257.7(a,3.682);298.9(a,13.22);304.4(a,29.33);  
355.3(a,0.2853);378.2(a,100.5);398.8(a,1.151);418.5(a,13.35);  
457.4(a,3.413);469.1(a,3.209);499.2(a,14.32);571.7(a,33.08);600.6(a,36.51);  
611.1(a,0.2139);628.0(a,1.092);632.3(a,13.11);692.6(a,83.30);  
699.1(a,64.39);726.0(a,2.251);738.6(a,8.336);777.5(a,85.62);780.0(a,129.6);  
797.8(a,4.967);800.3(a,17.29);847.1(a,35.49);878.4(a,4.552);897.1(a,69.39);  
987.8(a,11.65);991.2(a,140.5);1006.9(a,262.6);1013.7(a,38.72);  
1026.9(a,11.62);1038.1(a,4.787);1043.7(a,2.248);1051.2(a,3.021);  
1062.6(a,0.3399);1075.1(a,15.54);1090.2(a,28.06);1097.1(a,5.691);  
1131.6(a,4.529);1182.7(a,3.537);1216.3(a,24.52);1217.2(a,4.683);  
1229.5(a,52.90);1241.6(a,14.75);1314.3(a,173.1);1328.2(a,2.737);  
1347.9(a,4.037);1380.3(a,102.7);1406.6(a,56.58);1462.8(a,139.5);  
1486.3(a,16.40);1490.0(a,20.00);1492.5(a,14.24);1518.8(a,3.419);  
1573.3(a,397.4);1605.6(a,17.13);1642.6(a,326.2);2076.9(a,98.42);  
2355.4(a,35.05);2386.1(a,4.721);2388.4(a,16.68);2426.2(a,0.2342);  
3086.7(a,1.733);3093.0(a,3.068);3152.8(a,0.2858);3159.8(a,5.458);  
3165.1(a,1.006);3182.0(a,1.010);3203.6(a,1.266);3217.0(a,0.2580);  
3229.7(a,3.295);3241.2(a,9.726);3250.6(a,10.69);3269.3(a,0.6336);  
--- Zero-point energy (kcal/mol): 151.49 ---

Total number of freqs.

90

=== 1\_0-II.xyz ===

13

Structure 1(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | 0.000000  | 0.000000  | 1.147418  |
| P  | 0.000000  | 1.758791  | -0.485503 |
| P  | 0.000000  | -1.758791 | -0.485503 |
| C  | -0.365686 | 0.681071  | -2.051743 |
| C  | 0.365686  | -0.681071 | -2.051743 |
| H  | -1.452762 | 0.530948  | -2.071412 |
| H  | -0.090790 | 1.247356  | -2.950243 |
| H  | 1.452762  | -0.530948 | -2.071412 |
| H  | 0.090790  | -1.247356 | -2.950243 |
| H  | -1.219021 | -2.388752 | -0.942865 |
| H  | 0.865500  | -2.868107 | -0.833093 |
| H  | 1.219021  | 2.388752  | -0.942865 |
| H  | -0.865500 | 2.868107  | -0.833093 |

=== 2\_0-II.xyz ===

19

Structure 2(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | 0.000000  | 0.000000  | 0.771452  |
| P  | 0.000000  | 1.669209  | -1.053531 |
| P  | 0.000000  | -1.669209 | -1.053531 |
| C  | -0.353619 | 0.686018  | -2.675765 |
| C  | 0.353619  | -0.686018 | -2.675765 |
| H  | 1.199502  | 2.359470  | -1.463653 |
| H  | -0.898109 | 2.775947  | -1.275961 |
| H  | 0.898109  | -2.775947 | -1.275961 |
| H  | -1.199502 | -2.359470 | -1.463653 |
| H  | 0.042647  | -1.275750 | -3.545456 |
| H  | 1.441999  | -0.555624 | -2.731427 |
| H  | -1.441999 | 0.555624  | -2.731427 |
| H  | -0.042647 | 1.275750  | -3.545456 |
| C  | 0.005211  | 0.707517  | 2.846887  |
| C  | -0.005211 | -0.707517 | 2.846887  |
| H  | 0.910828  | -1.268492 | 3.025896  |
| H  | -0.931145 | -1.253047 | 3.023436  |
| H  | -0.910828 | 1.268492  | 3.025896  |
| H  | 0.931145  | 1.253047  | 3.023436  |

=== 3\_0-II.xyz ===

25

Structure 3(0-II)

|   |           |          |          |
|---|-----------|----------|----------|
| C | -1.677883 | 2.513295 | 1.665294 |
|---|-----------|----------|----------|

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.732907 | 1.135284  | 1.460933  |
| C  | -1.430199 | 0.588103  | 0.167596  |
| C  | -1.108128 | 1.478248  | -0.924122 |
| C  | -1.087129 | 2.890661  | -0.674142 |
| C  | -1.359893 | 3.399718  | 0.593648  |
| Pd | 0.709149  | 0.300966  | -0.162102 |
| P  | 1.896281  | -1.315024 | 1.347872  |
| C  | 3.770011  | -0.977743 | 1.048350  |
| C  | 4.077934  | -0.709584 | -0.440860 |
| P  | 2.945133  | 0.666659  | -1.171686 |
| I  | -2.321092 | -1.374573 | -0.316322 |
| H  | 1.930250  | -1.405638 | 2.788497  |
| H  | 1.882264  | -2.736920 | 1.102248  |
| H  | 3.360823  | 0.577026  | -2.550001 |
| H  | 3.741835  | 1.822512  | -0.839628 |
| H  | 5.130349  | -0.431531 | -0.567042 |
| H  | 3.897090  | -1.612616 | -1.037894 |
| H  | 4.363371  | -1.825087 | 1.409796  |
| H  | 4.032276  | -0.103048 | 1.657236  |
| H  | -1.140101 | 1.124375  | -1.950694 |
| H  | -0.884039 | 3.561652  | -1.506460 |
| H  | -1.350807 | 4.473385  | 0.766077  |
| H  | -1.891499 | 2.913704  | 2.654004  |
| H  | -2.006817 | 0.467740  | 2.272675  |

=== TS-3-4\_0-II.xyz ===

25

Structure TS-3-4(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.176699 | 2.422592  | -1.429913 |
| C  | -2.461034 | 3.201312  | -0.298537 |
| C  | -2.300248 | 2.649033  | 0.997296  |
| C  | -1.846327 | 1.334101  | 1.163777  |
| C  | -1.519182 | 0.557299  | 0.016222  |
| C  | -1.730622 | 1.084096  | -1.290777 |
| Pd | 0.537491  | 0.135332  | -0.327791 |
| I  | -1.656831 | -1.760240 | 0.209398  |
| P  | 2.069099  | 0.599321  | 1.724470  |
| C  | 3.823267  | 0.691729  | 0.926026  |
| C  | 4.024593  | -0.371674 | -0.174642 |
| P  | 2.656189  | -0.278372 | -1.523095 |
| H  | 3.013871  | -1.447865 | -2.284082 |
| H  | 3.264127  | 0.685546  | -2.407027 |
| H  | 2.221493  | 1.719465  | 2.629231  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.351044  | -0.415445 | 2.715963  |
| H | 4.588396  | 0.576466  | 1.701987  |
| H | 3.923518  | 1.701172  | 0.506917  |
| H | 5.010639  | -0.255189 | -0.638652 |
| H | 3.973814  | -1.380981 | 0.253216  |
| H | -1.619850 | 0.451063  | -2.164983 |
| H | -2.325675 | 2.828603  | -2.428221 |
| H | -2.822331 | 4.220549  | -0.412837 |
| H | -2.526785 | 3.249746  | 1.875739  |
| H | -1.726584 | 0.909163  | 2.155693  |

=== 4\_0-II.xyz ===

25

SCF Done: E(RB+HF-LYP) = -463.777785194 A.U.

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | -1.423957 | -1.630538 | 0.041301  |
| Pd | -0.749099 | 0.683748  | -0.021713 |
| I  | -0.061795 | 3.278136  | -0.105400 |
| P  | -3.226830 | 1.114513  | -0.034601 |
| C  | 1.214546  | 0.149831  | 0.000868  |
| C  | 3.918767  | -0.692784 | 0.036408  |
| C  | 1.903250  | -0.082970 | -1.209326 |
| C  | 1.886375  | -0.034558 | 1.228747  |
| C  | 3.233860  | -0.454321 | 1.243713  |
| C  | 3.250505  | -0.502630 | -1.188815 |
| H  | 1.409791  | 0.082624  | -2.164434 |
| H  | 1.380061  | 0.168928  | 2.169850  |
| H  | 3.745118  | -0.583667 | 2.196095  |
| H  | 3.775083  | -0.669321 | -2.128114 |
| H  | 4.958961  | -1.010905 | 0.049755  |
| C  | -3.304379 | -1.736832 | -0.316009 |
| H  | -1.304004 | -2.360184 | 1.269708  |
| H  | -0.885197 | -2.609423 | -0.853269 |
| C  | -4.070762 | -0.568746 | 0.347244  |
| H  | -3.893077 | 1.500100  | -1.245605 |
| H  | -3.908863 | 1.989501  | 0.871264  |
| H  | -3.416987 | -1.700556 | -1.406569 |
| H  | -5.113951 | -0.562562 | 0.013275  |
| H  | -4.072178 | -0.680786 | 1.438483  |
| H  | -3.697452 | -2.699995 | 0.027718  |

=== 5\_0-II.xyz ===

30

structure 5(0-II)

|   |           |           |           |
|---|-----------|-----------|-----------|
| P | -0.695222 | -1.843264 | -0.044688 |
|---|-----------|-----------|-----------|

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -0.362880 | 0.522921  | -0.025345 |
| P  | -2.896804 | 0.585614  | 0.005004  |
| C  | 1.634755  | -0.034431 | 0.003562  |
| C  | 4.341711  | -0.806862 | 0.079559  |
| C  | 2.338592  | -0.228056 | -1.201421 |
| C  | 2.268821  | -0.234641 | 1.246067  |
| C  | 3.627737  | -0.618539 | 1.278326  |
| C  | 3.696854  | -0.611933 | -1.157076 |
| H  | 1.857909  | -0.078934 | -2.166088 |
| H  | 1.734054  | -0.089057 | 2.182638  |
| H  | 4.119050  | -0.766797 | 2.236910  |
| H  | 4.242846  | -0.754678 | -2.086499 |
| H  | 5.387152  | -1.101206 | 0.108353  |
| C  | -2.544270 | -2.236194 | -0.312363 |
| H  | -0.346004 | -2.519923 | 1.161134  |
| H  | -0.008180 | -2.625980 | -1.015981 |
| C  | -3.445524 | -1.205226 | 0.398604  |
| H  | -3.591440 | 0.868554  | -1.214636 |
| H  | -3.684830 | 1.362783  | 0.911118  |
| H  | -2.717471 | -2.229403 | -1.394739 |
| H  | -4.489477 | -1.346213 | 0.101419  |
| H  | -3.391522 | -1.321149 | 1.487242  |
| H  | -2.758194 | -3.246898 | 0.051312  |
| C  | -0.505858 | 2.906458  | 0.039755  |
| H  | -0.923179 | 3.112127  | 1.022969  |
| H  | -1.125849 | 3.153674  | -0.818844 |
| C  | 0.831897  | 2.609408  | -0.115675 |
| H  | 1.502768  | 2.562694  | 0.735829  |
| H  | 1.296940  | 2.590874  | -1.097052 |

=== TS-5-6\_0-II.xyz ===

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Structure TS-5-6(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.530681 | 2.769386  | -0.038223 |
| Pd | -0.824804 | 0.632374  | -0.016885 |
| P  | -1.268608 | -1.809955 | 0.048213  |
| P  | -3.275901 | 0.781948  | -0.078750 |
| C  | -3.978221 | -0.947327 | 0.336060  |
| H  | -3.887068 | 1.091062  | -1.334404 |
| H  | -4.019692 | 1.652629  | 0.775922  |
| C  | -3.130022 | -2.067976 | -0.304902 |
| H  | -1.075856 | -2.490778 | 1.291403  |
| H  | -0.629992 | -2.730862 | -0.838135 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -5.016898 | -1.012772 | -0.003356 |
| H | -3.979704 | -1.034236 | 1.428868  |
| H | -3.450668 | -3.044907 | 0.070729  |
| H | -3.252320 | -2.076431 | -1.394283 |
| C | 0.853951  | 2.441411  | 0.015265  |
| H | -1.021216 | 3.129104  | 0.864955  |
| H | -0.953131 | 3.117971  | -0.979361 |
| H | 1.388707  | 2.553489  | 0.953189  |
| H | 1.459871  | 2.554943  | -0.877768 |
| C | 1.294897  | 0.319774  | 0.009352  |
| C | 3.605843  | -1.295049 | 0.012417  |
| C | 1.875774  | -0.076198 | 1.235344  |
| C | 1.886117  | -0.066835 | -1.215015 |
| C | 3.035682  | -0.881458 | -1.208678 |
| C | 3.025738  | -0.890709 | 1.231881  |
| H | 1.447999  | 0.244016  | 2.183082  |
| H | 1.466375  | 0.261758  | -2.163550 |
| H | 3.488187  | -1.179024 | -2.151158 |
| H | 3.470169  | -1.196138 | 2.175699  |
| H | 4.499794  | -1.912631 | 0.013778  |

=== 6\_0-II.xyz ===

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Structure 6(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.090013 | 2.539643  | 0.081574  |
| Pd | 0.578964  | 0.576763  | 0.036256  |
| P  | 1.478505  | -1.812973 | -0.049163 |
| P  | 2.884220  | 1.186912  | -0.018460 |
| C  | 3.938461  | -0.375469 | 0.287224  |
| H  | 3.403513  | 2.147364  | 0.900908  |
| H  | 3.384818  | 1.707152  | -1.251507 |
| C  | 3.344649  | -1.607645 | -0.430505 |
| H  | 1.095822  | -2.826165 | -0.984396 |
| H  | 1.505620  | -2.606960 | 1.142831  |
| H  | 3.965670  | -0.528873 | 1.372318  |
| H  | 4.964487  | -0.192522 | -0.048794 |
| H  | 3.441386  | -1.509709 | -1.518148 |
| H  | 3.889408  | -2.508938 | -0.132149 |
| C  | -1.562815 | 2.250442  | -0.252676 |
| H  | 0.441180  | 3.140116  | -0.660387 |
| H  | 0.091985  | 2.906035  | 1.096863  |
| H  | -1.793175 | 2.555610  | -1.278173 |
| H  | -2.242350 | 2.794103  | 0.415730  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | -1.783020 | 0.725877  | -0.107374 |
| C | -2.495473 | -2.009120 | 0.215308  |
| C | -2.096169 | -0.085848 | -1.236318 |
| C | -1.798891 | 0.120100  | 1.186299  |
| C | -2.156940 | -1.237455 | 1.340902  |
| C | -2.454760 | -1.433863 | -1.074653 |
| H | -2.101884 | 0.362625  | -2.226963 |
| H | -1.622917 | 0.732414  | 2.068235  |
| H | -2.200586 | -1.671458 | 2.335987  |
| H | -2.724465 | -2.028144 | -1.943367 |
| H | -2.803649 | -3.044050 | 0.337845  |

=== TS-6-7\_0-II.xyz ===

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Structure TS-6-7(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | -2.293599 | -1.266235 | 0.896657  |
| Pd | -0.561834 | -0.279165 | -0.371267 |
| H  | 1.234448  | -0.840868 | -2.051649 |
| P  | -2.100841 | 1.732633  | -0.584541 |
| H  | -4.260357 | 0.546572  | -0.745763 |
| C  | 0.634939  | -1.956572 | -0.279614 |
| H  | 0.107167  | -2.815077 | -0.706973 |
| H  | 0.953804  | -2.136948 | 0.749993  |
| C  | 1.714031  | -1.354016 | -1.186242 |
| H  | 2.269643  | -2.181514 | -1.657489 |
| C  | 2.636181  | -0.386503 | -0.460151 |
| C  | 4.255306  | 1.415827  | 1.008831  |
| C  | 2.278589  | 0.974991  | -0.342670 |
| C  | 3.822586  | -0.833621 | 0.156695  |
| C  | 4.627909  | 0.062318  | 0.885650  |
| C  | 3.075872  | 1.873402  | 0.392038  |
| H  | 1.402234  | 1.356283  | -0.878059 |
| H  | 4.122588  | -1.875566 | 0.065931  |
| H  | 5.543604  | -0.291854 | 1.351657  |
| H  | 2.792868  | 2.920125  | 0.466480  |
| H  | 4.881957  | 2.105143  | 1.567881  |
| C  | -3.564504 | 0.105473  | 1.283379  |
| H  | -2.012629 | -1.863205 | 2.161160  |
| H  | -3.054746 | -2.298457 | 0.269081  |
| C  | -3.765492 | 1.060822  | 0.086245  |
| H  | -1.894253 | 2.893953  | 0.227309  |
| H  | -2.509443 | 2.372037  | -1.797206 |
| H  | -4.407472 | 1.895204  | 0.385690  |

|   |           |           |          |
|---|-----------|-----------|----------|
| H | -3.185133 | 0.645578  | 2.158508 |
| H | -4.515804 | -0.358521 | 1.565026 |

=== 7\_0-II.xyz ===

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Structure 7(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| P  | 3.139204  | -0.609807 | -1.363744 |
| Pd | 1.374421  | -0.488209 | 0.235695  |
| H  | -0.232775 | -0.690236 | 1.245398  |
| P  | 2.921603  | 0.954559  | 1.566789  |
| H  | 5.079617  | -0.132215 | 1.066983  |
| C  | -0.052907 | -1.671839 | -0.702465 |
| H  | 0.312886  | -2.699130 | -0.742036 |
| H  | -0.340788 | -1.266504 | -1.671920 |
| C  | -0.910015 | -1.295411 | 0.474325  |
| H  | -1.156623 | -2.168162 | 1.089564  |
| C  | -2.110120 | -0.400050 | 0.210045  |
| C  | -4.364544 | 1.219226  | -0.313567 |
| C  | -1.956197 | 0.856160  | -0.414145 |
| C  | -3.398370 | -0.835043 | 0.582208  |
| C  | -4.522140 | -0.028966 | 0.316800  |
| C  | -3.077062 | 1.662057  | -0.677639 |
| H  | -0.961481 | 1.210402  | -0.688040 |
| H  | -3.530726 | -1.798558 | 1.070216  |
| H  | -5.512271 | -0.373501 | 0.602424  |
| H  | -2.950819 | 2.629255  | -1.156923 |
| H  | -5.231983 | 1.841948  | -0.514126 |
| C  | 4.441547  | 0.694591  | -0.858120 |
| H  | 2.913082  | -0.358526 | -2.749700 |
| H  | 3.873711  | -1.832355 | -1.430454 |
| C  | 4.607297  | 0.776408  | 0.675948  |
| H  | 2.724732  | 2.371259  | 1.589593  |
| H  | 3.271581  | 0.741789  | 2.935852  |
| H  | 5.253819  | 1.621019  | 0.934292  |
| H  | 4.101030  | 1.652805  | -1.267356 |
| H  | 5.398464  | 0.451913  | -1.331840 |

=== TS-7-8\_0-II.xyz ===

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Structure TS-7-8(0-II)

|    |          |           |           |
|----|----------|-----------|-----------|
| P  | 3.277681 | 0.970927  | 1.038316  |
| Pd | 1.343861 | 0.384562  | -0.376360 |
| H  | 0.084986 | 0.003585  | -1.312016 |
| P  | 2.697179 | -1.506294 | -1.083701 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 5.015533  | -2.142956 | -0.389946 |
| C | -0.035297 | 1.998177  | 0.058099  |
| H | 0.444109  | 2.865755  | -0.392171 |
| H | -0.192090 | 2.054341  | 1.132330  |
| C | -0.931083 | 1.228311  | -0.751251 |
| H | -1.027929 | 1.548761  | -1.790107 |
| C | -2.072568 | 0.419783  | -0.242101 |
| C | -4.326066 | -1.043102 | 0.635473  |
| C | -2.180257 | 0.016140  | 1.110042  |
| C | -3.101226 | 0.072120  | -1.148987 |
| C | -4.224380 | -0.650925 | -0.712582 |
| C | -3.300058 | -0.708453 | 1.544441  |
| H | -1.395850 | 0.259767  | 1.822840  |
| H | -3.029216 | 0.374766  | -2.192327 |
| H | -5.012749 | -0.904485 | -1.415459 |
| H | -3.378869 | -1.012534 | 2.584584  |
| H | -5.192529 | -1.603274 | 0.976102  |
| C | 4.709944  | -0.154526 | 0.447212  |
| H | 3.213644  | 0.701565  | 2.441493  |
| H | 3.878841  | 2.266551  | 1.068018  |
| C | 4.211448  | -1.570167 | 0.083328  |
| H | 3.280834  | -1.460038 | -2.386894 |
| H | 2.210885  | -2.847708 | -1.071388 |
| H | 3.898007  | -2.117726 | 0.979767  |
| H | 5.475711  | -0.213419 | 1.227275  |
| H | 5.160143  | 0.337628  | -0.422743 |

=== 8\_0-II.xyz ===

30

Structure 8(0-II)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -0.157364 | 2.135163  | -1.250967 |
| Pd | 1.411875  | 1.106758  | 0.046145  |
| P  | 3.351655  | 0.399137  | 1.261803  |
| P  | 1.680334  | -1.115491 | -1.174143 |
| C  | 3.416642  | -1.732968 | -0.649313 |
| H  | 1.707870  | -1.313909 | -2.591031 |
| H  | 0.840280  | -2.213096 | -0.803871 |
| C  | 3.706845  | -1.429325 | 0.836039  |
| H  | 3.374715  | 0.446876  | 2.685823  |
| H  | 4.564282  | 1.081459  | 0.946733  |
| H  | 4.142913  | -1.232816 | -1.300442 |
| H  | 3.496315  | -2.809498 | -0.831317 |
| H  | 3.072031  | -2.035501 | 1.492547  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 4.750023  | -1.660128 | 1.076352  |
| C | -0.930597 | 1.786956  | -0.144306 |
| H | -0.206910 | 1.574450  | -2.180057 |
| C | -1.825669 | 0.626243  | -0.007767 |
| H | -0.966860 | 2.498526  | 0.680415  |
| H | 1.505280  | 2.396162  | 0.912679  |
| H | 0.274012  | 3.130588  | -1.315446 |
| C | -3.609956 | -1.542653 | 0.347597  |
| C | -2.131049 | -0.240195 | -1.090424 |
| C | -2.439236 | 0.391917  | 1.249143  |
| C | -3.320692 | -0.686343 | 1.427777  |
| C | -3.015959 | -1.312662 | -0.912883 |
| H | -1.709093 | -0.056236 | -2.075780 |
| H | -2.226669 | 1.058870  | 2.082678  |
| H | -3.787431 | -0.852444 | 2.394395  |
| H | -3.261216 | -1.959139 | -1.751155 |
| H | -4.301031 | -2.370841 | 0.479194  |

=== l\_II-IV.xyz ===

14

Structure 1(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 3.463282  | 0.490543  | 0.358705  |
| C  | 2.709534  | 1.661903  | -0.301857 |
| P  | 0.831138  | 1.591417  | 0.033407  |
| Pd | 0.229484  | -0.658443 | -0.031279 |
| P  | 2.620197  | -1.175291 | -0.032882 |
| H  | 3.482008  | 0.593637  | 1.449172  |
| H  | 4.500508  | 0.471933  | 0.008992  |
| H  | 2.830183  | 1.650734  | -1.390817 |
| H  | 3.085939  | 2.622745  | 0.067498  |
| H  | 0.609863  | 2.205264  | 1.297134  |
| H  | 0.225741  | 2.484758  | -0.889851 |
| H  | 3.207274  | -1.603743 | -1.261572 |
| H  | 3.190330  | -2.099981 | 0.891427  |
| I  | -2.273491 | 0.090688  | 0.017319  |

=== 2\_II-IV.xyz ===

20

Structure 2(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.868252  | -1.858264 | 0.286596  |
| C  | 3.561356  | -0.653593 | -0.380664 |
| P  | 2.653433  | 0.974949  | 0.035170  |
| Pd | 0.253847  | 0.469716  | 0.020509  |
| I  | -2.229937 | -0.526436 | -0.021599 |
| P  | 0.979685  | -1.815284 | 0.003858  |
| H  | 3.216987  | 1.387375  | 1.282140  |
| H  | 3.225171  | 1.939195  | -0.849793 |
| H  | 4.603951  | -0.583165 | -0.054217 |
| H  | 3.558386  | -0.748537 | -1.472273 |
| H  | 3.027828  | -1.856631 | 1.370734  |
| H  | 3.271311  | -2.797399 | -0.107268 |
| H  | 0.758761  | -2.489800 | -1.230430 |
| H  | 0.426587  | -2.718186 | 0.952216  |
| C  | -0.536115 | 2.593441  | 0.709802  |
| C  | -0.527152 | 2.594683  | -0.673645 |
| H  | 0.279356  | 3.028043  | 1.283999  |
| H  | -1.432517 | 2.323683  | 1.261242  |
| H  | -1.416847 | 2.327200  | -1.236738 |
| H  | 0.295946  | 3.029797  | -1.236235 |

=== 3\_II-IV.xyz ===

26

Structure 3(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 2.253373  | -0.300336 | 0.697369  |
| C  | 1.035632  | -1.019134 | 0.905721  |
| C  | 0.379666  | -0.925161 | 2.169770  |
| C  | 0.918768  | -0.110903 | 3.194569  |
| C  | 2.125047  | 0.571034  | 2.973919  |
| C  | 2.795956  | 0.481373  | 1.727385  |
| Pd | -0.887642 | 0.291550  | 0.200038  |
| I  | -2.383127 | -1.915430 | -0.155414 |
| I  | 3.283203  | -0.503101 | -1.154146 |
| P  | -2.669699 | 1.392540  | -0.901642 |
| C  | -2.136067 | 3.189321  | -1.272207 |
| C  | -1.244164 | 3.751518  | -0.147668 |
| P  | 0.120394  | 2.503557  | 0.320860  |
| H  | -3.130634 | 0.867647  | -2.139087 |
| H  | -3.865476 | 1.489792  | -0.135461 |
| H  | 0.666990  | 3.002616  | 1.539648  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.181437  | 2.774341  | -0.595862 |
| H | -0.789354 | 4.697355  | -0.459694 |
| H | -1.826903 | 3.944722  | 0.759966  |
| H | -3.029898 | 3.808556  | -1.404156 |
| H | -1.600940 | 3.167973  | -2.228342 |
| H | 0.731415  | -1.784842 | 0.196754  |
| H | -0.479801 | -1.558442 | 2.367816  |
| H | 0.425863  | -0.060093 | 4.160652  |
| H | 2.572122  | 1.159270  | 3.771243  |
| H | 3.742989  | 0.994225  | 1.590096  |

=== TS-3-4\_II-IV.xyz ===

26

Structure TS-3-4(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.815160 | 0.401373  | -0.478910 |
| C  | -2.424876 | -0.548883 | -1.324927 |
| C  | -3.749756 | -0.315412 | -1.754065 |
| C  | -4.469463 | 0.801044  | -1.290742 |
| C  | -3.866182 | 1.702228  | -0.389603 |
| C  | -2.542222 | 1.496549  | 0.040882  |
| Pd | 0.273635  | 0.282653  | -0.399816 |
| I  | 0.628855  | -2.389497 | -0.614964 |
| I  | -0.327962 | -0.162865 | 2.196823  |
| P  | 2.787290  | 0.392302  | -0.678672 |
| C  | 3.322989  | 2.195631  | -0.343821 |
| C  | 2.303631  | 3.188623  | -0.935170 |
| P  | 0.516533  | 2.733557  | -0.437403 |
| H  | 3.618628  | -0.395365 | 0.168383  |
| H  | 3.330114  | 0.089678  | -1.964039 |
| H  | -0.312842 | 3.511603  | -1.298264 |
| H  | 0.308400  | 3.372848  | 0.821241  |
| H  | 2.517728  | 4.208606  | -0.598012 |
| H  | 2.337698  | 3.186008  | -2.030662 |
| H  | 4.315967  | 2.372472  | -0.770378 |
| H  | 3.402380  | 2.308654  | 0.743149  |
| H  | -1.907798 | -1.437867 | -1.662162 |
| H  | -4.213204 | -1.026886 | -2.432177 |
| H  | -5.498715 | 0.952244  | -1.603823 |
| H  | -4.425303 | 2.550567  | -0.003810 |
| H  | -2.118707 | 2.165753  | 0.782843  |

=== 3a\_II-IV.xyz ===

32

Structure 3a(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -4.172379 | -0.448748 | -0.906636 |
| C  | -3.390481 | 0.045614  | 0.151774  |
| C  | -3.651578 | -0.269409 | 1.495490  |
| C  | -4.737120 | -1.121454 | 1.782151  |
| C  | -5.535521 | -1.634362 | 0.741378  |
| C  | -5.255422 | -1.297147 | -0.596384 |
| Pd | 0.585038  | -0.244066 | -0.154929 |
| I  | -1.750343 | 1.373584  | -0.325454 |
| C  | 0.234474  | -1.133948 | -2.277044 |
| C  | -0.416539 | -1.967492 | -1.377910 |
| I  | 2.743517  | -1.799940 | 0.182901  |
| P  | 1.311745  | 0.900678  | 1.865333  |
| C  | 2.368266  | 2.458708  | 1.548437  |
| C  | 3.256475  | 2.341518  | 0.292575  |
| P  | 2.206163  | 2.183909  | -1.310820 |
| H  | -1.474781 | -1.851347 | -1.155944 |
| H  | 0.061309  | -2.869401 | -1.007823 |
| H  | -0.294280 | -0.342763 | -2.801774 |
| H  | 1.233848  | -1.373025 | -2.628746 |
| H  | 0.254596  | 1.375141  | 2.701249  |
| H  | 2.068713  | 0.128474  | 2.790643  |
| H  | 1.676489  | 3.305204  | 1.466112  |
| H  | 2.983790  | 2.620625  | 2.440684  |
| H  | 3.904570  | 1.460992  | 0.350457  |
| H  | 3.901856  | 3.223423  | 0.227566  |
| H  | 2.126580  | 3.581963  | -1.659113 |
| H  | 3.257328  | 1.849039  | -2.232703 |
| H  | -3.047617 | 0.131857  | 2.303002  |
| H  | -4.955462 | -1.374054 | 2.815861  |
| H  | -6.372526 | -2.287041 | 0.971918  |
| H  | -5.874186 | -1.683400 | -1.401312 |
| H  | -3.969891 | -0.180221 | -1.938781 |

=== TS-3a-5\_II-IV.xyz ===

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Structure TS-3a-5(II-IV)

|    |           |           |          |
|----|-----------|-----------|----------|
| Pd | 0.159451  | -0.213061 | 0.342304 |
| C  | -0.353148 | -0.512490 | 2.724149 |
| C  | 0.319721  | 0.689492  | 2.668634 |
| H  | -0.201755 | 1.639768  | 2.607220 |
| H  | 1.391228  | 0.739896  | 2.828236 |
| H  | -1.435858 | -0.565592 | 2.752557 |
| H  | 0.170030  | -1.441119 | 2.931631 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| I | 1.923264  | 1.955021  | 0.062557  |
| P | 0.870770  | -0.636581 | -1.918858 |
| H | -0.136077 | -1.269331 | -2.707602 |
| H | 1.213397  | 0.497645  | -2.705267 |
| C | 2.344063  | -1.840097 | -2.019137 |
| H | 1.915942  | -2.849069 | -2.035237 |
| H | 2.836055  | -1.669438 | -2.983976 |
| C | 3.346135  | -1.680891 | -0.862193 |
| H | 3.800678  | -0.685459 | -0.865413 |
| H | 4.147672  | -2.418505 | -0.972189 |
| P | 2.481373  | -1.903207 | 0.830670  |
| H | 2.483503  | -3.339515 | 0.929815  |
| H | 3.583457  | -1.642797 | 1.714784  |
| I | -1.987385 | -1.909031 | 0.015437  |
| C | -1.893540 | 0.700923  | -0.216339 |
| C | -2.041252 | 1.118166  | -1.550184 |
| C | -2.719313 | 2.329584  | -1.799024 |
| C | -3.273629 | 3.071322  | -0.739773 |
| C | -3.167896 | 2.591826  | 0.578216  |
| C | -2.492674 | 1.383330  | 0.854262  |
| H | -1.680235 | 0.535059  | -2.389204 |
| H | -2.822648 | 2.672542  | -2.825028 |
| H | -3.803667 | 3.997306  | -0.941741 |
| H | -3.620617 | 3.138287  | 1.401357  |
| H | -2.470382 | 1.013495  | 1.871544  |

=== 4a\_II-IV.xyz ===

26

Structure 4a(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 1.920867  | 1.966331  | -0.497515 |
| C  | 0.580569  | 1.584849  | -0.366868 |
| C  | -0.495437 | 2.468076  | -0.511902 |
| C  | -0.187180 | 3.817343  | -0.803988 |
| C  | 1.144961  | 4.244727  | -0.941446 |
| C  | 2.194709  | 3.323642  | -0.789150 |
| Pd | 0.200710  | -0.438075 | 0.081002  |
| I  | -1.535943 | 0.050788  | 2.048033  |
| P  | 1.905045  | -1.430501 | -1.414925 |
| C  | 3.304015  | -2.107528 | -0.295904 |
| C  | 3.580848  | -1.201827 | 0.923943  |
| P  | 1.961768  | -0.670409 | 1.796181  |
| I  | -1.631886 | -0.769598 | -1.824602 |
| H  | 2.303200  | 0.444372  | 2.613743  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 1.706036  | -1.690105 | 2.758894  |
| H | 4.215965  | -1.729527 | 1.643786  |
| H | 4.110714  | -0.289013 | 0.631605  |
| H | 2.983351  | -3.105615 | 0.024109  |
| H | 4.215691  | -2.230062 | -0.890870 |
| H | 1.523178  | -2.533607 | -2.230032 |
| H | 2.531342  | -0.560894 | -2.355370 |
| H | 2.753162  | 1.279261  | -0.393861 |
| H | 3.229457  | 3.639402  | -0.894999 |
| H | 1.362613  | 5.284754  | -1.166169 |
| H | -1.008491 | 4.519330  | -0.920334 |
| H | -1.526230 | 2.160075  | -0.410303 |

=== 4c\_II-IV.xyz ===

26

Structure 4c(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | 3.508347  | 2.266979  | -1.023346 |
| C  | 2.164210  | 1.830719  | -1.023857 |
| C  | 1.724427  | 1.020058  | 0.037374  |
| C  | 2.544324  | 0.670348  | 1.116125  |
| C  | 3.879799  | 1.134106  | 1.104552  |
| C  | 4.359518  | 1.924802  | 0.043520  |
| Pd | -0.167714 | 0.326174  | -0.425378 |
| I  | -0.733916 | -0.774523 | 1.990984  |
| I  | 0.669785  | -2.107762 | -1.038877 |
| P  | -1.107239 | 2.520809  | 0.144026  |
| C  | -3.005205 | 2.404629  | 0.011995  |
| C  | -3.442688 | 1.664019  | -1.270445 |
| P  | -2.528384 | -0.007768 | -1.460956 |
| H  | -2.769573 | -0.360367 | -2.824745 |
| H  | -3.385523 | -0.940014 | -0.799607 |
| H  | -4.524295 | 1.496208  | -1.251491 |
| H  | -3.218349 | 2.258432  | -2.163775 |
| H  | -3.348814 | 1.878477  | 0.909364  |
| H  | -3.428110 | 3.415013  | 0.034204  |
| H  | -0.842221 | 3.016581  | 1.451975  |
| H  | -0.744776 | 3.635118  | -0.674711 |
| H  | 1.517662  | 2.112846  | -1.854874 |
| H  | 3.869470  | 2.876515  | -1.847407 |
| H  | 5.387885  | 2.275008  | 0.049401  |
| H  | 4.537576  | 0.858619  | 1.924726  |
| H  | 2.200824  | 0.045102  | 1.931095  |

=== 4d\_II-IV.xyz ===

26

4d(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -2.285622 | 1.350638  | 1.126309  |
| C  | -1.237070 | 1.465568  | 0.195878  |
| C  | -1.083971 | 2.598421  | -0.627297 |
| C  | -2.065285 | 3.610707  | -0.556075 |
| C  | -3.129220 | 3.514338  | 0.360208  |
| C  | -3.236923 | 2.389231  | 1.200152  |
| Pd | 0.060708  | -0.077196 | -0.292908 |
| I  | -1.967586 | -1.836213 | -0.472689 |
| P  | 0.544937  | -0.404690 | 1.970636  |
| C  | 1.942201  | -1.692450 | 2.037576  |
| C  | 1.809588  | -2.789929 | 0.955256  |
| P  | 1.602811  | -2.078192 | -0.808033 |
| I  | 2.351759  | 1.445198  | -0.344883 |
| H  | 1.175443  | -3.216539 | -1.554246 |
| H  | 2.943958  | -1.912884 | -1.269872 |
| H  | 2.696980  | -3.429842 | 0.995202  |
| H  | 0.934804  | -3.421881 | 1.141886  |
| H  | 2.874009  | -1.129137 | 1.924232  |
| H  | 1.928243  | -2.144050 | 3.036877  |
| H  | 0.942412  | 0.741695  | 2.704749  |
| H  | -0.568039 | -0.922771 | 2.686417  |
| H  | -2.427357 | 0.468552  | 1.743009  |
| H  | -4.063653 | 2.301962  | 1.900005  |
| H  | -3.863843 | 4.312066  | 0.424119  |
| H  | -1.973844 | 4.476153  | -1.206745 |
| H  | -0.251286 | 2.715533  | -1.311604 |

=== 5a\_II-IV.xyz ===

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Step 6

|    |           |          |           |
|----|-----------|----------|-----------|
| Pd | 0.047561  | 0.416802 | 0.038666  |
| P  | -0.972810 | 1.992023 | -1.553655 |
| C  | -1.755104 | 3.412529 | -0.532646 |
| C  | -2.349396 | 2.942573 | 0.813747  |
| P  | -1.224196 | 1.681822 | 1.721510  |
| H  | -2.084073 | 0.981020 | 2.613837  |
| H  | -0.431784 | 2.460944 | 2.614102  |
| H  | -2.510710 | 3.805483 | 1.469077  |
| H  | -3.322144 | 2.461519 | 0.670762  |
| H  | -0.957075 | 4.144468 | -0.370378 |
| H  | -2.530260 | 3.900120 | -1.134159 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -0.162110 | 2.650090  | -2.521120 |
| H | -2.022095 | 1.455865  | -2.355056 |
| C | -1.459911 | -1.037393 | -0.243880 |
| C | -1.115720 | -2.388056 | -0.394905 |
| C | -2.158533 | -3.322515 | -0.581408 |
| C | -3.503241 | -2.913317 | -0.611398 |
| C | -3.818270 | -1.553923 | -0.454858 |
| C | -2.792398 | -0.598494 | -0.268968 |
| H | -3.080519 | 0.440831  | -0.159206 |
| H | -4.852521 | -1.219496 | -0.475414 |
| H | -4.293859 | -3.644137 | -0.754129 |
| H | -1.897933 | -4.370811 | -0.699799 |
| H | -0.091741 | -2.732465 | -0.370686 |
| C | 1.958204  | 2.770764  | -0.079410 |
| C | 2.508750  | 1.899650  | 0.806595  |
| H | 3.117322  | 1.063730  | 0.475272  |
| H | 2.425049  | 2.039138  | 1.881613  |
| H | 2.135150  | 2.664090  | -1.146757 |
| H | 1.434168  | 3.665611  | 0.255048  |
| I | 1.525016  | -0.613129 | -1.976971 |
| I | 1.056232  | -1.072107 | 2.071184  |

=== 5b\_II-IV.xyz ===

32

Structure 5b(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -1.181079 | -0.135706 | 0.032885  |
| Pd | 0.951356  | -0.550052 | 0.139505  |
| I  | 3.836730  | -0.617969 | 0.269534  |
| P  | 1.107977  | 1.318109  | 1.618231  |
| P  | 1.492135  | 1.088202  | -1.639104 |
| I  | 0.844514  | -2.031973 | 2.437399  |
| C  | -3.948173 | 0.425290  | -0.110517 |
| C  | -1.780778 | 0.147725  | -1.210933 |
| C  | -1.962801 | -0.153085 | 1.203124  |
| C  | -3.345309 | 0.130045  | 1.124115  |
| C  | -3.163022 | 0.429065  | -1.276744 |
| H  | -1.225004 | 0.136066  | -2.143228 |
| H  | -1.545460 | -0.411985 | 2.170076  |
| H  | -3.939306 | 0.105616  | 2.034277  |
| H  | -3.615278 | 0.637649  | -2.243301 |
| H  | -5.012127 | 0.637166  | -0.165186 |
| C  | 1.237742  | 2.889698  | 0.550885  |
| H  | 2.235760  | 1.280339  | 2.479408  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -0.004982 | 1.525539  | 2.478551  |
| C | 2.064375  | 2.659002  | -0.727955 |
| H | 0.434337  | 1.544389  | -2.486347 |
| H | 2.523181  | 0.787097  | -2.573379 |
| H | 1.691439  | 3.682031  | 1.157400  |
| H | 0.210716  | 3.188959  | 0.315470  |
| H | 1.960308  | 3.515802  | -1.402376 |
| H | 3.124860  | 2.521681  | -0.500754 |
| C | 0.110415  | -2.474124 | -1.107723 |
| H | -0.415216 | -2.057330 | -1.959932 |
| H | -0.499352 | -2.941167 | -0.340751 |
| C | 1.484940  | -2.623317 | -1.119685 |
| H | 2.085161  | -2.310892 | -1.969666 |
| H | 1.999426  | -3.189526 | -0.350250 |

=== 5c\_II-IV.xyz ===

32

Structure 5c(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -4.595152 | -1.311377 | -0.306340 |
| C  | -4.131671 | -0.159173 | 0.351406  |
| C  | -2.765124 | 0.199067  | 0.308888  |
| C  | -1.875424 | -0.607502 | -0.417074 |
| C  | -2.319956 | -1.768398 | -1.077947 |
| C  | -3.687661 | -2.114435 | -1.019550 |
| Pd | 0.193040  | -0.085085 | -0.530093 |
| P  | 2.754897  | 0.330893  | -0.440181 |
| C  | 3.637729  | -1.334698 | -0.773289 |
| C  | 2.803210  | -2.526735 | -0.261887 |
| P  | 0.987295  | -2.418806 | -0.828235 |
| I  | 0.229511  | -0.632150 | 2.130120  |
| I  | -0.045735 | 2.578416  | 0.056005  |
| H  | 3.466425  | 1.246956  | -1.276795 |
| H  | 3.217291  | 0.726112  | 0.849273  |
| H  | 4.620668  | -1.334524 | -0.290863 |
| H  | 3.803937  | -1.403992 | -1.854652 |
| H  | 2.781333  | -2.553900 | 0.832056  |
| H  | 3.226982  | -3.472654 | -0.616925 |
| H  | 0.305866  | -3.441964 | -0.109694 |
| H  | 1.000991  | -2.951948 | -2.158641 |
| H  | -2.437246 | 1.080201  | 0.845547  |
| H  | -4.818348 | 0.467103  | 0.914982  |
| H  | -5.645973 | -1.582649 | -0.260417 |
| H  | -4.030439 | -3.006648 | -1.537882 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -1.658816 | -2.404302 | -1.659866 |
| C | 0.622974  | 0.590602  | -2.971646 |
| C | -0.739507 | 0.453336  | -2.861766 |
| H | -1.369472 | 1.293030  | -2.586023 |
| H | -1.245637 | -0.454088 | -3.172742 |
| H | 1.235539  | -0.202245 | -3.396046 |
| H | 1.097514  | 1.551919  | -2.800146 |

=== 5d\_II-IV.xyz ===

32

Structure 5d(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| Pd | -0.016359 | -0.102154 | -0.300780 |
| P  | 0.023844  | -0.285685 | 2.073382  |
| C  | 0.027695  | -2.131393 | 2.536317  |
| C  | -0.854437 | -2.977803 | 1.595101  |
| P  | -0.471849 | -2.648438 | -0.246995 |
| H  | -1.583577 | -3.240127 | -0.919685 |
| H  | 0.573354  | -3.572457 | -0.554895 |
| H  | -0.702397 | -4.040658 | 1.810049  |
| H  | -1.915980 | -2.752358 | 1.738373  |
| H  | 1.073034  | -2.454494 | 2.500110  |
| H  | -0.323745 | -2.225518 | 3.570361  |
| H  | 1.146913  | 0.301231  | 2.714156  |
| H  | -1.094408 | 0.309617  | 2.719000  |
| C  | 0.323300  | 1.991359  | 0.163834  |
| C  | 1.608576  | 2.535599  | -0.010280 |
| C  | 1.816951  | 3.901766  | 0.281466  |
| C  | 0.761893  | 4.707195  | 0.746634  |
| C  | -0.512842 | 4.143128  | 0.921197  |
| C  | -0.743781 | 2.777699  | 0.633929  |
| H  | -1.743497 | 2.382053  | 0.763939  |
| H  | -1.341141 | 4.750377  | 1.277421  |
| H  | 0.931503  | 5.757024  | 0.968308  |
| H  | 2.809474  | 4.321664  | 0.139011  |
| H  | 2.445883  | 1.944100  | -0.359054 |
| C  | 0.093945  | 0.952424  | -2.502497 |
| C  | -0.079802 | -0.397618 | -2.737070 |
| H  | -1.072339 | -0.806923 | -2.903081 |
| H  | 0.774448  | -1.039754 | -2.933913 |
| H  | 1.084144  | 1.395621  | -2.507714 |
| H  | -0.752608 | 1.631610  | -2.469000 |
| I  | 2.652349  | -0.880595 | -0.249933 |
| I  | -2.793585 | -0.005522 | -0.295069 |

=== TS-5-6\_II-IV.xyz ===

32

Structure TS-5-6(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| H  | 1.199776  | -2.547465 | 2.395899  |
| H  | -0.206913 | -2.503463 | 3.471990  |
| H  | -1.765565 | -2.954034 | 1.595257  |
| H  | -0.477696 | -4.171532 | 1.557921  |
| H  | 1.105406  | 0.152082  | 2.864757  |
| H  | -1.114608 | 0.031349  | 2.873361  |
| H  | -1.423115 | -3.153338 | -1.108065 |
| H  | 0.756373  | -3.420604 | -0.774345 |
| P  | -0.338093 | -2.603152 | -0.365977 |
| C  | -0.692526 | -3.104182 | 1.439439  |
| C  | 0.138041  | -2.287217 | 2.455394  |
| P  | 0.020819  | -0.413399 | 2.133626  |
| Pd | -0.018024 | -0.127937 | -0.325548 |
| I  | -2.802358 | -0.166554 | -0.253970 |
| I  | 2.687835  | -0.775951 | -0.305770 |
| H  | 0.653663  | 5.566846  | 1.597443  |
| H  | -1.631639 | 4.686014  | 1.075168  |
| H  | 2.669329  | 4.218383  | 0.972762  |
| H  | 2.417764  | 2.030695  | -0.130588 |
| H  | -1.908167 | 2.501277  | -0.027898 |
| H  | 1.100466  | 1.936571  | -2.410235 |
| H  | -0.735481 | 2.128189  | -2.377315 |
| H  | 0.844619  | -0.483795 | -2.851450 |
| H  | -0.998769 | -0.289457 | -2.825963 |
| C  | -0.023188 | 0.083748  | -2.527054 |
| C  | 0.126483  | 1.476152  | -2.283305 |
| C  | -0.908695 | 2.850648  | 0.201560  |
| C  | 0.234086  | 2.083477  | -0.114972 |
| C  | 1.528630  | 2.585458  | 0.144052  |
| C  | 1.670909  | 3.838917  | 0.772155  |
| C  | 0.536946  | 4.597267  | 1.121323  |
| C  | -0.748603 | 4.102137  | 0.829402  |

=== 6\_II-IV.xyz ===

32

Structure 6(II-IV)

|    |          |           |           |
|----|----------|-----------|-----------|
| Pd | 0.183227 | -0.045168 | -0.163614 |
| P  | 1.374549 | 1.697843  | -1.287105 |
| C  | 2.241265 | 2.765258  | 0.025810  |
| C  | 1.359808 | 2.991824  | 1.272889  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| P | 0.693234  | 1.347233  | 1.985345  |
| H | -0.312618 | 1.802559  | 2.893558  |
| H | 1.720135  | 0.957705  | 2.903300  |
| H | 1.942610  | 3.516573  | 2.036570  |
| H | 0.488062  | 3.609181  | 1.032579  |
| H | 2.505617  | 3.724086  | -0.434681 |
| H | 3.167100  | 2.239986  | 0.282087  |
| H | 0.589177  | 2.576648  | -2.084786 |
| H | 2.388030  | 1.254273  | -2.181532 |
| I | -2.078676 | 1.498178  | -0.429645 |
| I | 2.652258  | -1.279975 | 0.087948  |
| C | -1.582682 | -2.277153 | -0.394665 |
| C | -0.933038 | -1.966978 | 0.848180  |
| C | -1.714912 | -1.658682 | 2.002582  |
| C | -3.740324 | -1.956002 | 0.693191  |
| C | -3.108700 | -1.640615 | 1.922788  |
| C | -2.986059 | -2.265866 | -0.454647 |
| H | -3.491246 | -2.492937 | -1.389254 |
| H | -4.825941 | -1.961623 | 0.637286  |
| H | -3.709923 | -1.412996 | 2.797692  |
| H | -1.216770 | -1.479088 | 2.951840  |
| H | 0.100010  | -2.279627 | 0.995925  |
| C | -0.153839 | -1.107028 | -2.023011 |
| H | -0.882571 | -0.466298 | -2.521752 |
| H | 0.812443  | -1.140907 | -2.527747 |
| C | -0.706521 | -2.476117 | -1.620786 |
| H | -1.282298 | -2.892397 | -2.459289 |
| H | 0.113153  | -3.170147 | -1.403239 |

=== TS-6-7\_II-IV.xyz ===

32

Structure TS-6-7(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -3.765434 | -1.238719 | -1.084763 |
| C  | -2.728623 | -1.658666 | -0.224068 |
| C  | -2.956065 | -1.666298 | 1.167850  |
| C  | -4.192378 | -1.243599 | 1.694620  |
| C  | -5.216753 | -0.812601 | 0.830827  |
| C  | -5.000944 | -0.813092 | -0.561175 |
| C  | -1.399385 | -2.131720 | -0.787144 |
| C  | -0.585635 | -1.133779 | -1.607319 |
| Pd | 0.433470  | -0.048401 | -0.054746 |
| I  | 2.376165  | -1.951771 | 0.165132  |
| P  | 1.834404  | 1.084178  | -1.562256 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| C | 3.132243  | 1.963692  | -0.483524 |
| C | 2.551863  | 2.542621  | 0.829709  |
| P | 1.597015  | 1.248668  | 1.867740  |
| I | -1.338054 | 1.991693  | -0.138729 |
| H | 0.910888  | 2.072573  | 2.810703  |
| H | 2.614921  | 0.672885  | 2.689636  |
| H | 3.376314  | 2.954564  | 1.420581  |
| H | 1.850353  | 3.357245  | 0.621976  |
| H | 3.575729  | 2.766484  | -1.084155 |
| H | 3.905119  | 1.214720  | -0.281432 |
| H | 1.197554  | 2.055712  | -2.381324 |
| H | 2.532060  | 0.258614  | -2.484172 |
| H | -3.621062 | -1.255379 | -2.164237 |
| H | -5.793097 | -0.494958 | -1.233826 |
| H | -6.172862 | -0.491090 | 1.234645  |
| H | -4.356268 | -1.257119 | 2.768955  |
| H | -2.178186 | -2.018373 | 1.844439  |
| H | -1.176156 | -0.421354 | -2.186009 |
| H | 0.230714  | -1.585198 | -2.175460 |
| H | -1.578920 | -2.959784 | -1.506343 |
| H | -0.781234 | -2.598663 | -0.007344 |

=== 7\_II-IV.xyz ===

32

Structure 7(II-VI)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -5.267639 | -1.027445 | -0.962153 |
| C  | -3.885806 | -1.244111 | -1.100543 |
| C  | -3.046440 | -1.240090 | 0.037999  |
| C  | -3.612539 | -1.010365 | 1.312455  |
| C  | -4.992661 | -0.791532 | 1.449020  |
| C  | -5.824506 | -0.797573 | 0.310904  |
| C  | -1.566435 | -1.552949 | -0.096004 |
| C  | -0.865928 | -1.053145 | -1.335815 |
| Pd | 0.486685  | -0.043643 | -0.027570 |
| I  | -0.968051 | 2.261567  | -0.096551 |
| I  | 2.111594  | -2.241727 | 0.120719  |
| P  | 2.007700  | 0.868132  | -1.616151 |
| C  | 3.467010  | 1.527791  | -0.587127 |
| C  | 3.023062  | 2.184391  | 0.742129  |
| P  | 1.887909  | 1.055583  | 1.786303  |
| H  | 1.341068  | 1.957346  | 2.746873  |
| H  | 2.796420  | 0.297047  | 2.585256  |
| H  | 3.913742  | 2.445458  | 1.322695  |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | 2.461793  | 3.106009  | 0.556463  |
| H | 4.015985  | 2.253833  | -1.197257 |
| H | 4.120132  | 0.667692  | -0.406271 |
| H | 1.525425  | 1.944961  | -2.410790 |
| H | 2.558541  | -0.034330 | -2.566768 |
| H | -3.474988 | -1.444258 | -2.087656 |
| H | -5.907281 | -1.045195 | -1.840283 |
| H | -6.892740 | -0.629531 | 0.416085  |
| H | -5.418467 | -0.616213 | 2.432978  |
| H | -2.978011 | -1.000130 | 2.197307  |
| H | -1.381496 | -0.298634 | -1.927269 |
| H | -0.282661 | -1.771629 | -1.909109 |
| H | -1.331260 | -2.615388 | 0.062388  |
| H | -1.064311 | -1.086493 | 0.835176  |

=== TS-7-8\_II-IV.xyz ===

32

Structure TS-7-8(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -5.656531 | -0.895806 | 0.541221  |
| C  | -5.080881 | -0.053266 | -0.433878 |
| C  | -3.740183 | -0.217694 | -0.806571 |
| C  | -2.957058 | -1.240608 | -0.210093 |
| C  | -3.547190 | -2.082631 | 0.772640  |
| C  | -4.886655 | -1.912880 | 1.144163  |
| C  | -1.560750 | -1.514673 | -0.592396 |
| Pd | 0.450424  | -0.026307 | -0.110506 |
| P  | 1.609962  | 0.795508  | 1.913472  |
| C  | 2.914895  | 2.024029  | 1.263024  |
| C  | 3.563823  | 1.548095  | -0.057368 |
| P  | 2.268770  | 1.086403  | -1.380177 |
| C  | -0.822805 | -0.897533 | -1.675894 |
| I  | -0.948866 | 2.335361  | -0.058645 |
| I  | 2.012575  | -2.293301 | -0.015498 |
| H  | 0.881701  | 1.531786  | 2.891144  |
| H  | 2.337816  | -0.138725 | 2.707378  |
| H  | 3.688889  | 2.162181  | 2.025344  |
| H  | 2.399044  | 2.980299  | 1.127150  |
| H  | 4.214890  | 2.334765  | -0.452757 |
| H  | 4.174494  | 0.653467  | 0.103540  |
| H  | 1.989539  | 2.305240  | -2.066410 |
| H  | 3.010950  | 0.355531  | -2.353548 |
| H  | -3.314712 | 0.437316  | -1.559680 |
| H  | -5.680093 | 0.723684  | -0.899293 |

|   |           |           |           |
|---|-----------|-----------|-----------|
| H | -6.696932 | -0.762927 | 0.825287  |
| H | -5.332200 | -2.564385 | 1.889828  |
| H | -2.954602 | -2.870766 | 1.234080  |
| H | -1.274674 | -0.089960 | -2.243586 |
| H | -0.112267 | -1.521563 | -2.211749 |
| H | -1.184392 | -2.494224 | -0.288984 |
| H | -0.784516 | -0.831682 | 0.616582  |

=== 8\_II-IV.xyz ===

32

Structure 8(II-IV)

|    |           |           |           |
|----|-----------|-----------|-----------|
| C  | -5.112552 | 1.756272  | -0.910712 |
| C  | -5.761754 | 0.593347  | -0.439583 |
| C  | -5.098204 | -0.295083 | 0.437615  |
| C  | -3.788157 | -0.029984 | 0.845670  |
| C  | -3.115270 | 1.140143  | 0.378564  |
| C  | -3.802849 | 2.028207  | -0.504985 |
| C  | -1.780195 | 1.495821  | 0.785184  |
| C  | -0.894580 | 0.776568  | 1.623047  |
| Pd | 0.513251  | 0.006374  | 0.022885  |
| I  | 1.756307  | 2.450031  | -0.131935 |
| P  | 2.017129  | -0.851631 | -1.674633 |
| C  | 3.299498  | -1.949488 | -0.794627 |
| C  | 3.749948  | -1.342884 | 0.551562  |
| P  | 2.261607  | -0.901550 | 1.667726  |
| I  | -0.830791 | -2.371652 | -0.147737 |
| H  | 1.451834  | -1.655766 | -2.702836 |
| H  | 2.759273  | 0.128097  | -2.393550 |
| H  | 4.160637  | -2.081826 | -1.459193 |
| H  | 2.825176  | -2.926357 | -0.652743 |
| H  | 4.402711  | -2.050442 | 1.072775  |
| H  | 4.315099  | -0.417352 | 0.397341  |
| H  | 2.013990  | -2.115896 | 2.381161  |
| H  | 2.866252  | -0.109688 | 2.692465  |
| H  | -3.289216 | -0.714846 | 1.523208  |
| H  | -5.610785 | -1.182666 | 0.795779  |
| H  | -6.781511 | 0.381682  | -0.750339 |
| H  | -5.630764 | 2.435002  | -1.580998 |
| H  | -3.297796 | 2.923707  | -0.861490 |
| H  | -1.239921 | -0.115218 | 2.137867  |
| H  | -0.136821 | 1.361903  | 2.139874  |
| H  | -1.415000 | 2.459958  | 0.428082  |
| H  | -0.411352 | 0.492590  | -1.124320 |