Electronic Supplementary Material (ESI) for Reaction Chemistry & Engineering.

The mechanism of MOF as the heterogeneous catalyst for propene hydroformylation: The DFT study

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Tianjin 300072, China

The mechanism study of H_2 activation and spillover on precious metal cluster supported on M-Cu-BTC

As we have mentioned before, MOF are a kind of porous materials with high specific surface area and adjustable pore size. Recently, H_2 storage and spillover mechanism has been studied extensively, [1-3] directly doping precious group metals is effective for enhancing the hydrogen storage capacity.

Palladium is highly recommended for hydrogen spillover because of its low dissociation barrier. In addition, the moderate interaction of palladium catalyst with free H atoms can promote H migrate to the substrate with low energy cost. [4-6] Pd_4 cluster is the smallest three dimension model catalyst which has been applied in relative theoretically study, [5] and this model is enough to reveal the mechanism, reducing the computational cost greatly at the same time. In this work, we build the Pd_4,

Rh_4, Ir_4, cluster deposited on the M-Cu-BTC models to investigate H_2 activation and spillover mechanism. In Figure S1 (a)-(c), the H-H bond breaks easily without activation barrier, and in Figure S1(d)-(f) represent the process of adsorbed H_2 migrate from hydrogen saturated Pd_4 cluster to the Rh metal node, it involves the break of H-H bond and the H-Rh bond formation. The DFT calculation shows that reaction energy is 0.13 eV, and activation barrier is 0.39 eV. The result indicates that the H_2 dissociation and the H* migrate process is energetically favorable. Therefore, the assumption we applied in this work is reasonable for the investigated catalyst system.

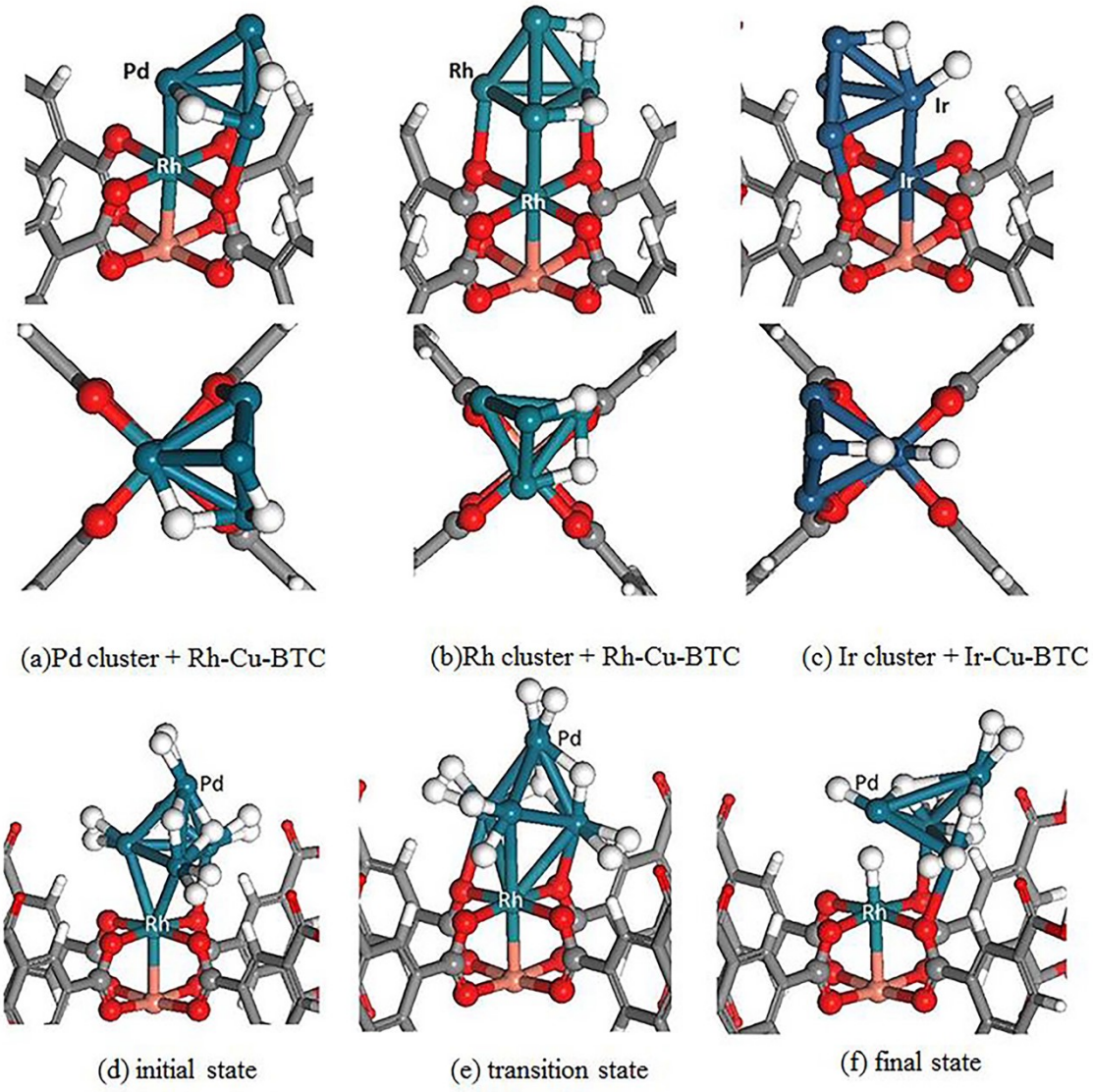

Figure S1 (a)-(c) are the geometrical structures of H_2 dissociation on precious metal cluster

supported on M-Cu-BTC, (d)-(e) are the motifs of H spillover from Hydrogen saturated Pd clusters

The Cartesian coordinates, total energies of the reactants, intermediates and transition states located along the reaction coordinate:

$HRh(CO)_2(PPh_3)_2$

E = -2444.0433350 Ha

ATOM	X	Y	Z
1	Rh	-0.731751	1.737285	-0.215817
2	P	1.243987	0.640785	0.380726
3	P	-2.594344	0.398919	0.188050
4	C	-3.463086	0.517876	1.804610
5	C	-3.962944	0.645885	-1.010838
6	C	2.363715	0.249018	-1.019052
7	C	2.309256	1.567981	1.550318
8	C	-2.323925	-1.421395	0.071237
9	C	1.133493	-1.017537	1.175699
10	C	3.758806	0.298986	-0.900389
11	C	4.568079	-0.130491	-1.954464
12	C	3.995739	-0.624782	-3.127052
13	C	2.605472	-0.672650	-3.252381
14	C	1.798133	-0.227750	-2.208100
15	C	1.946098	-2.100868	0.819200
16	C	1.759827	-3.347810	1.418868
17	C	0.766510	-3.528676	2.380681
18	C	-0.037567	-2.450512	2.751506
19	C	0.145071	-1.210622	2.148394
20	C	2.641626	2.893810	1.230740
21	C	3.387052	3.667823	2.116074
22	C	3.792370	3.135840	3.343127
23	C	3.461662	1.821594	3.668926
24	C	2.730707	1.035389	2.774596
25	C	-4.833627	0.247980	1.933696
26	C	-5.429895	0.208527	3.194764
27	C	-4.668231	0.439430	4.341761
28	C	-3.308785	0.731583	4.220573
29	C	-2.717471	0.782153	2.959890
30	C	-4.461346	1.945274	-1.185983
31	C	-5.483647	2.191059	-2.098597
32	C	-6.005364	1.146698	-2.868898
33	C	-5.504491	-0.144122	-2.709327
34	C	-4.494383	-0.398033	-1.778340
35	C	-3.040155	-2.337904	0.852838
36	C	-2.793165	-3.706546	0.744467
37	C	-1.828065	-4.180360	-0.143407
38	C	-1.111864	-3.275293	-0.928160
39	C	-1.357938	-1.908792	-0.818382
40	C	-0.779992	2.966769	1.274005
41	O	-0.782962	3.716023	2.159890
42	H	4.212421	0.660739	0.021619
43	H	5.650997	-0.083809	-1.853072
44	H	4.630127	-0.963883	-3.944147
45	H	2.147884	-1.045107	-4.167443
46	H	0.712232	-0.240200	-2.308399
47	H	2.714402	-1.984602	0.057245
48	H	2.385312	-4.185580	1.114688
49	H	0.604943	-4.509119	2.825299
50	H	-0.839811	-2.577928	3.476086
51	H	-0.518184	-0.390358	2.410525
52	H	2.298073	3.323433	0.289610
53	H	3.636644	4.694534	1.855263
54	H	4.356535	3.748212	4.044350
55	H	3.771678	1.399527	4.623595
56	H	2.481358	0.008831	3.037278
57	H	-5.431214	0.049861	1.045018
58	H	-6.493095	-0.008828	3.280298
59	H	-5.133208	0.401824	5.325151
60	H	-2.704596	0.929196	5.104007
61	H	-1.660098	1.024861	2.875599
62	H	-4.031117	2.769037	-0.616393
63	H	-5.863158	3.204003	-2.221457
64	H	-6.791697	1.343608	-3.595639
65	H	-5.896312	-0.963647	-3.310005
66	H	-4.115798	-1.411659	-1.657974
67	H	-3.787285	-1.987608	1.561433
68	H	-3.351742	-4.401104	1.369701
69	H	-1.622228	-5.246934	-0.212515

70 H -0.335028 -3.624447 -1.605590
71 H -0.766800 -1.203639 -1.401902
72 H -0.686972 0.706090 -1.453453
73 C -0.748001 3.019589 -1.640764
74 O -0.745364 3.764072 -2.534074

H_2

E = -1.1688573 Ha

ATOM X Y Z
1 H -2.380593 0.508957 0.000000
2 H -1.631483 0.533122 0.000000

CO

E = -113.3201192 Ha

ATOM X Y Z
1 C -2.488581 1.286484 0.000113
2 O -1.347954 1.302804 -0.000105

Propene

E = -117.9034770 Ha

ATOM X Y Z
1 C -1.771396 1.282791 0.103998
2 C -0.463513 1.192612 -0.135931
3 C 0.506106 2.312531 0.031404
4 H -2.439882 0.437176 -0.032213
5 H -2.214625 2.216474 0.448606
6 H -0.050267 0.242510 -0.479505
7 H 1.015207 2.541295 -0.914308
8 H 1.293217 2.052460 0.751811
9 H 0.005475 3.222069 0.381462

$HRh(CO)(PPh_3)_2$－catalyst

E = -2330.6638861 Ha

ATOM X Y Z
1 Rh -0.822925 0.713113 1.707241
2 P 1.321764 0.515035 1.001312
3 P -2.785154 0.072229 0.767919
4 C -4.434112 0.248041 1.558640
5 C -3.091953 0.642859 -0.953457
6 C 1.388413 0.365092 -0.836241
7 C 2.674833 1.689446 1.402133
8 C -2.665233 -1.754565 0.582903
9 C 2.041598 -1.068024 1.582490
10 C 2.404503 -0.341181 -1.496412
11 C 2.406494 -0.437599 -2.888251
12 C 1.390433 0.157026 -3.639018
13 C 0.373739 0.854996 -2.990241
14 C 0.382746 0.963112 -1.602864
15 C 1.538269 -2.275066 1.079567
16 C 1.870129 -3.484731 1.681122
17 C 2.708589 -3.506306 2.796884
18 C 3.227372 -2.310736 3.291665
19 C 2.899874 -1.097551 2.687940
20 C 3.955976 1.571049 0.847763
21 C 4.982127 2.410878 1.270982
22 C 4.739564 3.374857 2.252210
23 C 3.464911 3.504008 2.800474
24 C 2.434964 2.664703 2.373662
25 C -5.634304 0.010137 0.877114
26 C -6.848834 0.075788 1.555792
27 C -6.875944 0.378377 2.918675
28 C -5.685356 0.621265 3.601059
29 C -4.469245 0.561029 2.921591
30 C -2.769223 1.962576 -1.287449
31 C -2.981240 2.444277 -2.576150
32 C -3.505470 1.600650 -3.556546
33 C -3.821265 0.280815 -3.237222
34 C -3.621739 -0.197014 -1.941482
35 C -3.433627 -2.620278 1.368779
36 C -3.188571 -3.993760 1.352337
37 C -2.184573 -4.518662 0.542607
38 C -1.426818 -3.662680 -0.259337
39 C -1.659412 -2.290733 -0.236664
40 H -0.838853 1.934997 0.639062
41 C -0.778503 -0.588864 3.121489
42 O -0.756959 -1.321147 4.023334
43 H 3.192226 -0.824837 -0.921663
44 H 3.203602 -0.982936 -3.388382
45 H 1.388477 0.066487 -4.723167
46 H -0.445684 1.308967 -3.544986
47 H -0.418906 1.492413 -1.095423
48 H 0.845859 -2.267264 0.241476
49 H 1.443009 -4.406737 1.292904
50 H 2.946135 -4.448025 3.286200
51 H 3.879899 -2.315364 4.161595

52 H 3.297658 -0.169778 3.094286
53 H 4.153172 0.810804 0.093659
54 H 5.976042 2.310034 0.840618
55 H 5.544186 4.025516 2.586580
56 H 3.269123 4.253998 3.563551
57 H 1.436123 2.748603 2.801907
58 H -5.618701 -0.234097 -0.183480
59 H -7.776607 -0.110470 1.019391
60 H -7.825976 0.429104 3.445513
61 H -5.699244 0.860142 4.661701
62 H -3.534103 0.745987 3.449589
63 H -2.276579 2.579373 -0.535582
64 H -2.711297 3.468869 -2.820686
65 H -3.654131 1.968699 -4.569287
66 H -4.216366 -0.386093 -4.000257
67 H -3.863525 -1.230724 -1.703727
68 H -4.212844 -2.223906 2.016167
69 H -3.783158 -4.648756 1.985086
70 H -1.985728 -5.587698 0.543410
71 H -0.625124 -4.058451 -0.879502
72 H -1.028344 -1.629876 -0.831411

(1) propene － $HRh(CO)(PPh_3)_2$

E = -2448.6465945 Ha

ATOM X Y Z
1 Rh -0.970043 0.984587 2.257743
2 P 1.065760 0.314925 1.410114
3 P -2.587921 -0.004918 0.914830
4 C -4.284489 -0.201778 1.602020
5 C -2.926633 0.895971 -0.656602
6 C 1.051780 0.078335 -0.413844
7 C 2.492873 1.443600 1.634891
8 C -2.273256 -1.726361 0.361818
9 C 1.763335 -1.271640 2.015223
10 C 1.633215 -1.029668 -1.041226
11 C 1.492911 -1.211703 -2.418079
12 C 0.772274 -0.293740 -3.181237
13 C 0.216526 0.830489 -2.567187
14 C 0.365130 1.015820 -1.196340
15 C 0.936372 -2.404026 2.008226
16 C 1.406595 -3.626364 2.476594
17 C 2.704498 -3.734739 2.978789
18 C 3.529708 -2.611959 2.996230
19 C 3.066015 -1.387814 2.513475
20 C 3.475886 1.616213 0.654681
21 C 4.591113 2.413339 0.911952
22 C 4.738754 3.034655 2.151553
23 C 3.755964 2.875031 3.129125
24 C 2.633593 2.091920 2.867970
25 C -5.310214 -0.746109 0.816937
26 C -6.578742 -0.938555 1.354218
27 C -6.837002 -0.592723 2.682994
28 C -5.822568 -0.048531 3.467497
29 C -4.550083 0.147131 2.927899
30 C -2.699448 2.276947 -0.692500
31 C -2.891507 2.998567 -1.867627
32 C -3.311736 2.347139 -3.027757
33 C -3.566099 0.976710 -2.996154
34 C -3.384670 0.258428 -1.815578
35 C -2.653924 -2.794184 1.191067
36 C -2.255659 -4.096963 0.898087
37 C -1.471554 -4.360786 -0.226846
38 C -1.096550 -3.307206 -1.058546
39 C -1.491943 -2.003618 -0.768293
40 H -0.801621 1.982423 1.025926
41 C -1.024462 -0.196647 3.784949
42 O -1.028629 -0.930903 4.686131
43 H 2.161138 -1.774981 -0.451081
44 H 1.928279 -2.090659 -2.887896
45 H 0.631603 -0.458705 -4.247266
46 H -0.379447 1.539913 -3.137109
47 H -0.115569 1.862062 -0.710522
48 H -0.082477 -2.337941 1.633551
49 H 0.744222 -4.488750 2.451900
50 H 3.069093 -4.686884 3.357120
51 H 4.543071 -2.681029 3.386002
52 H 3.727187 -0.524477 2.526263
53 H 3.374448 1.119621 -0.308122
54 H 5.348448 2.540145 0.141362
55 H 5.613655 3.649187 2.350550
56 H 3.857334 3.370369 4.091805
57 H 1.841876 1.993393 3.610423
58 H -5.109150 -1.026141 -0.215643
59 H -7.367347 -1.363032 0.736798

60	H	-7.828406	-0.746035	3.103008
61	H	-6.017641	0.222521	4.502318
62	H	-3.753658	0.581540	3.529159
63	H	-2.307819	2.765209	0.200969
64	H	-2.691240	4.067345	-1.880433
65	H	-3.439469	2.905505	-3.952339
66	H	-3.893863	0.459764	-3.895241
67	H	-3.572590	-0.812503	-1.804313
68	H	-3.255007	-2.606279	2.078821
69	H	-2.556391	-4.907535	1.557787
70	H	-1.156939	-5.377081	-0.451461
71	H	-0.473533	-3.481175	-1.932949
72	H	-1.176372	-1.199953	-1.427374
73	C	-2.137270	2.640261	3.088858
74	C	-0.766516	2.941206	3.283051
75	C	-0.111237	4.016778	2.457793
76	H	-2.759978	2.300281	3.912114
77	H	-2.674376	3.154864	2.291941
78	H	-0.340322	2.787534	4.275093
79	H	0.951408	3.818849	2.288112
80	H	-0.198131	4.996476	2.950244
81	H	-0.601870	4.070706	1.478060

TS-1a

E = -2448.6263469 Ha

Imaginary Frequency = -828.32 cm^{-1}

ATOM	X	Y	Z
1	Rh	-0.964585	0.239864	2.500135
2	P	1.025012	-0.023755	1.303718
3	P	-2.658242	-0.490688	1.124581
4	C	-4.293337	-0.779102	1.918367
5	C	-3.182948	0.605276	-0.260167
6	C	0.847210	0.183928	-0.514994
7	C	2.366085	1.154495	1.706378
8	C	-2.315000	-2.087995	0.299016
9	C	1.883227	-1.642165	1.385034
10	C	1.397715	-0.699230	-1.451806
11	C	1.079403	-0.577404	-2.804768
12	C	0.215621	0.427867	-3.239334
13	C	-0.313299	1.331525	-2.315878
14	C	0.000475	1.205142	-0.966506
15	C	1.094232	-2.798150	1.407376
16	C	1.681809	-4.057805	1.325028
17	C	3.069296	-4.179384	1.251091
18	C	3.864612	-3.033096	1.253915
19	C	3.276894	-1.769352	1.313633
20	C	2.882381	2.085364	0.796318
21	C	3.847799	3.007910	1.202445
22	C	4.315641	3.009300	2.515800
23	C	3.807825	2.084144	3.429512
24	C	2.834012	1.173060	3.031141
25	C	-5.329171	-1.448449	1.255224
26	C	-6.573165	-1.592357	1.863580
27	C	-6.795122	-1.055662	3.134228
28	C	-5.769605	-0.382732	3.795026
29	C	-4.520530	-0.246541	3.189647
30	C	-3.053168	1.989751	-0.114052
31	C	-3.467317	2.857155	-1.121295
32	C	-4.004736	2.347163	-2.303335
33	C	-4.144858	0.967816	-2.457292
34	C	-3.747462	0.103959	-1.438770
35	C	-2.571296	-3.289402	0.976399
36	C	-2.090289	-4.497940	0.474876
37	C	-1.343206	-4.524031	-0.703122
38	C	-1.093069	-3.334404	-1.385974
39	C	-1.576350	-2.126204	-0.892273
40	H	-1.081480	1.715131	1.748167
41	C	-1.171659	-1.204591	3.712832
42	O	-1.288302	-2.117666	4.431671
43	H	2.042142	-1.511226	-1.123480
44	H	1.487846	-1.291017	-3.517413
45	H	-0.057405	0.497666	-4.289685
46	H	-1.021358	2.095461	-2.629756
47	H	-0.469666	1.860952	-0.234077
48	H	0.011274	-2.715912	1.467206
49	H	1.042587	-4.937695	1.317229
50	H	3.530819	-5.162776	1.194366
51	H	4.947707	-3.119930	1.199822
52	H	3.903452	-0.879898	1.290154
53	H	2.535432	2.084775	-0.235268
54	H	4.238024	3.724726	0.482843
55	H	5.068064	3.729458	2.828802
56	H	4.162630	2.078079	4.457847
57	H	2.422346	0.468231	3.752031

58 H -5.158360 -1.863023 0.262753
59 H -7.372533 -2.118227 1.346465
60 H -7.767521 -1.166527 3.608480
61 H -5.937841 0.036010 4.784725
62 H -3.701176 0.269933 3.691696
63 H -2.592110 2.384658 0.790509
64 H -3.351458 3.930804 -0.989734
65 H -4.312883 3.021392 -3.098857
66 H -4.563258 0.558928 -3.373852
67 H -3.858751 -0.970011 -1.570875
68 H -3.128827 -3.278978 1.911137
69 H -2.286242 -5.418479 1.019989
70 H -0.949809 -5.465105 -1.079574
71 H -0.496306 -3.329489 -2.295264
72 H -1.357297 -1.208150 -1.432255
73 C -0.321699 1.662929 4.020813
74 C -1.124027 2.451083 3.141918
75 C -2.535594 2.842934 3.493159
76 H 0.754323 1.823446 4.032730
77 H -0.766501 1.357677 4.965554
78 H -0.579191 3.215444 2.582294
79 H -2.981444 2.099061 4.160447
80 H -3.168859 2.904057 2.601385
81 H -2.550277 3.824319 3.986642

TS-1b

E = -2448.6217063 Ha

Imaginary Frequency = -832.38 cm^{-1}

ATOM X Y Z
1 Rh -0.945911 1.128082 2.110278
2 P 1.074162 0.270965 1.312213
3 P -2.657099 0.092017 0.959020
4 C -4.364342 0.161103 1.648474
5 C -2.975476 0.667508 -0.762755
6 C 1.039930 -0.119470 -0.494907
7 C 2.504560 1.407631 1.432510
8 C -2.415585 -1.713251 0.754635
9 C 1.703104 -1.312367 1.990037
10 C 1.574304 -1.297754 -1.032586
11 C 1.351884 -1.627081 -2.370092
12 C 0.598962 -0.788199 -3.191394
13 C 0.096109 0.407163 -2.676956
14 C 0.316695 0.730418 -1.341843
15 C 0.766903 -2.251593 2.437047
16 C 1.175082 -3.515494 2.855810
17 C 2.527451 -3.852549 2.854063
18 C 3.470181 -2.921584 2.413686
19 C 3.061208 -1.663126 1.978166
20 C 2.680342 2.409971 0.466655
21 C 3.630677 3.412508 0.649216
22 C 4.426685 3.429293 1.794911
23 C 4.262821 2.433116 2.758100
24 C 3.306406 1.436996 2.583894
25 C -5.421798 -0.509677 1.019971
26 C -6.713583 -0.413400 1.526737
27 C -6.963081 0.352641 2.668517
28 C -5.915092 1.017833 3.301065
29 C -4.619411 0.924344 2.789671
30 C -2.699865 2.001083 -1.083305
31 C -2.922161 2.486488 -2.369767
32 C -3.415841 1.635768 -3.359483
33 C -3.702057 0.307028 -3.048377
34 C -3.492504 -0.171537 -1.756416
35 C -2.884878 -2.602957 1.732267
36 C -2.499099 -3.943254 1.711105
37 C -1.639105 -4.413902 0.718745
38 C -1.181101 -3.537770 -0.265054
39 C -1.567772 -2.201458 -0.251046
40 H -0.762776 2.120497 0.811301
41 C -1.285913 0.232976 3.745784
42 O -1.483084 -0.351741 4.737379
43 H 2.126517 -1.987448 -0.399357
44 H 1.746472 -2.562387 -2.760888
45 H 0.394915 -1.067798 -4.222158
46 H -0.523874 1.059742 -3.287552
47 H -0.143070 1.623986 -0.923409
48 H -0.292577 -2.006616 2.433630
49 H 0.423701 -4.233147 3.176762
50 H 2.847824 -4.837111 3.187690
51 H 4.527335 -3.177376 2.403176
52 H 3.800554 -0.950147 1.620285
53 H 2.067143 2.409688 -0.433204
54 H 3.748366 4.182408 -0.110460
55 H 5.167661 4.212706 1.935038

56	H	4.876473	2.435306	3.656276
57	H	3.176465	0.679691	3.354313
58	H	-5.231083	-1.106490	0.129329
59	H	-7.530117	-0.933435	1.030725
60	H	-7.974015	0.424170	3.063756
61	H	-6.101613	1.609705	4.194430
62	H	-3.787041	1.439149	3.271153
63	H	-2.267819	2.647804	-0.320692
64	H	-2.691415	3.523305	-2.603229
65	H	-3.573004	2.006536	-4.369759
66	H	-4.082927	-0.365688	-3.813436
67	H	-3.711906	-1.211083	-1.523971
68	H	-3.545244	-2.246589	2.520720
69	H	-2.864910	-4.618763	2.481164
70	H	-1.320060	-5.453422	0.718549
71	H	-0.495205	-3.877726	-1.037691
72	H	-1.190768	-1.532110	-1.019989
73	C	-0.947888	3.407651	1.756551
74	C	-0.565106	3.118369	3.085091
75	C	0.811404	3.456630	3.580732
76	H	-1.971288	3.661691	1.503182
77	H	-0.190510	3.851382	1.108300
78	H	-1.359141	3.129799	3.830422
79	H	1.191705	2.718132	4.292043
80	H	0.796805	4.431532	4.090049
81	H	1.523583	3.521890	2.752858

2a

E = -2448.6338606 Ha

ATOM	X	Y	Z
1	Rh	-1.274819	0.109276	2.524263
2	P	0.830679	-0.002928	1.516929
3	P	-2.658790	-0.688576	0.847346
4	C	-4.398053	-0.983584	1.365106
5	C	-2.981973	0.405771	-0.597273
6	C	0.941773	0.048312	-0.320326
7	C	2.093247	1.235681	2.003621
8	C	-2.167714	-2.286272	0.110089
9	C	1.686444	-1.590624	1.864641
10	C	1.594556	-0.925222	-1.086614
11	C	1.512277	-0.896115	-2.478975
12	C	0.785186	0.103778	-3.124203
13	C	0.150707	1.092507	-2.369765
14	C	0.233620	1.061172	-0.981087
15	C	0.911579	-2.753859	1.923432
16	C	1.514482	-4.001574	2.056573
17	C	2.901791	-4.099478	2.160187
18	C	3.681044	-2.942806	2.122011
19	C	3.080162	-1.694366	1.963205
20	C	2.604459	2.199570	1.124868
21	C	3.501005	3.166228	1.580412
22	C	3.902818	3.184478	2.915566
23	C	3.398827	2.229518	3.799301
24	C	2.498264	1.267935	3.348630
25	C	-5.255692	-1.783349	0.600002
26	C	-6.589881	-1.931573	0.967656
27	C	-7.081130	-1.270615	2.094924
28	C	-6.234539	-0.463733	2.853847
29	C	-4.894466	-0.322167	2.492475
30	C	-2.844254	1.789006	-0.444174
31	C	-3.123810	2.654649	-1.498713
32	C	-3.546505	2.144624	-2.725874
33	C	-3.699493	0.766778	-2.884802
34	C	-3.430057	-0.095310	-1.824722
35	C	-2.434330	-3.472110	0.813382
36	C	-1.876573	-4.677715	0.394350
37	C	-1.040010	-4.715720	-0.722436
38	C	-0.772831	-3.542010	-1.423897
39	C	-1.334221	-2.334876	-1.013590
40	H	2.127318	-1.737371	-0.598146
41	H	2.000922	-1.676875	-3.057886
42	H	0.699399	0.105423	-4.208326
43	H	-0.450023	1.861082	-2.850612
44	H	-0.301240	1.807376	-0.397129
45	H	-0.170875	-2.685262	1.852859
46	H	0.888711	-4.890956	2.077849
47	H	3.376790	-5.071185	2.275144
48	H	4.763563	-3.010582	2.206271
49	H	3.697657	-0.800216	1.908218
50	H	2.313534	2.190152	0.076792
51	H	3.891529	3.902707	0.881196
52	H	4.606279	3.936513	3.265381
53	H	3.704468	2.232132	4.842973
54	H	2.105754	0.528150	4.043498

55 H -4.873398 -2.294217 -0.282282
56 H -7.246164 -2.562138 0.372155
57 H -8.123688 -1.387854 2.381483
58 H -6.614852 0.050839 3.733419
59 H -4.219827 0.296014 3.087753
60 H -2.483474 2.189436 0.502562
61 H -3.001461 3.727054 -1.362893
62 H -3.755245 2.815767 -3.555472
63 H -4.032878 0.360484 -3.836697
64 H -3.552964 -1.168183 -1.957669
65 H -3.065140 -3.449179 1.699987
66 H -2.083758 -5.586818 0.954314
67 H -0.592130 -5.655408 -1.036488
68 H -0.106124 -3.546557 -2.282913
69 H -1.105208 -1.427179 -1.566847
70 C -0.705658 1.477596 4.027748
71 C -1.363888 2.492426 3.139470
72 C -2.736161 2.979494 3.580038
73 H 0.362396 1.631020 4.182437
74 H -1.232833 1.302298 4.966579
75 H -1.511956 2.038371 2.084469
76 H -3.360153 2.117726 3.842792
77 H -3.238646 3.522687 2.772434
78 H -2.659854 3.638447 4.451319
79 H -0.680826 3.318312 2.900197
80 C -1.829788 -1.181772 3.750549
81 O -2.038085 -2.093924 4.455468

2b

E = -2448.6308109 Ha

ATOM X Y Z
1 Rh -1.184601 0.993297 2.384277
2 P 0.817422 0.515515 1.295472
3 P -2.513879 -0.392488 1.047240
4 C -4.295422 -0.484570 1.509584
5 C -2.720032 0.392733 -0.601852
6 C 0.805665 0.545886 -0.548323
7 C 2.376561 1.432918 1.635870
8 C -2.100525 -2.148880 0.750543
9 C 1.383602 -1.182437 1.721777
10 C 1.214816 -0.503780 -1.377827
11 C 1.102921 -0.397297 -2.764680
12 C 0.598793 0.766568 -3.341544
13 C 0.201006 1.824460 -2.525695
14 C 0.290485 1.707557 -1.142046
15 C 0.610317 -1.990532 2.558042
16 C 1.022291 -3.284178 2.871377
17 C 2.218615 -3.780083 2.359420
18 C 3.011481 -2.971789 1.543283
19 C 2.600475 -1.678406 1.231853
20 C 2.905903 2.381165 0.754201
21 C 4.021163 3.135799 1.116424
22 C 4.621291 2.949546 2.360099
23 C 4.107883 1.993675 3.237788
24 C 2.993953 1.241538 2.879956
25 C -5.157414 -1.397951 0.886307
26 C -6.515388 -1.403582 1.191587
27 C -7.033323 -0.483731 2.105319
28 C -6.185114 0.440235 2.711452
29 C -4.821711 0.438311 2.416179
30 C -2.876386 1.786013 -0.599722
31 C -3.124984 2.473492 -1.782745
32 C -3.203756 1.778931 -2.989957
33 C -3.036611 0.395899 -3.001685
34 C -2.806691 -0.297569 -1.813631
35 C -2.544130 -3.114479 1.667942
36 C -2.075297 -4.423487 1.598746
37 C -1.145896 -4.789321 0.624333
38 C -0.693453 -3.836009 -0.285821
39 C -1.167235 -2.528402 -0.225141
40 C -1.921400 0.543571 4.036787
41 O -2.191723 0.112209 5.090626
42 H 1.591064 -1.424910 -0.940437
43 H 1.402272 -1.233878 -3.392023
44 H 0.499534 0.844630 -4.421641
45 H -0.229428 2.722002 -2.961244
46 H -0.073342 2.516390 -0.508245
47 H -0.324935 -1.599071 2.952218
48 H 0.392954 -3.905587 3.503315
49 H 2.537005 -4.791652 2.601236
50 H 3.955485 -3.345102 1.153082
51 H 3.225596 -1.048126 0.603012
52 H 2.448216 2.537474 -0.219651

53 H 4.418164 3.870968 0.419760
54 H 5.487457 3.543041 2.643122
55 H 4.570644 1.840135 4.209762
56 H 2.587957 0.513226 3.579958
57 H -4.763783 -2.113862 0.167031
58 H -7.171780 -2.124815 0.709810
59 H -8.094522 -0.489551 2.342396
60 H -6.577886 1.162404 3.423605
61 H -4.155603 1.154960 2.894690
62 H -2.778106 2.339451 0.334065
63 H -3.239167 3.554843 -1.760554
64 H -3.382996 2.315703 -3.918642
65 H -3.084496 -0.151637 -3.940142
66 H -2.682385 -1.376979 -1.836738
67 H -3.258981 -2.840218 2.441272
68 H -2.428249 -5.156911 2.320249
69 H -0.764272 -5.806933 0.588422
70 H 0.047148 -4.101108 -1.037003
71 H -0.786089 -1.793064 -0.927947
72 C -1.285477 3.723699 2.000877
73 C -0.714638 2.930309 3.169068
74 C 0.668244 3.412377 3.543403
75 H -2.350337 3.521108 1.833272
76 H -0.745970 3.521750 1.062238
77 H -1.363306 3.082336 4.036699
78 H 1.141686 2.779723 4.300507
79 H 0.594178 4.430570 3.958688
80 H 1.344883 3.462868 2.684660
81 H -1.186988 4.806008 2.194096

3a

E = -2562.0098319 Ha

ATOM X Y Z
1 Rh -0.672594 1.220828 1.946700
2 P 1.272294 0.238715 1.042822
3 P -2.405278 0.084907 0.763778
4 C -4.028410 0.045187 1.623816
5 C -2.859261 0.787769 -0.872349
6 C 1.255040 -0.136296 -0.755477
7 C 2.723842 1.341645 1.233007
8 C -2.142344 -1.700245 0.401704
9 C 1.882700 -1.334333 1.761870
10 C 1.842913 -1.291812 -1.284929
11 C 1.682554 -1.606334 -2.634269
12 C 0.928712 -0.777839 -3.465047
13 C 0.361739 0.389429 -2.950049
14 C 0.525272 0.707587 -1.604510
15 C 0.957920 -2.364242 1.973116
16 C 1.379208 -3.605695 2.438089
17 C 2.726494 -3.828526 2.720842
18 C 3.649845 -2.800131 2.537757
19 C 3.232708 -1.558281 2.057544
20 C 3.794491 1.319936 0.329990
21 C 4.912260 2.123721 0.550071
22 C 4.969489 2.952121 1.671156
23 C 3.901375 2.985572 2.566417
24 C 2.780556 2.187063 2.347983
25 C -5.241902 0.293026 0.972677
26 C -6.442027 0.251729 1.681769
27 C -6.447727 -0.044453 3.043855
28 C -5.243015 -0.287974 3.702196
29 C -4.042731 -0.231121 2.998934
30 C -2.799879 2.180408 -1.010750
31 C -3.105568 2.787052 -2.226035
32 C -3.466809 2.008133 -3.326228
33 C -3.546191 0.622431 -3.193496
34 C -3.256627 0.016144 -1.971416
35 C -2.560437 -2.686892 1.308648
36 C -2.192495 -4.019804 1.127382
37 C -1.406435 -4.394797 0.037862
38 C -0.999726 -3.424543 -0.876290
39 C -1.364940 -2.093446 -0.698780
40 H 2.397606 -1.966645 -0.636540
41 H 2.125646 -2.518536 -3.027352
42 H 0.778062 -1.044124 -4.508494
43 H -0.252957 1.031743 -3.576202
44 H 0.027984 1.588567 -1.206771
45 H -0.096036 -2.205432 1.765299
46 H 0.641421 -4.393461 2.572312
47 H 3.056140 -4.797488 3.088903
48 H 4.700765 -2.960462 2.767160
49 H 3.963644 -0.765903 1.913770
50 H 3.752814 0.673486 -0.544566

51 H 5.736357 2.106891 -0.159256
52 H 5.843163 3.577833 1.838515
53 H 3.930241 3.642129 3.432651
54 H 1.930156 2.238767 3.028089
55 H -5.253687 0.525444 -0.089718
56 H -7.376689 0.450691 1.162112
57 H -7.386248 -0.074240 3.592720
58 H -5.230725 -0.499940 4.768275
59 H -3.100932 -0.377295 3.523706
60 H -2.499106 2.790310 -0.160876
61 H -3.048595 3.869298 -2.314133
62 H -3.688567 2.480836 -4.280290
63 H -3.835305 0.005485 -4.041260
64 H -3.322725 -1.064710 -1.881157
65 H -3.166048 -2.416903 2.170597
66 H -2.521190 -4.764856 1.848304
67 H -1.108617 -5.432062 -0.094270
68 H -0.376557 -3.685468 -1.728378
69 H -1.033140 -1.359499 -1.426510
70 C -2.148464 2.501864 2.948166
71 C -1.670565 3.189537 4.217283
72 C -0.393071 4.010130 4.103383
73 H -3.000891 1.862630 3.184357
74 H -2.491517 3.246663 2.219235
75 H -1.544498 2.445390 5.014751
76 H 0.459545 3.364336 3.861658
77 H -0.183499 4.531220 5.043639
78 H -0.471517 4.759807 3.307301
79 H -2.480303 3.859621 4.549360
80 C -0.218234 2.867641 1.105735
81 O 0.011010 3.883500 0.578798
82 C -0.461475 0.331802 3.634921
83 O -0.372870 -0.204611 4.666085

3b

E = -2562.0162392 Ha

ATOM X Y Z
1 Rh -0.752632 1.135055 2.215309
2 P 1.202833 0.239786 1.202982
3 P -2.426581 0.043056 0.894499
4 C -4.091096 -0.084587 1.665949
5 C -2.819516 0.809449 -0.732525
6 C 1.160357 -0.014052 -0.613648
7 C 2.656587 1.333911 1.425824
8 C -2.125000 -1.723114 0.463626
9 C 1.853430 -1.366836 1.804155
10 C 1.730821 -1.136005 -1.227176
11 C 1.556860 -1.352773 -2.593468
12 C 0.810163 -0.456654 -3.358168
13 C 0.264079 0.679552 -2.758381
14 C 0.444999 0.902638 -1.396153
15 C 0.948353 -2.407106 2.042252
16 C 1.403196 -3.664297 2.427984
17 C 2.767645 -3.892294 2.602508
18 C 3.674964 -2.855676 2.385335
19 C 3.223419 -1.598889 1.984023
20 C 3.615021 1.516395 0.422633
21 C 4.745966 2.296016 0.667623
22 C 4.930516 2.892410 1.913856
23 C 3.973665 2.719153 2.914184
24 C 2.838654 1.950202 2.670527
25 C -5.273816 0.151926 0.956117
26 C -6.511765 0.010244 1.581048
27 C -6.583398 -0.372806 2.920138
28 C -5.409915 -0.602345 3.637125
29 C -4.171741 -0.446974 3.018091
30 C -2.700558 2.200937 -0.842156
31 C -2.944980 2.839610 -2.055319
32 C -3.301281 2.094531 -3.180158
33 C -3.441958 0.711155 -3.075333
34 C -3.216082 0.074516 -1.856209
35 C -2.528698 -2.747831 1.333884
36 C -2.157929 -4.070524 1.095674
37 C -1.376580 -4.398408 -0.012208
38 C -0.979212 -3.389353 -0.886788
39 C -1.352133 -2.068132 -0.654106
40 H 2.273430 -1.865642 -0.630896
41 H 1.985366 -2.240624 -3.052714
42 H 0.643072 -0.649027 -4.415508
43 H -0.347312 1.370969 -3.333420
44 H -0.028205 1.764021 -0.931561
45 H -0.118775 -2.245449 1.918304
46 H 0.679906 -4.460800 2.586418

47 H 3.122901 -4.872462 2.912554
48 H 4.741003 -3.021021 2.526045
49 H 3.940361 -0.799678 1.810213
50 H 3.480918 1.045818 -0.549052
51 H 5.482175 2.434173 -0.120972
52 H 5.814091 3.497925 2.101824
53 H 4.104070 3.192764 3.884087
54 H 2.078051 1.838518 3.441765
55 H -5.231794 0.453372 -0.088041
56 H -7.421759 0.199747 1.016170
57 H -7.549911 -0.486069 3.405305
58 H -5.453424 -0.892203 4.684252
59 H -3.256073 -0.600293 3.585513
60 H -2.410565 2.781532 0.032026
61 H -2.843013 3.920238 -2.122519
62 H -3.469339 2.591184 -4.132923
63 H -3.722779 0.120351 -3.944266
64 H -3.324359 -1.004570 -1.788036
65 H -3.131802 -2.517724 2.208933
66 H -2.481699 -4.844814 1.787415
67 H -1.079155 -5.428923 -0.189787
68 H -0.362134 -3.611134 -1.754416
69 H -1.035842 -1.306112 -1.359151
70 C -0.233228 2.875572 1.640074
71 O 0.079552 3.955032 1.324833
72 C -0.514583 0.161495 3.850038
73 O -0.411277 -0.394766 4.869355
74 C -3.216594 3.098488 2.460797
75 C -2.312179 2.240992 3.328246
76 C -1.715924 3.074094 4.451816
77 H -3.786698 2.508208 1.737899
78 H -2.662839 3.864405 1.904154
79 H -2.925731 1.448629 3.767240
80 H -1.133788 2.471050 5.154574
81 H -2.531595 3.562772 5.008973
82 H -1.061495 3.866911 4.070381
83 H -3.940642 3.621078 3.105801

TS-3a

E = -2561.9937529 Ha

Imaginary Frequency = -329.47 cm^{-1}

ATOM X Y Z
1 Rh -0.717480 0.559155 2.021124
2 P 1.408368 0.247515 1.225403
3 P -2.568447 -0.033868 0.775110
4 C -4.260430 0.026241 1.484941
5 C -2.869770 0.509764 -0.957304
6 C 1.369325 -0.171947 -0.568140
7 C 2.724397 1.497087 1.391835
8 C -2.215078 -1.820494 0.598346
9 C 2.146605 -1.265889 1.943563
10 C 1.900026 -1.364389 -1.077029
11 C 1.651440 -1.738195 -2.399937
12 C 0.875008 -0.928388 -3.226216
13 C 0.370324 0.277810 -2.734679
14 C 0.617816 0.654381 -1.418780
15 C 1.315200 -2.389568 2.069572
16 C 1.817518 -3.588189 2.565360
17 C 3.151853 -3.673040 2.967107
18 C 3.976695 -2.553085 2.868897
19 C 3.481139 -1.354587 2.353156
20 C 3.731653 1.657493 0.435207
21 C 4.719303 2.624135 0.617244
22 C 4.706696 3.432632 1.753382
23 C 3.699274 3.279516 2.706715
24 C 2.707370 2.320813 2.523208
25 C -5.354827 -0.583856 0.859751
26 C -6.620097 -0.506110 1.435397
27 C -6.802848 0.189716 2.633099
28 C -5.718877 0.806824 3.255008
29 C -4.448176 0.718523 2.685647
30 C -2.582307 1.833596 -1.309614
31 C -2.758175 2.274567 -2.619293
32 C -3.214502 1.392894 -3.598683
33 C -3.512232 0.074030 -3.256472
34 C -3.348970 -0.362474 -1.943664
35 C -2.654543 -2.726305 1.575901
36 C -2.233799 -4.054600 1.541809
37 C -1.369361 -4.494503 0.538060
38 C -0.931743 -3.599424 -0.438643
39 C -1.349069 -2.271687 -0.410711
40 H 2.474515 -2.025711 -0.432784
41 H 2.048158 -2.680033 -2.772419

42 H 0.652361 -1.237095 -4.245009
43 H -0.263688 0.906878 -3.355534
44 H 0.186799 1.573558 -1.032720
45 H 0.272668 -2.338565 1.759391
46 H 1.157089 -4.449615 2.636447
47 H 3.546045 -4.606510 3.361994
48 H 5.015050 -2.608915 3.188489
49 H 4.136651 -0.490570 2.264462
50 H 3.737471 1.030285 -0.454677
51 H 5.497863 2.746287 -0.132637
52 H 5.474771 4.190917 1.888292
53 H 3.671764 3.922127 3.583605
54 H 1.891714 2.233066 3.241238
55 H -5.213816 -1.118353 -0.078376
56 H -7.465802 -0.988665 0.950634
57 H -7.793269 0.251365 3.078328
58 H -5.857891 1.353221 4.184979
59 H -3.590033 1.193482 3.164439
60 H -2.191787 2.525022 -0.567974
61 H -2.515666 3.303009 -2.874815
62 H -3.331861 1.730067 -4.625932
63 H -3.865404 -0.623101 -4.012934
64 H -3.574558 -1.395563 -1.689272
65 H -3.323332 -2.389129 2.365610
66 H -2.577804 -4.746582 2.306948
67 H -1.029098 -5.527421 0.524827
68 H -0.236355 -3.915246 -1.212552
69 H -0.981697 -1.582199 -1.167122
70 C -1.955958 3.207115 1.997633
71 C -1.935041 3.372043 3.517237
72 C -0.600275 3.868152 4.054430
73 H -2.880465 2.696220 1.710390
74 H -1.944205 4.195968 1.521760
75 H -2.193261 2.413022 3.980294
76 H 0.196938 3.148048 3.835516
77 H -0.645925 4.002983 5.138541
78 H -0.324130 4.821087 3.590169
79 H -2.729297 4.080322 3.780951
80 C -0.729939 2.453075 1.422542
81 O 0.104016 3.081255 0.793471
82 C -0.669138 0.240675 3.962508
83 O -0.563578 0.447193 5.105837

TS-3b

E = -2561.9968928 Ha

Imaginary Frequency = -276.28 cm^{-1}

ATOM X Y Z
1 Rh -1.066623 1.013657 2.050317
2 P 1.092041 0.496293 1.515316
3 P -2.431934 -0.350721 0.684895
4 C -4.191367 -0.428844 1.228262
5 C -2.633191 0.032665 -1.101387
6 C 1.307249 -0.100803 -0.208431
7 C 2.301660 1.868917 1.609350
8 C -1.914453 -2.106987 0.715847
9 C 1.908292 -0.828119 2.481483
10 C 2.064899 -1.232758 -0.531644
11 C 2.105772 -1.699433 -1.845589
12 C 1.394536 -1.041979 -2.848763
13 C 0.657396 0.101772 -2.536489
14 C 0.620313 0.572057 -1.227627
15 C 1.239613 -2.053060 2.616654
16 C 1.842293 -3.115679 3.281281
17 C 3.108727 -2.961668 3.846589
18 C 3.768380 -1.738317 3.738697
19 C 3.174774 -0.675578 3.056169
20 C 3.436023 1.896714 0.789137
21 C 4.383638 2.907199 0.937906
22 C 4.207661 3.892913 1.908740
23 C 3.074036 3.874967 2.720691
24 C 2.119850 2.871204 2.567768
25 C -5.237618 -0.731736 0.346954
26 C -6.556182 -0.742843 0.796010
27 C -6.848447 -0.453633 2.129419
28 C -5.814049 -0.153181 3.013732
29 C -4.495566 -0.135660 2.563264
30 C -2.661964 1.383883 -1.470276
31 C -2.794893 1.753474 -2.805998
32 C -2.898813 0.775956 -3.796191
33 C -2.888418 -0.571420 -3.437748
34 C -2.767619 -0.940787 -2.098952
35 C -2.310144 -2.924059 1.786142
36 C -1.753934 -4.190732 1.950345

37	C	-0.801724	-4.668009 1.047640
38	C	-0.411941	-3.866391 -0.023993
39	C	-0.960024	-2.596525 -0.188603
40	H	2.594259	-1.773630 0.248965
41	H	2.681098	-2.593478 -2.076487
42	H	1.402880	-1.424796 -3.866806
43	H	0.071227	0.609829 -3.298633
44	H	0.014982	1.444516 -0.992896
45	H	0.250496	-2.187049 2.186981
46	H	1.307726	-4.060078 3.355944
47	H	3.579357	-3.790942 4.370087
48	H	4.751229	-1.605638 4.184895
49	H	3.707514	0.268148 2.964184
50	H	3.577440	1.125735 0.034054
51	H	5.257630	2.925136 0.290793
52	H	4.946415	4.683469 2.020187
53	H	2.925222	4.651546 3.467404
54	H	1.218339	2.862608 3.180657
55	H	-5.024252	-0.947213 -0.697735
56	H	-7.358523	-0.975779 0.099551
57	H	-7.879483	-0.455917 2.475634
58	H	-6.031231	0.082665 4.052745
59	H	-3.689823	0.131289 3.245013
60	H	-2.569052	2.153971 -0.708281
61	H	-2.805608	2.807716 -3.071364
62	H	-2.981623	1.063299 -4.841819
63	H	-2.968665	-1.342173 -4.201037
64	H	-2.752022	-1.994124 -1.832799
65	H	-3.039972	-2.561799 2.507932
66	H	-2.062204	-4.804239 2.793526
67	H	-0.359025	-5.651265 1.186633
68	H	0.342350	-4.207328 -0.729357
69	H	-0.622133	-1.979316 -1.016518
70	C	-1.063055	2.731680 1.278139
71	O	-0.821049	3.711133 0.653026
72	C	-1.056613	0.063425 3.738725
73	O	-1.053489	-0.451269 4.784118
74	C	-3.688339	3.198843 1.482725
75	C	-2.614726	2.821720 2.481906
76	C	-2.197022	3.952620 3.397105
77	H	-4.007671	2.336801 0.889843
78	H	-3.346693	3.984772 0.799338
79	H	-3.003491	1.997025 3.087071
80	H	-1.474378	3.610490 4.142390
81	H	-3.082097	4.341103 3.921685
82	H	-1.752460	4.781736 2.834446
83	H	-4.566793	3.574611 2.024912

4a

E = -2562.0066748 Ha

ATOM	X	Y	Z
1	Rh	-0.712004	0.993630 1.963281
2	P	1.269571	0.074207 1.037437
3	P	-2.413705	0.123307 0.644905
4	C	-4.047587	0.091891 1.497538
5	C	-2.826057	0.739352 -1.041502
6	C	1.268003	-0.233687 -0.770563
7	C	2.631957	1.286618 1.224653
8	C	-2.152006	-1.669665 0.325017
9	C	1.962419	-1.480414 1.709627
10	C	1.771091	-1.401858 -1.353068
11	C	1.572978	-1.647099 -2.712608
12	C	0.871236	-0.733739 -3.497795
13	C	0.391487	0.448711 -2.928103
14	C	0.596583	0.698208 -1.575514
15	C	1.098299	-2.579576 1.812507
16	C	1.566506	-3.801432 2.285162
17	C	2.896769	-3.935475 2.685024
18	C	3.754433	-2.839201 2.607617
19	C	3.293268	-1.616619 2.119041
20	C	3.764782	1.241081 0.401162
21	C	4.803351	2.151360 0.584939
22	C	4.714396	3.121755 1.584232
23	C	3.583918	3.180003 2.398415
24	C	2.546392	2.267264 2.221369
25	C	-5.255504	-0.097942 0.815758
26	C	-6.456524	-0.170458 1.519579
27	C	-6.466693	-0.060093 2.910631
28	C	-5.267676	0.127844 3.596161
29	C	-4.067886	0.206436 2.892784
30	C	-2.471846	2.056276 -1.363236
31	C	-2.698343	2.554589 -2.646276
32	C	-3.271983	1.741359 -3.623704

33 C -3.632984 0.430874 -3.309329
34 C -3.419516 -0.064132 -2.024885
35 C -2.583505 -2.633036 1.248118
36 C -2.272350 -3.980148 1.059556
37 C -1.523479 -4.383588 -0.046310
38 C -1.097347 -3.431528 -0.971874
39 C -1.411866 -2.087996 -0.790991
40 H 2.272700 -2.144964 -0.737257
41 H 1.942570 -2.572451 -3.148421
42 H 0.683336 -0.947336 -4.547324
43 H -0.193011 1.151883 -3.517111
44 H 0.167034 1.593255 -1.127964
45 H 0.056110 -2.487073 1.517838
46 H 0.878703 -4.641937 2.343717
47 H 3.261661 -4.887855 3.062574
48 H 4.790154 -2.929389 2.927482
49 H 3.975183 -0.771691 2.056300
50 H 3.830864 0.489551 -0.383839
51 H 5.680365 2.103531 -0.056554
52 H 5.525691 3.832393 1.723351
53 H 3.502918 3.940973 3.171391
54 H 1.655153 2.321585 2.848201
55 H -5.262234 -0.188981 -0.268623
56 H -7.388610 -0.315767 0.978339
57 H -7.405903 -0.118469 3.455932
58 H -5.260975 0.221249 4.680049
59 H -3.129503 0.375874 3.419005
60 H -1.987421 2.681532 -0.614524
61 H -2.411647 3.576105 -2.884282
62 H -3.433386 2.124821 -4.628695
63 H -4.078777 -0.211345 -4.065756
64 H -3.691984 -1.090393 -1.790655
65 H -3.163165 -2.334284 2.119151
66 H -2.610702 -4.714350 1.786931
67 H -1.271092 -5.432413 -0.183491
68 H -0.499012 -3.715589 -1.834380
69 H -1.073314 -1.365116 -1.527571
70 C -2.415767 3.165414 3.605663
71 C -1.496441 3.290560 4.827288
72 C -0.231965 4.091243 4.549555
73 H -3.216726 2.451044 3.825850
74 H -2.860025 4.143570 3.380723
75 H -1.225225 2.294130 5.187331
76 H 0.420337 3.546362 3.856139
77 H 0.325860 4.264752 5.474424
78 H -0.467576 5.059616 4.094521
79 H -2.080003 3.770574 5.620937
80 C -1.676880 2.691770 2.380876
81 O -1.378003 3.458629 1.465565
82 C -0.350985 0.421144 3.706579
83 O -0.224954 -0.170336 4.710477

4b

E = -2562.0103363 Ha

ATOM X Y Z
1 Rh -0.863760 0.346266 2.255133
2 P 1.237200 0.080231 1.432440
3 P -2.632169 -0.238918 0.895527
4 C -4.315127 -0.203214 1.630357
5 C -2.959509 0.634319 -0.688652
6 C 1.172095 -0.047615 -0.405111
7 C 2.538708 1.343341 1.689523
8 C -2.396698 -1.982190 0.393666
9 C 2.069546 -1.490787 1.871963
10 C 1.787494 -1.091112 -1.108134
11 C 1.599094 -1.219065 -2.485499
12 C 0.801605 -0.305838 -3.173424
13 C 0.211395 0.754247 -2.482462
14 C 0.400041 0.889657 -1.109309
15 C 1.345539 -2.682529 1.709044
16 C 1.942751 -3.912202 1.963978
17 C 3.264653 -3.969583 2.410429
18 C 3.981933 -2.789191 2.595475
19 C 3.391843 -1.553578 2.322394
20 C 3.562360 1.543547 0.755667
21 C 4.536487 2.513548 0.980588
22 C 4.495354 3.292899 2.136964
23 C 3.475418 3.100864 3.068699
24 C 2.499841 2.132814 2.842191
25 C -5.451463 -0.571932 0.899105
26 C -6.716251 -0.457691 1.469225
27 C -6.857723 0.033753 2.769267
28 C -5.731323 0.402011 3.502316

29 C -4.463680 0.280774 2.932979
30 C -3.041576 2.032668 -0.643972
31 C -3.288255 2.766228 -1.800548
32 C -3.454030 2.115499 -3.023739
33 C -3.385061 0.724270 -3.075846
34 C -3.142121 -0.012313 -1.917267
35 C -3.025248 -3.030612 1.076501
36 C -2.695564 -4.355050 0.787537
37 C -1.738442 -4.647982 -0.184731
38 C -1.113831 -3.607816 -0.873508
39 C -1.438450 -2.285539 -0.586675
40 H 2.385067 -1.830214 -0.580777
41 H 2.068164 -2.047020 -3.012873
42 H 0.635421 -0.422503 -4.242285
43 H -0.433637 1.462231 -2.998000
44 H -0.079866 1.712375 -0.583730
45 H 0.317289 -2.653157 1.351849
46 H 1.367433 -4.822815 1.811864
47 H 3.732843 -4.929519 2.615790
48 H 5.009877 -2.823376 2.950014
49 H 3.968436 -0.640248 2.453783
50 H 3.591490 0.945003 -0.153041
51 H 5.325208 2.665496 0.247111
52 H 5.250408 4.057609 2.305162
53 H 3.424255 3.718090 3.962873
54 H 1.678803 2.006414 3.547447
55 H -5.344264 -0.934627 -0.122062
56 H -7.595743 -0.739552 0.894614
57 H -7.848202 0.130547 3.207897
58 H -5.835361 0.791299 4.512484
59 H -3.573747 0.586921 3.485918
60 H -2.903215 2.558441 0.296918
61 H -3.337392 3.850816 -1.742562
62 H -3.632946 2.689599 -3.930032
63 H -3.513442 0.203461 -4.022006
64 H -3.074397 -1.095035 -1.979832
65 H -3.767126 -2.812856 1.842740
66 H -3.188945 -5.160328 1.326790
67 H -1.480257 -5.681566 -0.402642
68 H -0.353380 -3.812163 -1.623942
69 H -0.932102 -1.487322 -1.122138
70 C -0.858199 2.291920 1.876170
71 O -0.490036 3.139981 1.081655
72 C -0.890782 -1.169196 3.477250
73 O -0.920044 -1.935695 4.350696
74 C -2.894104 3.379890 2.834531
75 C -1.581635 2.693858 3.203948
76 C -0.682675 3.595798 4.042655
77 H -3.528581 2.726162 2.228120
78 H -2.682604 4.289165 2.261796
79 H -1.836977 1.792857 3.799010
80 H 0.237060 3.079228 4.331714
81 H -1.210582 3.909470 4.949941
82 H -0.411594 4.484615 3.463104
83 H -3.448128 3.645656 3.741064

5a

E = -2563.1931863 Ha

ATOM X Y Z
1 Rh -0.478282 0.964203 2.091178
2 P 1.410414 0.065754 0.917909
3 P -2.237420 0.141629 0.824880
4 C -3.886377 0.249345 1.633304
5 C -2.599198 0.823633 -0.841251
6 C 1.251808 -0.358713 -0.859982
7 C 2.816420 1.241738 0.882168
8 C -2.052077 -1.667898 0.545365
9 C 2.128739 -1.464276 1.622048
10 C 1.622510 -1.598372 -1.392240
11 C 1.345158 -1.897133 -2.726718
12 C 0.691915 -0.969125 -3.535822
13 C 0.351854 0.282980 -3.018600
14 C 0.638840 0.589148 -1.692272
15 C 1.236467 -2.496760 1.940346
16 C 1.705192 -3.703226 2.449845
17 C 3.070407 -3.885878 2.672680
18 C 3.962144 -2.856717 2.370929
19 C 3.497019 -1.651135 1.843721
20 C 3.811017 1.162316 -0.102554
21 C 4.897854 2.033287 -0.072735
22 C 4.999144 2.992730 0.935795
23 C 4.007314 3.081962 1.912557
24 C 2.917747 2.212838 1.884733

25 C -5.010555 0.794501 1.001516
26 C -6.217695 0.915406 1.691140
27 C -6.323123 0.480145 3.010586
28 C -5.210964 -0.073722 3.644184
29 C -4.001063 -0.169854 2.966845
30 C -2.156329 2.126969 -1.096612
31 C -2.372533 2.715986 -2.340029
32 C -3.032450 2.007398 -3.343276
33 C -3.487358 0.711715 -3.092732
34 C -3.277830 0.123596 -1.847102
35 C -2.341444 -2.573401 1.578863
36 C -2.054192 -3.928653 1.439881
37 C -1.461274 -4.406436 0.270110
38 C -1.171690 -3.516009 -0.760972
39 C -1.468593 -2.160050 -0.629804
40 H 2.086762 -2.348451 -0.755441
41 H 1.618659 -2.872764 -3.121664
42 H 0.445853 -1.219726 -4.564497
43 H -0.176261 1.012434 -3.627273
44 H 0.351721 1.559201 -1.288668
45 H 0.169208 -2.361037 1.784596
46 H 0.992580 -4.491618 2.681948
47 H 3.438695 -4.821536 3.088152
48 H 5.027248 -2.987771 2.549431
49 H 4.201514 -0.857093 1.605002
50 H 3.735071 0.415126 -0.890139
51 H 5.666375 1.966003 -0.839727
52 H 5.845067 3.676877 0.954650
53 H 4.074672 3.835506 2.693916
54 H 2.133103 2.281052 2.637746
55 H -4.947859 1.142067 -0.027216
56 H -7.073556 1.365843 1.192731
57 H -7.258120 0.597822 3.552108
58 H -5.265301 -0.372577 4.687924
59 H -3.114964 -0.518987 3.493505
60 H -1.610280 2.672039 -0.327432
61 H -2.007089 3.723277 -2.525575
62 H -3.194842 2.463461 -4.316791
63 H -4.005746 0.155856 -3.870207
64 H -3.626758 -0.890153 -1.661077
65 H -2.778324 -2.220026 2.508133
66 H -2.282106 -4.606626 2.259127
67 H -1.220442 -5.461987 0.169293
68 H -0.685918 -3.858344 -1.672107
69 H -1.222964 -1.487870 -1.448042
70 C 0.165060 0.520110 3.799131
71 O 0.457202 0.070874 4.838542
72 C -2.485802 2.367766 4.095543
73 C -3.851324 3.049269 4.056860
74 C -4.593685 2.808847 5.362745
75 H -1.850116 2.838125 4.861538
76 H -2.607329 1.322732 4.399263
77 H -4.430936 2.631143 3.225863
78 H -4.647852 1.733416 5.570272
79 H -5.616613 3.194720 5.316877
80 H -4.079300 3.290365 6.201357
81 H -3.736054 4.121938 3.869918
82 C -1.697925 2.405546 2.805742
83 O -1.661793 3.396601 2.083846
84 H 0.273682 3.150603 0.092172
85 H 0.684358 3.355407 -0.503446

5b

E = -2563.1920706 Ha

ATOM X Y Z
1 Rh -0.730883 0.724534 2.321516
2 P 1.246528 -0.025627 1.184676
3 P -2.458279 -0.059895 0.934225
4 C -4.157438 -0.094250 1.653062
5 C -2.742237 0.781443 -0.673425
6 C 1.210955 -0.218893 -0.634253
7 C 2.517309 1.267888 1.458188
8 C -2.230630 -1.826705 0.485106
9 C 2.058703 -1.561022 1.746466
10 C 1.723155 -1.336972 -1.302458
11 C 1.527141 -1.480693 -2.676774
12 C 0.819434 -0.515042 -3.392280
13 C 0.323952 0.612648 -2.734128
14 C 0.523530 0.759627 -1.365440
15 C 1.296565 -2.737607 1.782322
16 C 1.877395 -3.933530 2.193809
17 C 3.215191 -3.963306 2.591703
18 C 3.972838 -2.793523 2.569674

19	C	3.400413	-1.595225	2.143205
20	C	3.388329	1.700250	0.452676
21	C	4.303024	2.723049	0.708091
22	C	4.366120	3.311407	1.971000
23	C	3.508800	2.875013	2.981881
24	C	2.586513	1.864640	2.727625
25	C	-5.301179	-0.068503	0.846957
26	C	-6.571038	-0.141679	1.415835
27	C	-6.715571	-0.238851	2.799653
28	C	-5.581946	-0.264434	3.610294
29	C	-4.311449	-0.189645	3.041480
30	C	-2.417199	2.140168	-0.744987
31	C	-2.617254	2.854708	-1.923354
32	C	-3.138535	2.215507	-3.048821
33	C	-3.468233	0.861173	-2.986464
34	C	-3.278940	0.149718	-1.802594
35	C	-2.657059	-2.817915	1.382726
36	C	-2.352504	-4.158098	1.156134
37	C	-1.614140	-4.532319	0.032758
38	C	-1.189927	-3.554087	-0.866282
39	C	-1.494504	-2.211823	-0.644503
40	H	2.247466	-2.112137	-0.748426
41	H	1.922782	-2.358122	-3.183799
42	H	0.648823	-0.643756	-4.458832
43	H	-0.257974	1.359837	-3.268736
44	H	0.091611	1.616068	-0.851774
45	H	0.249022	-2.724086	1.485287
46	H	1.274724	-4.838545	2.211850
47	H	3.663791	-4.894877	2.928722
48	H	5.013672	-2.807699	2.885226
49	H	3.998988	-0.686803	2.119091
50	H	3.342386	1.248607	-0.536390
51	H	4.966218	3.062848	-0.083920
52	H	5.072192	4.115402	2.164871
53	H	3.541593	3.333129	3.967776
54	H	1.875334	1.562724	3.496322
55	H	-5.206614	0.018630	-0.233010
56	H	-7.448134	-0.111250	0.773167
57	H	-7.708124	-0.283065	3.242042
58	H	-5.681431	-0.326322	4.691548
59	H	-3.433346	-0.196428	3.685430
60	H	-1.978031	2.619191	0.131655
61	H	-2.355541	3.909493	-1.963574
62	H	-3.287394	2.770681	-3.972233
63	H	-3.879562	0.357525	-3.858329
64	H	-3.538892	-0.905616	-1.760323
65	H	-3.227778	-2.543707	2.267958
66	H	-2.690923	-4.908546	1.867087
67	H	-1.373354	-5.578756	-0.139430
68	H	-0.602667	-3.822124	-1.741600
69	H	-1.147354	-1.467346	-1.356934
70	C	-2.017342	1.909263	3.449136
71	O	-2.718368	2.756047	2.927482
72	C	-0.462759	-0.544192	3.711373
73	O	-0.343048	-1.430230	4.462114
74	C	-3.045902	2.533264	5.688004
75	C	-1.911992	1.809167	4.977208
76	C	-0.545712	2.338015	5.430756
77	H	-4.019698	2.158803	5.356764
78	H	-3.008238	3.607371	5.482704
79	H	-1.957169	0.740634	5.223663
80	H	0.271917	1.818858	4.920728
81	H	-0.440547	2.200235	6.511764
82	H	-0.464008	3.408753	5.209341
83	H	-2.952143	2.381241	6.768715
84	H	0.039182	2.282309	2.296603
85	H	-0.443317	2.273988	1.527821

TS-5a

E = -2563.1713976 Ha

Imaginary Frequency = -825.78 cm^{-1}

ATOM	X	Y	Z
1	Rh	-0.194237	0.786661	2.393226
2	P	1.406851	0.086691	0.760366
3	P	-2.157806	-0.065949	1.426256
4	C	-3.691648	0.033206	2.461906
5	C	-2.762408	0.634237	-0.162953
6	C	0.865027	-0.253187	-0.953014
7	C	2.690589	1.361552	0.482374
8	C	-2.049262	-1.867703	1.090290
9	C	2.316468	-1.448364	1.178252
10	C	1.052845	-1.484400	-1.592458
11	C	0.532592	-1.692493	-2.870020

12 C -0.174229 -0.679820 -3.516584
13 C -0.342245 0.557012 -2.891651
14 C 0.180820 0.769874 -1.621100
15 C 1.546009 -2.554490 1.563765
16 C 2.147990 -3.785511 1.803282
17 C 3.533726 -3.918033 1.699360
18 C 4.308490 -2.813035 1.351133
19 C 3.705308 -1.583225 1.084465
20 C 3.629110 1.221915 -0.551298
21 C 4.603072 2.196474 -0.747758
22 C 4.638488 3.324278 0.075058
23 C 3.694779 3.475497 1.088728
24 C 2.720142 2.498956 1.294835
25 C -4.954564 0.221242 1.885851
26 C -6.100213 0.261224 2.678491
27 C -6.009238 0.108835 4.060969
28 C -4.758342 -0.074638 4.646450
29 C -3.613812 -0.101722 3.853237
30 C -2.471735 1.968219 -0.464803
31 C -2.965563 2.557387 -1.626879
32 C -3.742732 1.812256 -2.512923
33 C -4.034217 0.479112 -2.224616
34 C -3.557031 -0.101847 -1.052362
35 C -2.170741 -2.774778 2.154026
36 C -1.874186 -4.122624 1.970495
37 C -1.440435 -4.588939 0.727079
38 C -1.330221 -3.696099 -0.336516
39 C -1.635337 -2.348603 -0.159713
40 H 1.565970 -2.295510 -1.081919
41 H 0.667016 -2.658638 -3.351032
42 H -0.599876 -0.853111 -4.502097
43 H -0.911085 1.347897 -3.373365
44 H 0.024106 1.722773 -1.120013
45 H 0.467469 -2.457132 1.666975
46 H 1.523421 -4.633127 2.076178
47 H 4.010021 -4.875588 1.896998
48 H 5.390270 -2.904036 1.284208
49 H 4.320746 -0.732868 0.801643
50 H 3.592291 0.350865 -1.203222
51 H 5.328155 2.081617 -1.550347
52 H 5.397169 4.087942 -0.082805
53 H 3.706178 4.355928 1.726682
54 H 1.971551 2.631955 2.076605
55 H -5.054016 0.351130 0.811680
56 H -7.066617 0.421600 2.207010
57 H -6.902890 0.149736 4.678848
58 H -4.663460 -0.176048 5.724992
59 H -2.637989 -0.202245 4.325941
60 H -1.824418 2.526474 0.211903
61 H -2.725693 3.594887 -1.847094
62 H -4.118117 2.266217 -3.427026
63 H -4.638883 -0.112686 -2.907707
64 H -3.798266 -1.137505 -0.829415
65 H -2.480271 -2.424580 3.137045
66 H -1.967474 -4.808875 2.808961
67 H -1.189392 -5.638119 0.592283
68 H -0.982896 -4.030962 -1.311446
69 H -1.530041 -1.670113 -1.000658
70 C 1.115457 0.296729 3.668757
71 O 1.919318 0.004520 4.458226
72 C -1.923970 2.958934 3.840815
73 C -2.854211 3.401278 2.715199
74 C -4.279350 3.574395 3.214618
75 H -1.889808 3.739184 4.613179
76 H -2.328786 2.034746 4.270815
77 H -2.842476 2.648548 1.922966
78 H -4.647866 2.627641 3.623785
79 H -4.944864 3.873987 2.399460
80 H -4.330096 4.333713 4.002962
81 H -2.480866 4.332838 2.273084
82 C -0.511425 2.685816 3.356688
83 O 0.384106 3.477245 3.565756
84 H -0.320591 2.072433 1.335512
85 H -1.111862 0.335205 3.608456

Ts-5b

E = -2563.1663786 Ha

Imaginary Frequency = -455.47 cm^{-1}

ATOM X Y Z
1 Rh -0.663533 1.002164 1.944432
2 P 1.264471 -0.191347 1.216217
3 P -2.433252 0.191648 0.790422
4 C -4.102135 0.366280 1.540561

5	C	-2.599536	1.008008	-0.847918
6	C	1.221163	-0.510017	-0.586027
7	C	2.848697	0.705990	1.439597
8	C	-2.414192	-1.587244	0.353507
9	C	1.639285	-1.833448	1.935395
10	C	1.553952	-1.742513	-1.159019
11	C	1.374744	-1.949377	-2.527052
12	C	0.857023	-0.934243	-3.330919
13	C	0.546001	0.305214	-2.767646
14	C	0.738648	0.518913	-1.406667
15	C	0.655130	-2.827174	1.828796
16	C	0.852016	-4.083253	2.390217
17	C	2.026579	-4.360942	3.090400
18	C	3.001461	-3.373035	3.219344
19	C	2.814858	-2.116121	2.642487
20	C	3.986528	0.334506	0.712205
21	C	5.199705	0.984209	0.927634
22	C	5.288964	2.003241	1.877382
23	C	4.158181	2.379037	2.601266
24	C	2.939624	1.740616	2.375454
25	C	-5.236828	-0.018779	0.814694
26	C	-6.506928	0.127271	1.364471
27	C	-6.659000	0.663057	2.644584
28	C	-5.534136	1.040513	3.374057
29	C	-4.262696	0.890536	2.824144
30	C	-2.005785	2.259391	-1.044722
31	C	-2.083736	2.885099	-2.287851
32	C	-2.746625	2.265063	-3.346002
33	C	-3.349842	1.021985	-3.154036
34	C	-3.282066	0.400092	-1.909668
35	C	-2.945142	-2.527470	1.249122
36	C	-2.781749	-3.891605	1.014726
37	C	-2.093678	-4.335404	-0.115066
38	C	-1.577903	-3.406446	-1.018142
39	C	-1.732712	-2.042676	-0.785585
40	H	1.909746	-2.556175	-0.531350
41	H	1.616997	-2.918447	-2.957816
42	H	0.685532	-1.110546	-4.390365
43	H	0.108714	1.097776	-3.370486
44	H	0.455079	1.472707	-0.967024
45	H	-0.273515	-2.622620	1.305187
46	H	0.070222	-4.832397	2.287533
47	H	2.176858	-5.337979	3.543796
48	H	3.917177	-3.575922	3.770354
49	H	3.590263	-1.359806	2.741651
50	H	3.922554	-0.464069	-0.025074
51	H	6.075400	0.698669	0.349208
52	H	6.235795	2.512024	2.042608
53	H	4.215820	3.183224	3.331327
54	H	2.032713	2.073347	2.884670
55	H	-5.126439	-0.432330	-0.186021
56	H	-7.380563	-0.168630	0.788281
57	H	-7.652267	0.783676	3.070576
58	H	-5.635053	1.466424	4.369721
59	H	-3.394766	1.197438	3.402529
60	H	-1.482665	2.739727	-0.221329
61	H	-1.614930	3.856241	-2.426495
62	H	-2.796095	2.748604	-4.319006
63	H	-3.867936	0.530912	-3.974461
64	H	-3.747202	-0.572727	-1.769790
65	H	-3.467417	-2.193637	2.141487
66	H	-3.181178	-4.607773	1.728933
67	H	-1.956251	-5.400800	-0.286827
68	H	-1.023802	-3.729719	-1.896178
69	H	-1.306767	-1.335112	-1.492232
70	C	-1.651405	2.762955	2.473771
71	O	-2.293227	3.547161	1.798105
72	C	-0.970091	-0.247361	3.401531
73	O	-1.544278	-1.245696	3.745887
74	C	-2.659454	3.686453	4.601371
75	C	-1.414070	3.072097	3.974028
76	C	-0.194036	3.985998	4.080979
77	H	-3.508719	2.998143	4.525649
78	H	-2.925996	4.612878	4.084670
79	H	-1.178345	2.134109	4.490060
80	H	0.664729	3.520833	3.581040
81	H	0.048069	4.165572	5.133336
82	H	-0.396115	4.946589	3.595327
83	H	-2.475351	3.904657	5.658396
84	H	-0.309758	0.360523	4.106693
85	H	0.358378	2.353814	1.838919

6a

E = -2563.1987585 Ha

ATOM	X	Y	Z
1	Rh	-0.460091	1.202654	1.978127
2	P	1.399282	0.046782	1.004608
3	P	-2.192959	0.222689	0.747580
4	C	-3.795563	0.255770	1.650128
5	C	-2.594092	0.969102	-0.874979
6	C	1.228925	-0.371453	-0.774850
7	C	2.906271	1.097269	0.855127
8	C	-1.995862	-1.573700	0.391850
9	C	1.996752	-1.488574	1.789976
10	C	1.701748	-1.549731	-1.360556
11	C	1.517404	-1.774438	-2.723764
12	C	0.864491	-0.827173	-3.512603
13	C	0.419634	0.364795	-2.937931
14	C	0.614854	0.595565	-1.579338
15	C	1.326811	-2.695283	1.540123
16	C	1.708225	-3.865192	2.188974
17	C	2.757717	-3.848348	3.108316
18	C	3.414599	-2.648628	3.379844
19	C	3.034305	-1.474458	2.732290
20	C	4.154079	0.524506	0.568512
21	C	5.263182	1.333066	0.338415
22	C	5.138940	2.723017	0.377127
23	C	3.898419	3.298116	0.642852
24	C	2.786666	2.489811	0.884600
25	C	-4.973168	0.750411	1.079081
26	C	-6.153205	0.782456	1.822666
27	C	-6.176576	0.312955	3.134478
28	C	-5.005843	-0.179919	3.709413
29	C	-3.823760	-0.191752	2.977968
30	C	-2.104207	2.250572	-1.143835
31	C	-2.332730	2.845791	-2.381788
32	C	-3.049141	2.163666	-3.364392
33	C	-3.561378	0.893533	-3.095045
34	C	-3.347047	0.302336	-1.851455
35	C	-2.224251	-2.501881	1.417454
36	C	-2.032114	-3.863194	1.201953
37	C	-1.589382	-4.322755	-0.038741
38	C	-1.343332	-3.406305	-1.058988
39	C	-1.544765	-2.041852	-0.848483
40	H	2.184771	-2.309073	-0.751564
41	H	1.876017	-2.702007	-3.164034
42	H	0.703910	-1.017257	-4.571429
43	H	-0.108985	1.107291	-3.531381
44	H	0.255027	1.514107	-1.117222
45	H	0.511453	-2.729580	0.823051
46	H	1.172605	-4.787000	1.971539
47	H	3.063173	-4.763982	3.609506
48	H	4.228510	-2.621678	4.100507
49	H	3.565542	-0.549599	2.946110
50	H	4.258264	-0.557268	0.520467
51	H	6.224753	0.874649	0.119256
52	H	6.006412	3.352203	0.191716
53	H	3.788889	4.379943	0.665070
54	H	1.805874	2.928996	1.064484
55	H	-4.969126	1.136351	0.062672
56	H	-7.053204	1.197236	1.375435
57	H	-7.092783	0.363906	3.717716
58	H	-4.994213	-0.488861	4.751389
59	H	-2.882208	-0.478623	3.446417
60	H	-1.501946	2.747087	-0.382217
61	H	-1.932516	3.837176	-2.581232
62	H	-3.209129	2.620740	-4.338190
63	H	-4.125621	0.358677	-3.855221
64	H	-3.744339	-0.689887	-1.650359
65	H	-2.549381	-2.162903	2.396691
66	H	-2.216087	-4.561399	2.014833
67	H	-1.432152	-5.386324	-0.203996
68	H	-0.975396	-3.738822	-2.026391
69	H	-1.331423	-1.349616	-1.658396
70	C	-2.440714	2.386621	4.040473
71	C	-3.833630	2.930463	4.326740
72	C	-4.317883	2.484265	5.697693
73	H	-1.689004	2.885461	4.673273
74	H	-2.374447	1.322739	4.293164
75	H	-4.523531	2.558853	3.560634
76	H	-4.326301	1.388410	5.747964
77	H	-5.335679	2.836597	5.894817
78	H	-3.661607	2.854493	6.493693
79	H	-3.833925	4.022260	4.247897
80	C	-1.970486	2.558810	2.604346
81	O	-2.447245	3.418450	1.890862
82	C	0.630971	1.911933	3.354547

83 O 1.287667 2.301344 4.227408
84 H -0.070968 2.319584 0.828172
85 H -0.971925 0.020551 3.025446

6b

E =-2563.1999243 Ha

ATOM X Y Z
1 Rh -0.384224 1.468264 1.686868
2 P 1.409803 0.130646 0.843733
3 P -2.111191 0.323959 0.595718
4 C -3.678053 0.240287 1.556088
5 C -2.637953 0.953248 -1.041593
6 C 1.289740 -0.292968 -0.939264
7 C 3.011805 1.027433 0.802489
8 C -1.835508 -1.475011 0.272662
9 C 1.774200 -1.403223 1.757751
10 C 1.838668 -1.442637 -1.518080
11 C 1.656031 -1.696587 -2.875779
12 C 0.939531 -0.801601 -3.672030
13 C 0.436944 0.372447 -3.111394
14 C 0.622322 0.627843 -1.755298
15 C 1.320809 -2.659166 1.342855
16 C 1.476653 -3.774941 2.164134
17 C 2.086330 -3.651993 3.409684
18 C 2.534243 -2.399772 3.837013
19 C 2.372020 -1.283132 3.023684
20 C 4.242525 0.391924 1.003737
21 C 5.430889 1.106802 0.866490
22 C 5.402448 2.455692 0.512825
23 C 4.178132 3.089138 0.300456
24 C 2.987246 2.381742 0.446112
25 C -4.928759 0.499626 0.985258
26 C -6.089400 0.381466 1.749806
27 C -6.016805 -0.005352 3.086598
28 C -4.772303 -0.253559 3.665465
29 C -3.612897 -0.126057 2.907086
30 C -2.196845 2.209985 -1.462764
31 C -2.561844 2.696758 -2.717325
32 C -3.366254 1.930349 -3.559670
33 C -3.821403 0.680104 -3.139049
34 C -3.463918 0.195610 -1.884361
35 C -1.997286 -2.400647 1.311896
36 C -1.802082 -3.761213 1.088989
37 C -1.423377 -4.221471 -0.171913
38 C -1.232846 -3.305224 -1.204321
39 C -1.438053 -1.943832 -0.986123
40 H 2.375665 -2.161301 -0.905541
41 H 2.065449 -2.606209 -3.308837
42 H 0.776586 -1.018744 -4.725220
43 H -0.140267 1.075075 -3.708689
44 H 0.205874 1.525581 -1.299322
45 H 0.825899 -2.775260 0.383598
46 H 1.099707 -4.735911 1.821478
47 H 2.209056 -4.523331 4.048827
48 H 3.005544 -2.289466 4.810636
49 H 2.712530 -0.310488 3.374160
50 H 4.275930 -0.660854 1.274999
51 H 6.380569 0.602832 1.030315
52 H 6.331190 3.010481 0.401308
53 H 4.147685 4.140188 0.023269
54 H 2.023440 2.868540 0.290903
55 H -5.003079 0.811525 -0.052843
56 H -7.052081 0.600015 1.293885
57 H -6.923436 -0.093513 3.680500
58 H -4.699927 -0.524169 4.716018
59 H -2.628752 -0.253245 3.359205
60 H -1.537885 2.779278 -0.804918
61 H -2.208634 3.674453 -3.036567
62 H -3.642739 2.305431 -4.542642
63 H -4.451697 0.077068 -3.788306
64 H -3.815099 -0.782385 -1.564039
65 H -2.280027 -2.061816 2.305150
66 H -1.925097 -4.458156 1.914004
67 H -1.263037 -5.283748 -0.342661
68 H -0.908056 -3.634340 -2.188465
69 H -1.279390 -1.254234 -1.809664
70 C 0.797606 2.396909 2.835999
71 O 1.531893 2.929976 3.558171
72 H -0.058763 2.446080 0.398800
73 H -0.836580 0.438652 2.904886
74 C -1.894779 2.879429 2.212949
75 O -2.243428 3.770443 1.465942
76 C -3.997928 3.141800 3.592354

77 C -2.522331 2.757092 3.610079
78 C -1.766941 3.652641 4.595368
79 H -4.564787 2.545991 2.872760
80 H -4.111170 4.199035 3.334077
81 H -2.402122 1.718503 3.930765
82 H -0.726736 3.349895 4.727070
83 H -2.264667 3.589872 5.569095
84 H -1.794750 4.695500 4.261221
85 H -4.422011 2.973827 4.588152

TS-6a

E = -2563.1885902 Ha

Imaginary Frequency = -1813.54 cm^{-1}

ATOM X Y Z
1 Rh -0.972185 0.751973 2.274618
2 P 0.829269 -0.714201 1.634230
3 P -2.349056 0.382751 0.402419
4 C -4.149666 0.453634 0.777245
5 C -2.107183 1.479918 -1.048143
6 C 1.266268 -0.666269 -0.146708
7 C 2.435639 -0.175348 2.350888
8 C -2.257409 -1.307608 -0.328214
9 C 0.697441 -2.465780 2.118058
10 C 1.745212 -1.754276 -0.884966
11 C 1.995214 -1.616243 -2.249216
12 C 1.784511 -0.391940 -2.885125
13 C 1.350249 0.707026 -2.143922
14 C 1.099479 0.570117 -0.781924
15 C 0.149459 -3.423624 1.256960
16 C -0.093307 -4.720735 1.702035
17 C 0.203356 -5.080223 3.014629
18 C 0.735839 -4.127983 3.886130
19 C 0.976686 -2.829629 3.445774
20 C 3.494853 -1.070933 2.548132
21 C 4.720492 -0.610603 3.023072
22 C 4.906728 0.746089 3.289855
23 C 3.861432 1.643527 3.077949
24 C 2.629966 1.185512 2.612723
25 C -5.095983 0.672732 -0.228277
26 C -6.457384 0.627492 0.065507
27 C -6.889363 0.355589 1.363042
28 C -5.948983 0.138418 2.368686
29 C -4.587723 0.188716 2.078208
30 C -1.346955 2.642671 -0.892376
31 C -1.099732 3.480026 -1.976658
32 C -1.603826 3.160836 -3.237197
33 C -2.364837 2.004010 -3.403721
34 C -2.621568 1.172934 -2.315437
35 C -2.931386 -2.350342 0.323005
36 C -2.883774 -3.647342 -0.179121
37 C -2.153551 -3.928929 -1.334519
38 C -1.465137 -2.902022 -1.977321
39 C -1.514879 -1.600262 -1.478475
40 H 1.882330 -2.720450 -0.407664
41 H 2.340777 -2.475724 -2.819420
42 H 1.955321 -0.296638 -3.955049
43 H 1.158158 1.662969 -2.626025
44 H 0.721518 1.411752 -0.201179
45 H -0.098979 -3.161830 0.233356
46 H -0.526824 -5.439869 1.010342
47 H 0.013002 -6.093276 3.361410
48 H 0.963526 -4.393387 4.915549
49 H 1.383613 -2.097262 4.140606
50 H 3.360218 -2.130222 2.340043
51 H 5.534465 -1.314574 3.180249
52 H 5.865834 1.101598 3.659100
53 H 4.000396 2.703126 3.280672
54 H 1.799602 1.872429 2.443491
55 H -4.779863 0.894000 -1.244282
56 H -7.180489 0.808727 -0.726504
57 H -7.952470 0.321879 1.589160
58 H -6.270742 -0.065481 3.387480
59 H -3.841525 0.033621 2.857000
60 H -0.898375 2.843026 0.081168
61 H -0.499210 4.375805 -1.835601
62 H -1.398899 3.804972 -4.089083
63 H -2.756745 1.740380 -4.383388
64 H -3.205226 0.267298 -2.460047
65 H -3.497790 -2.148767 1.229615
66 H -3.405520 -4.444180 0.344890
67 H -2.113979 -4.944561 -1.722140
68 H -0.866163 -3.102255 -2.862494
69 H -0.961561 -0.818256 -1.991328
70 C -1.622519 3.400133 3.740497

71 C -2.120645 4.836402 3.679014
72 C -1.519945 5.666553 4.804257
73 H -0.525535 3.381721 3.764684
74 H -1.947670 2.925516 4.679180
75 H -3.214292 4.854270 3.730749
76 H -1.807598 5.265514 5.783395
77 H -1.851754 6.708529 4.753595
78 H -0.424703 5.653133 4.749222
79 H -1.848712 5.268791 2.708850
80 C -2.079777 2.505523 2.591618
81 O -2.964010 2.897466 1.847876
82 C -0.322526 0.744490 4.055168
83 O 0.053174 0.661819 5.149384
84 H -0.026964 1.931565 1.578532
85 H -1.982420 -0.427203 2.803529

TS-6b

E = -2563.1934203 Ha

Imaginary Frequency = -194.38 cm^{-1}

ATOM X Y Z
1 Rh -0.396364 1.306088 1.710243
2 P 1.437061 0.181476 0.774869
3 P -2.139383 0.229467 0.611482
4 C -3.747322 0.148239 1.522934
5 C -2.612235 0.915727 -1.042912
6 C 1.308382 -0.337571 -0.974682
7 C 3.058600 1.040350 0.713117
8 C -1.914382 -1.555051 0.255953
9 C 1.797923 -1.341595 1.745626
10 C 1.810323 -1.521458 -1.516654
11 C 1.616236 -1.807354 -2.868352
12 C 0.925358 -0.907130 -3.688154
13 C 0.449595 0.286095 -3.154832
14 C 0.642808 0.570891 -1.811434
15 C 1.241454 -2.583153 1.414097
16 C 1.448274 -3.697480 2.225678
17 C 2.209660 -3.591591 3.385183
18 C 2.768905 -2.358147 3.732490
19 C 2.559256 -1.243005 2.921455
20 C 4.274522 0.356163 0.683938
21 C 5.471752 1.062792 0.553409
22 C 5.450574 2.454631 0.433667
23 C 4.241684 3.132962 0.446339
24 C 3.046174 2.432540 0.590878
25 C -4.980737 0.133124 0.872525
26 C -6.164075 -0.003780 1.603018
27 C -6.120819 -0.124727 2.990332
28 C -4.892016 -0.103396 3.651525
29 C -3.713364 0.030261 2.912502
30 C -2.184275 2.202779 -1.387162
31 C -2.514822 2.759904 -2.625758
32 C -3.265480 2.032136 -3.544622
33 C -3.698197 0.744765 -3.214721
34 C -3.382858 0.201104 -1.970883
35 C -2.118817 -2.469112 1.296416
36 C -1.909318 -3.828933 1.088828
37 C -1.478664 -4.289653 -0.155922
38 C -1.246413 -3.380279 -1.185206
39 C -1.461394 -2.018762 -0.982624
40 H 2.314264 -2.240853 -0.879576
41 H 1.985692 -2.739640 -3.275041
42 H 0.758469 -1.152181 -4.733843
43 H -0.120868 0.986115 -3.771599
44 H 0.234264 1.485471 -1.384731
45 H 0.647579 -2.703015 0.508815
46 H 1.002663 -4.648682 1.933543
47 H 2.369303 -4.462509 4.020792
48 H 3.369894 -2.258481 4.630963
49 H 3.012623 -0.294114 3.205800
50 H 4.296574 -0.729989 0.769663
51 H 6.409765 0.529052 0.539519
52 H 6.390624 3.001307 0.332156
53 H 4.219480 4.217597 0.348183
54 H 2.092227 2.965942 0.606670
55 H -5.038266 0.229012 -0.213613
56 H -7.119678 -0.007175 1.084829
57 H -7.045826 -0.216808 3.564893
58 H -4.838645 -0.151866 4.733203
59 H -2.753325 0.118940 3.426560
60 H -1.571359 2.777459 -0.693664
61 H -2.179959 3.765434 -2.868599
62 H -3.522285 2.465140 -4.513674
63 H -4.283280 0.171175 -3.928136
64 H -3.730124 -0.809499 -1.733289

65 H -2.438986 -2.120113 2.275861
66 H -2.075689 -4.520583 1.909348
67 H -1.319310 -5.352525 -0.317621
68 H -0.891118 -3.713343 -2.157257
69 H -1.261254 -1.326967 -1.797637
70 C 0.554008 2.318229 2.973035
71 O 1.070978 2.961143 3.792272
72 H -1.699514 3.785964 1.000520
73 H -1.664183 2.031717 2.400200
74 C -2.597202 4.446001 1.114625
75 O -2.580782 5.616232 0.771282
76 C -4.862858 3.499341 0.659454
77 C -3.786721 3.738098 1.722998
78 C -4.355083 4.518327 2.904680
79 H -4.486818 2.894028 -0.170754
80 H -5.226368 4.454734 0.265927
81 H -3.417592 2.767107 2.073618
82 H -3.612105 4.629201 3.700486
83 H -5.219626 3.982035 3.310035
84 H -4.674389 5.514937 2.583132
85 H -5.694756 2.957837 1.120885

n-pro+cat

E = -2563.1968249 Ha

ATOM X Y Z

1 Rh -0.345947 0.581907 2.359416
2 P 1.450814 -0.051407 0.991071
3 P -2.176983 -0.033618 1.069553
4 C -3.818609 0.036778 1.909837
5 C -2.519358 0.835536 -0.506130
6 C 1.201736 -0.385164 -0.799314
7 C 2.854776 1.126475 0.900334
8 C -2.059071 -1.809601 0.619786
9 C 2.209045 -1.609375 1.587377
10 C 1.524664 -1.589460 -1.432727
11 C 1.210277 -1.781081 -2.779220
12 C 0.567552 -0.776780 -3.502061
13 C 0.268353 0.437972 -2.882609
14 C 0.590885 0.632232 -1.543977
15 C 1.391125 -2.748084 1.633205
16 C 1.890062 -3.958504 2.101889
17 C 3.206958 -4.043758 2.557532
18 C 4.017940 -2.910986 2.535348
19 C 3.526129 -1.698795 2.047973
20 C 3.920751 0.905648 0.016163
21 C 4.980214 1.805582 -0.045284
22 C 4.980342 2.941074 0.767314
23 C 3.918294 3.173149 1.638743
24 C 2.857483 2.269144 1.705675
25 C -5.012756 0.193953 1.195575
26 C -6.234070 0.237251 1.867028
27 C -6.280766 0.103180 3.253829
28 C -5.097027 -0.070031 3.968357
29 C -3.874749 -0.091494 3.302107
30 C -2.120503 2.174151 -0.595803
31 C -2.379481 2.914339 -1.747077
32 C -3.019696 2.315343 -2.831181
33 C -3.416957 0.979979 -2.753373
34 C -3.177339 0.246363 -1.593481
35 C -2.335183 -2.771107 1.604454
36 C -2.087868 -4.119697 1.363603
37 C -1.560195 -4.532960 0.137961
38 C -1.292496 -3.584245 -0.846615
39 C -1.539526 -2.232767 -0.610442
40 H 1.987856 -2.396290 -0.869696
41 H 1.449255 -2.729819 -3.254840
42 H 0.300714 -0.939679 -4.543518
43 H -0.250023 1.227347 -3.421614
44 H 0.333754 1.574796 -1.066424
45 H 0.359398 -2.695440 1.294366
46 H 1.236212 -4.827692 2.116962
47 H 3.595530 -4.986331 2.935907
48 H 5.042321 -2.963210 2.897607
49 H 4.174030 -0.825405 2.029604
50 H 3.916022 0.027212 -0.626976
51 H 5.804468 1.624093 -0.731042
52 H 5.805669 3.647365 0.715118
53 H 3.910293 4.059430 2.268841
54 H 2.020331 2.448963 2.378787
55 H -4.994446 0.313643 0.115161
56 H -7.150095 0.390269 1.301189
57 H -7.231766 0.160732 3.777506
58 H -5.118707 -0.136920 5.053085
59 H -2.938746 -0.154776 3.856779
60 H -1.597299 2.642298 0.235022

61 H -2.071234 3.955690 -1.788618
62 H -3.208714 2.887515 -3.736767
63 H -3.914912 0.505850 -3.595931
64 H -3.492334 -0.792661 -1.539132
65 H -2.728191 -2.462175 2.570917
66 H -2.299100 -4.848393 2.142806
67 H -1.353780 -5.585006 -0.043575
68 H -0.863242 -3.879085 -1.801236
69 H -1.300044 -1.510098 -1.385993
70 C -3.027637 3.279760 3.762688
71 C -4.539735 3.389990 3.600578
72 C -5.249682 3.138268 4.921534
73 H -2.688094 3.963564 4.557495
74 H -2.740680 2.266406 4.073272
75 H -4.868962 2.648151 2.863258
76 H -4.971873 2.154577 5.316055
77 H -6.336447 3.152266 4.793742
78 H -4.972764 3.895703 5.663893
79 H -4.796468 4.379104 3.206813
80 C -2.236271 3.602543 2.526872
81 O -2.484144 4.509908 1.749898
82 C 0.640151 0.633060 3.954020
83 O 1.143346 0.598197 5.003013
84 H -1.507676 1.014051 3.375779
85 H -1.380362 2.885943 2.352253

i-pro+cat

E = -2563.1979407 Ha

ATOM X Y Z
1 Rh -0.459614 1.251351 1.737042
2 P 1.402770 0.148581 0.850745
3 P -2.189085 0.163174 0.631113
4 C -3.788597 0.161163 1.537071
5 C -2.615249 0.929135 -0.976483
6 C 1.262780 -0.375829 -0.905087
7 C 2.958000 1.122134 0.748764
8 C -2.036204 -1.629628 0.269422
9 C 1.910726 -1.360302 1.753182
10 C 1.727452 -1.593442 -1.411426
11 C 1.530636 -1.914377 -2.754433
12 C 0.871104 -1.025705 -3.603767
13 C 0.426481 0.202192 -3.110603
14 C 0.634021 0.526236 -1.772994
15 C 1.183958 -2.548123 1.590497
16 C 1.469800 -3.665099 2.370103
17 C 2.476864 -3.608483 3.334087
18 C 3.198488 -2.427668 3.508780
19 C 2.918296 -1.308106 2.726306
20 C 4.131451 0.535217 0.253522
21 C 5.296964 1.285555 0.134911
22 C 5.300684 2.635031 0.496827
23 C 4.135831 3.226532 0.979999
24 C 2.966826 2.473671 1.103531
25 C -4.965685 -0.270158 0.913921
26 C -6.166070 -0.277320 1.619014
27 C -6.197349 0.130462 2.954506
28 C -5.025979 0.550863 3.580514
29 C -3.825886 0.569146 2.871031
30 C -2.182795 2.247131 -1.161455
31 C -2.440545 2.924789 -2.348870
32 C -3.115050 2.273380 -3.381089
33 C -3.548931 0.957323 -3.209220
34 C -3.309996 0.289743 -2.009533
35 C -2.330472 -2.543554 1.293216
36 C -2.109860 -3.905809 1.109463
37 C -1.595679 -4.378542 -0.098956
38 C -1.308029 -3.477281 -1.122776
39 C -1.524825 -2.111887 -0.941813
40 H 2.206787 -2.311558 -0.750180
41 H 1.878437 -2.874172 -3.129825
42 H 0.697317 -1.291944 -4.643634
43 H -0.111892 0.899494 -3.748454
44 H 0.264129 1.476451 -1.393480
45 H 0.395688 -2.609156 0.845514
46 H 0.888668 -4.572725 2.221081
47 H 2.694821 -4.478879 3.948691
48 H 3.981657 -2.373258 4.261470
49 H 3.489454 -0.393767 2.873478
50 H 4.129935 -0.513770 -0.038646
51 H 6.201477 0.820996 -0.250601
52 H 6.210576 3.222157 0.394535
53 H 4.130196 4.277386 1.259292
54 H 2.053501 2.935021 1.474225
55 H -4.945836 -0.593155 -0.125547

56 H -7.079847 -0.599257 1.124992
57 H -7.137674 0.126860 3.501130
58 H -5.046086 0.886155 4.614985
59 H -2.907152 0.956840 3.313021
60 H -1.618451 2.730289 -0.364623
61 H -2.109227 3.955075 -2.451725
62 H -3.305458 2.791483 -4.318297
63 H -4.073531 0.447579 -4.014087
64 H -3.646343 -0.737350 -1.883423
65 H -2.726839 -2.187620 2.241842
66 H -2.334228 -4.597251 1.918086
67 H -1.417656 -5.442396 -0.238711
68 H -0.889727 -3.822122 -2.065094
69 H -1.271765 -1.426373 -1.746409
70 C 0.333769 2.016362 3.253153
71 O 0.681794 2.414022 4.292281
72 H -1.701777 2.158513 2.205396
73 C -4.088275 3.689557 2.138270
74 C -3.379468 5.030380 1.939597
75 C -4.321638 6.173597 1.614181
76 C -2.285272 4.823107 0.926638
77 O -2.088826 5.498958 -0.069931
78 H -4.821151 3.751371 2.947741
79 H -3.357480 2.917974 2.394686
80 H -4.604857 3.364620 1.227657
81 H -2.844908 5.236956 2.881978
82 H -3.777728 7.110298 1.464504
83 H -5.038178 6.305112 2.431220
84 H -4.881014 5.959346 0.697025
85 H -1.656152 3.925659 1.164307

Adsorption configurations of reactants (H, CO, propene, H_2) on the M(Rh, Ir)-Cu-BTC

Rh-Cu-BTC

E = -3556.7390521 Ha

ATOM X Y Z
1 Cu 13.170547 18.916244 5.761842
2 Rh 13.171328 20.613263 7.453734
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.410072 17.860412 6.961959
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.931109 20.113624 4.702861
15 O 14.768147 19.860527 4.953284
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.572951 18.111453 6.709396
19 O 11.543456 19.705711 8.328755
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.799187 21.484584 6.542683
23 O 11.909628 21.745132 6.283984
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.433001 19.446442 8.588649
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.777716 18.316656 8.093866
44 C 15.682254 17.466275 8.925476
45 C 11.564155 21.247060 5.155870
46 C 10.659622 22.076531 4.303381
47 C 15.247225 20.913888 5.487162

48 C 16.429917 21.548372 4.830414
49 C 11.094635 18.648736 7.761389
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134

Ir-Cu-BTC

E = -3591.0276450 Ha

ATOM X Y Z
1 Cu 13.170585 18.902176 5.747821
2 Ir 13.171320 20.602182 7.442657
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.421230 17.842145 6.959518
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.919883 20.111052 4.684639
15 O 14.777599 19.860170 4.932258
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.563497 18.090605 6.709129
19 O 11.548150 19.697159 8.322434
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.794444 21.478173 6.534050
23 O 11.913791 21.737206 6.277573
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.428838 19.440060 8.580767
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.779387 18.302827 8.086596

44 C 15.682254 17.466275 8.925476
45 C 11.562464 21.239693 5.142017
46 C 10.659622 22.076531 4.303381
47 C 15.248754 20.907728 5.471727
48 C 16.429917 21.548372 4.830414
49 C 11.093079 18.633350 7.755318
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134

H ─ Rh-Cu-BTC

E = -3557.3427820 Ha

ATOM X Y Z
1 Cu 13.170663 18.887194 5.728988
2 Rh 13.171479 20.652020 7.494609
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.401178 17.878054 6.960443
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.938760 20.109802 4.711213
15 O 14.755188 19.861054 4.960172
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.587128 18.126136 6.711351
19 O 11.537101 19.715384 8.342253
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.804424 21.490766 6.550500
23 O 11.910491 21.754096 6.286698
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.433539 19.451812 8.606659
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492

40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.769750 18.326924 8.097513
44 C 15.682254 17.466275 8.925476
45 C 11.572604 21.246674 5.161632
46 C 10.659622 22.076531 4.303381
47 C 15.239902 20.914254 5.494352
48 C 16.429917 21.548372 4.830414
49 C 11.102034 18.659241 7.765168
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134
83 H 13.172392 21.773446 8.545641

CO ─ Rh-Cu-BTC

E = -3670.1083410 Ha

ATOM X Y Z
1 Cu 13.170795 18.896593 5.740916
2 Rh 13.170313 20.643662 7.483725
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.414058 17.852534 6.964896
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.927698 20.116641 4.693372
15 O 14.774953 19.861699 4.944793
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.566895 18.105160 6.710824
19 O 11.532083 19.699902 8.333553
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.809884 21.487842 6.536418
23 O 11.902179 21.752155 6.274830
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.438846 19.437739 8.596673
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858

36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.777191 18.304908 8.087827
44 C 15.682254 17.466275 8.925476
45 C 11.565092 21.240970 5.143186
46 C 10.659622 22.076531 4.303381
47 C 15.250276 20.904976 5.476711
48 C 16.429917 21.548372 4.830414
49 C 11.093377 18.637352 7.755062
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134
83 C 13.184777 22.028619 8.845868
84 O 13.198806 22.860762 9.632252

Propene ─ Rh-Cu-BTC

E = -3674.7085111 Ha

ATOM X Y Z
1 Cu 7.441652 10.930569 4.464562
2 Rh 7.438185 12.671853 6.208130
3 O 2.452180 6.486551 5.488709
4 O 3.537079 17.906239 4.258778
5 O 3.597830 12.741590 -0.786195
6 O 2.374813 11.560483 10.624687
7 O 11.352737 10.738728 11.444691
8 O 12.432766 11.932922 0.020749
9 O 12.515003 17.084483 5.078782
10 O 11.287115 5.677883 6.295653
11 O 8.687215 9.868816 5.674108
12 O 0.879342 9.859273 10.583894
13 O 14.009642 17.037730 3.376993
14 O 6.195244 12.127713 3.398120
15 O 9.042266 11.882479 3.652022
16 O 2.388936 18.101381 2.315609
17 O 12.500047 8.795621 11.645278
18 O 5.842631 10.107459 5.419193
19 O 5.786696 11.727469 7.015448
20 O 12.465819 5.429624 8.214479
21 O 2.419922 14.660204 -1.039808
22 O 9.097986 13.487566 5.265276
23 O 6.171208 13.760724 4.983530
24 O 13.962946 13.603662 0.014480
25 O 0.922795 6.486165 7.160190
26 O 8.707750 11.450571 7.309620
27 C 1.999239 6.999528 6.495820
28 C 2.536403 8.231346 7.137687
29 C 3.210851 17.439805 3.182449

30 C 3.645733 16.114065 2.660452
31 C 3.249094 13.823506 -0.349829
32 C 3.663018 14.382452 0.967045
33 C 1.949180 10.551317 10.092815
34 C 2.513792 9.933876 8.860268
35 C 11.678229 9.660810 10.981423
36 C 11.242466 9.134934 9.657506
37 C 12.886431 12.941393 0.530403
38 C 12.350161 13.587312 1.760490
39 C 12.939900 16.549299 4.071058
40 C 12.374407 15.315123 3.457690
41 C 11.636576 6.117416 7.376052
42 C 11.223547 7.436205 7.931132
43 C 9.047951 10.322340 6.798626
44 C 9.955016 9.480805 7.634041
45 C 5.835832 13.252536 3.853784
46 C 4.932384 14.091061 3.011947
47 C 9.524083 12.919452 4.194822
48 C 10.702678 13.562902 3.538980
49 C 5.361175 10.655270 6.452773
50 C 4.184722 10.008964 7.107008
51 C 3.642190 8.850221 6.544866
52 H 4.074984 8.422049 5.644453
53 C 4.496930 15.342332 3.458374
54 H 4.815411 15.723758 4.425026
55 C 4.514509 13.612921 1.767040
56 H 4.847753 12.641225 1.411878
57 C 3.619316 10.550723 8.265200
58 H 4.032964 11.451745 8.710607
59 C 10.391280 9.930880 8.883722
60 H 10.073442 10.898856 9.262317
61 C 11.244388 12.996930 2.381718
62 H 10.810960 12.095408 1.956531
63 C 11.268894 14.722489 4.076896
64 H 10.855889 15.170869 4.976737
65 C 10.372069 8.234230 7.159543
66 H 10.038191 7.876233 6.189106
67 C 1.971371 8.773539 8.297029
68 H 1.113194 8.295625 8.759160
69 C 12.916005 14.748050 2.298837
70 H 13.774173 15.208295 1.819091
71 C 3.228054 15.634795 1.413983
72 H 2.567173 16.234080 0.795493
73 C 11.659322 7.886794 9.181883
74 H 12.320194 7.269840 9.782758
75 H 0.596723 10.350955 11.381058
76 H 14.292875 17.836271 3.866080
77 H 2.170924 18.945802 2.758915
78 H 12.718674 9.241424 12.488223
79 H 12.667207 4.592333 7.750316
80 H 14.224450 13.094591 -0.778944
81 H 0.660670 5.691300 6.653692
82 H 2.217912 14.193558 -1.875568
83 C 7.461879 14.681995 7.309506
84 C 7.447237 13.801262 8.363571
85 C 6.247989 13.478933 9.177862
86 H 8.397404 15.064378 6.911956
87 H 6.546529 15.175976 6.989386
88 H 8.399358 13.413020 8.724727
89 H 6.363521 13.950295 10.164708
90 H 6.152021 12.400817 9.344897
91 H 5.325625 13.845178 8.717763

H_2 — Rh-Cu-BTC

E = -3557.9338489 Ha

ATOM X Y Z
1 Cu 13.172191 18.916243 5.761815
2 Rh 13.172036 20.631437 7.471603
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.412609 17.856315 6.963682
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.932947 20.118214 4.698241
15 O 14.773839 19.859179 4.953098
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712

18 O 11.570432 18.110407 6.711308
19 O 11.538701 19.701790 8.336168
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.804593 21.490899 6.537871
23 O 11.908196 21.753972 6.278089
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.435187 19.439942 8.596185
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.771915 18.308616 8.095183
44 C 15.682254 17.466275 8.925476
45 C 11.567045 21.247842 5.149706
46 C 10.659622 22.076531 4.303381
47 C 15.249608 20.910447 5.484416
48 C 16.429917 21.548372 4.830414
49 C 11.093857 18.644729 7.760462
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134
83 H 12.805135 22.011696 8.759397
84 H 13.584416 21.915358 8.839980

H－Ir-Cu-BTC

E = -3591.6471132 Ha

ATOM X Y Z
1 Cu 13.171220 18.881408 5.721813
2 Ir 13.170990 20.654408 7.498428
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.411250 17.880596 6.954985
12 O 6.606580 17.844743 11.875328

13 O 19.736880 25.023200 4.668428
14 O 11.929937 20.105217 4.713473
15 O 14.749763 19.867533 4.950129
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.593025 18.117277 6.717500
19 O 11.533745 19.715186 8.342170
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.808227 21.489169 6.551252
23 O 11.907955 21.754954 6.286835
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.434131 19.450390 8.607671
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.775594 18.322635 8.093242
44 C 15.682254 17.466275 8.925476
45 C 11.566060 21.242318 5.158731
46 C 10.659622 22.076531 4.303381
47 C 15.239625 20.914857 5.485626
48 C 16.429917 21.548372 4.830414
49 C 11.101317 18.650986 7.765256
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134
83 H 13.173028 21.791942 8.569844

CO ─Ir-Cu-BTC

E = -3704.4261324 Ha

ATOM X Y Z
1 Cu 13.170460 18.862951 5.709251
2 Ir 13.171587 20.625519 7.465810
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125

8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.433684 17.841470 6.958969
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.907358 20.110273 4.684308
15 O 14.778637 19.866133 4.923296
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.562957 18.082271 6.715610
19 O 11.531045 19.694010 8.322210
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.812733 21.476567 6.531224
23 O 11.909113 21.746963 6.265147
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.435696 19.429002 8.589601
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.783705 18.291521 8.079398
44 C 15.682254 17.466275 8.925476
45 C 11.558887 21.232889 5.130538
46 C 10.659622 22.076531 4.303381
47 C 15.252650 20.899580 5.459898
48 C 16.429917 21.548372 4.830414
49 C 11.089512 18.621620 7.747950
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318
74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134
83 C 13.172932 21.957611 8.792842
84 O 13.174208 22.773487 9.605514

Propene ─Ir-Cu-BTC

E = -3709.0098981 Ha

ATOM X Y Z
1 Cu 13.167246 18.886417 5.732988
2 Ir 13.178679 20.646332 7.484149

3	O	8.179418	14.472021	6.780144
4	O	9.264318	25.891709	5.550213
5	O	9.325069	20.727060	0.505239
6	O	8.102052	19.545954	11.916121
7	O	17.079976	18.724198	12.736125
8	O	18.160004	19.918392	1.312183
9	O	18.242241	25.069953	6.370217
10	O	17.014354	13.663353	7.587088
11	O	14.527872	17.936679	6.917482
12	O	6.606580	17.844743	11.875328
13	O	19.736880	25.023200	4.668428
14	O	11.816578	20.070585	4.768988
15	O	14.710086	19.929845	4.817772
16	O	8.116175	26.086851	3.607044
17	O	18.227286	16.781091	12.936712
18	O	11.626219	17.987152	6.777945
19	O	11.489985	19.718808	8.254317
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.865042	21.393184	6.555866
23	O	12.005909	21.810536	6.222201
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.349327	19.393031	8.655260
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605
32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.786162	18.315775	8.091287
44	C	15.682254	17.466275	8.925476
45	C	11.560652	21.244121	5.149742
46	C	10.659622	22.076531	4.303381
47	C	15.239915	20.890834	5.428252
48	C	16.429917	21.548372	4.830414
49	C	11.103159	18.596685	7.744886
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887
53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	C	12.494360	22.063286	9.008264
84	C	13.880988	22.222232	8.986305
85	C	14.557765	23.409717	8.392630
86	H	12.015231	21.441393	9.757397

87 H 11.861615 22.792101 8.505620
88 H 14.476746 21.619225 9.671147
89 H 15.556691 23.167324 8.023048
90 H 14.669574 24.164442 9.183852
91 H 13.973088 23.847119 7.578577

H_2 —Ir-Cu-BTC

E = -3592.2272608 Ha

ATOM X Y Z
1 Cu 13.170395 18.885338 5.731910
2 Ir 13.170475 20.614970 7.453264
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.431740 17.852650 6.961000
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.909118 20.111203 4.692426
15 O 14.779651 19.864109 4.925330
16 O 8.116175 26.086851 3.607044
17 O 18.227286 16.781091 12.936712
18 O 11.563445 18.088952 6.716294
19 O 11.537570 19.691710 8.331252
20 O 18.193058 13.415094 9.505913
21 O 8.147161 22.645674 0.251626
22 O 14.802655 21.484134 6.521924
23 O 11.916542 21.754644 6.264699
24 O 19.690185 21.589132 1.305915
25 O 6.650033 14.471635 8.451624
26 O 14.426288 19.430191 8.599241
27 C 7.726478 14.984999 7.787255
28 C 8.263642 16.216816 8.429122
29 C 8.938090 25.425276 4.473884
30 C 9.372971 24.099535 3.951886
31 C 8.976333 21.808976 0.941605
32 C 9.390256 22.367923 2.258479
33 C 7.676419 18.536787 11.384250
34 C 8.241030 17.919346 10.151702
35 C 17.405468 17.646280 12.272858
36 C 16.969704 17.120405 10.948941
37 C 18.613670 20.926864 1.821837
38 C 18.077400 21.572782 3.051925
39 C 18.667139 24.534769 5.362492
40 C 18.101645 23.300593 4.749125
41 C 17.363815 14.102886 8.667487
42 C 16.950785 15.421675 9.222567
43 C 14.780484 18.299104 8.089089
44 C 15.682254 17.466275 8.925476
45 C 11.560246 21.239960 5.136860
46 C 10.659622 22.076531 4.303381
47 C 15.251443 20.904128 5.461064
48 C 16.429917 21.548372 4.830414
49 C 11.092383 18.625528 7.756681
50 C 9.911960 17.994434 8.398443
51 C 9.369428 16.835691 7.836300
52 H 9.802223 16.407519 6.935887
53 C 10.224168 23.327802 4.749809
54 H 10.542649 23.709229 5.716460
55 C 10.241747 21.598391 3.058475
56 H 10.574992 20.626695 2.703312
57 C 9.346555 18.536193 9.556635
58 H 9.760203 19.437215 10.002041
59 C 16.118519 17.916351 10.175156
60 H 15.800681 18.884326 10.553752
61 C 16.971627 20.982400 3.673152
62 H 16.538199 20.080879 3.247965
63 C 16.996133 22.707959 5.368330
64 H 16.583127 23.156339 6.268171
65 C 16.099308 16.219700 8.450978
66 H 15.765430 15.861703 7.480541
67 C 7.698610 16.759010 9.588463
68 H 6.840433 16.281095 10.050594
69 C 18.643243 22.733520 3.590272
70 H 19.501412 23.193765 3.110526
71 C 8.955292 23.620265 2.705417
72 H 8.294412 24.219550 2.086928
73 C 17.386561 15.872264 10.473318

74 H 18.047433 15.255310 11.074192
75 H 6.323961 18.336425 12.672492
76 H 20.020114 25.821741 5.157515
77 H 7.898162 26.931272 4.050349
78 H 18.445913 17.226894 13.779658
79 H 18.394446 12.577803 9.041751
80 H 19.951689 21.080061 0.512491
81 H 6.387908 13.676770 7.945126
82 H 7.945151 22.179028 -0.584134
83 H 12.758102 21.854494 8.636018
84 H 13.613896 21.842803 8.636067

The species below are reaction intermediates shown in Figure 8 and Figure 9

Figure 8:

(1) H+propene

E = -3675.2793012 Ha

ATOM X Y Z
1 Cu 9.819813 13.882136 2.847211
2 Rh 9.817356 15.628844 4.585906
3 O 4.828605 9.449493 3.876568
4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.069399 12.828162 4.051448
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.580721 15.094836 1.811509
15 O 11.412509 14.842791 2.050644
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.229848 13.089847 3.812677
19 O 8.181869 14.689967 5.435642
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.462232 16.467345 3.649642
23 O 8.556992 16.747861 3.382643
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.070968 14.409206 5.689827
27 C 4.375664 9.962471 4.883679
28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916
40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.420809 13.286073 5.182224
44 C 12.331441 12.443747 6.021900
45 C 8.220054 16.231059 2.261321
46 C 7.308809 17.054003 1.399805
47 C 11.892102 15.891346 2.590291
48 C 13.079103 16.525844 1.926839
49 C 7.749117 13.631947 4.860089
50 C 6.561147 12.971906 5.494867
51 C 6.018615 11.813163 4.932724
52 H 6.451410 11.384991 4.032312
53 C 6.873355 18.305274 1.846233
54 H 7.191836 18.686701 2.812885
55 C 6.890934 16.575863 0.154899
56 H 7.224179 15.604167 -0.200264
57 C 5.995741 13.513665 6.653059
58 H 6.409389 14.414687 7.098466
59 C 12.767705 12.893823 7.271581
60 H 12.449867 13.861798 7.650176
61 C 13.620813 15.959872 0.769576
62 H 13.187385 15.058351 0.344389
63 C 13.645319 17.685431 2.464754
64 H 13.232314 18.133811 3.364595
65 C 12.748494 11.197173 5.547402
66 H 12.414616 10.839175 4.576965

67 C 4.347796 11.736482 6.684887
68 H 3.489619 11.258567 7.147018
69 C 15.292430 17.710992 0.686696
70 H 16.150598 18.171237 0.206950
71 C 5.604479 18.597737 -0.198159
72 H 4.943598 19.197022 -0.816648
73 C 14.035747 10.849736 7.569742
74 H 14.696619 10.232782 8.170616
75 H 2.973148 13.313897 9.768916
76 H 16.669301 20.799213 2.253939
77 H 4.547349 21.908744 1.146773
78 H 15.095100 12.204366 10.876082
79 H 15.043633 7.555275 6.138175
80 H 16.600875 16.057533 -2.391085
81 H 3.037095 8.654242 5.041551
82 H 4.594337 17.156500 -3.487709
83 H 10.051642 16.604754 5.956380
84 C 10.225406 17.276999 7.039388
85 C 11.147026 16.563756 7.804175
86 C 12.606821 16.679138 7.651320
87 H 10.574699 18.203423 6.578543
88 H 9.188726 17.291070 7.375637
89 H 10.782586 15.777721 8.465561
90 H 12.892140 17.466200 6.947137
91 H 13.018106 15.720131 7.301075
92 H 13.087474 16.856446 8.624498

TS-1a
E = -3675.2694376 Ha
Imaginary Frequency = -1626.34 cm^{-1}

ATOM X Y Z
1 Cu 9.818907 13.879560 2.841141
2 Rh 9.818543 15.633769 4.588500
3 O 4.828605 9.449493 3.876568
4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.068554 12.817145 4.055391
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.570897 15.095658 1.798422
15 O 11.425202 14.840697 2.037816
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.223744 13.076259 3.817561
19 O 8.169554 14.690772 5.427250
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.455060 16.468873 3.633493
23 O 8.552543 16.740418 3.380516
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.107026 14.418388 5.674408
27 C 4.375664 9.962471 4.883679
28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916
40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.430828 13.282613 5.174159
44 C 12.331441 12.443747 6.021900
45 C 8.215869 16.223776 2.254329
46 C 7.308809 17.054003 1.399805
47 C 11.893680 15.886487 2.576608
48 C 13.079103 16.525844 1.926839
49 C 7.744654 13.623590 4.854369
50 C 6.561147 12.971906 5.494867
51 C 6.018615 11.813163 4.932724
52 H 6.451410 11.384991 4.032312
53 C 6.873355 18.305274 1.846233

54 H 7.191836 18.686701 2.812885
55 C 6.890934 16.575863 0.154899
56 H 7.224179 15.604167 -0.200264
57 C 5.995741 13.513665 6.653059
58 H 6.409389 14.414687 7.098466
59 C 12.767705 12.893823 7.271581
60 H 12.449867 13.861798 7.650176
61 C 13.620813 15.959872 0.769576
62 H 13.187385 15.058351 0.344389
63 C 13.645319 17.685431 2.464754
64 H 13.232314 18.133811 3.364595
65 C 12.748494 11.197173 5.547402
66 H 12.414616 10.839175 4.576965
67 C 4.347796 11.736482 6.684887
68 H 3.489619 11.258567 7.147018
69 C 15.292430 17.710992 0.686696
70 H 16.150598 18.171237 0.206950
71 C 5.604479 18.597737 -0.198159
72 H 4.943598 19.197022 -0.816648
73 C 14.035747 10.849736 7.569742
74 H 14.696619 10.232782 8.170616
75 H 2.973148 13.313897 9.768916
76 H 16.669301 20.799213 2.253939
77 H 4.547349 21.908744 1.146773
78 H 15.095100 12.204366 10.876082
79 H 15.043633 7.555275 6.138175
80 H 16.600875 16.057533 -2.391085
81 H 3.037095 8.654242 5.041551
82 H 4.594337 17.156500 -3.487709
83 C 10.001982 17.454932 6.094141
84 C 10.144054 16.938963 7.421005
85 C 11.462412 16.524688 7.976257
86 H 9.056766 17.896191 5.802704
87 H 10.898920 17.735747 5.551682
88 H 9.841211 16.138965 6.384114
89 H 12.231026 16.542430 7.199666
90 H 11.431309 15.511463 8.392594
91 H 11.765744 17.199908 8.786650
92 H 9.250308 16.871021 8.035559

TS-1b
E = -3675.2800779 Ha

Imaginary Frequency = -625.05 cm^{-1}

ATOM X Y Z
1 Cu 9.818929 13.940957 2.903603
2 Rh 9.802907 15.735306 4.672715
3 O 4.828605 9.449493 3.876568
4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.104571 12.824093 4.024670
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.532870 15.059898 1.787555
15 O 11.380749 14.883459 2.064185
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.265492 13.103755 3.861371
19 O 8.132226 14.742523 5.450390
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.486486 16.495172 3.680471
23 O 8.581863 16.726157 3.341161
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.028482 14.357262 5.704524
27 C 4.375664 9.962471 4.883679
28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916

40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.415008 13.264003 5.168930
44 C 12.331441 12.443747 6.021900
45 C 8.213026 16.199501 2.231794
46 C 7.308809 17.054003 1.399805
47 C 11.885285 15.913206 2.607174
48 C 13.079103 16.525844 1.926839
49 C 7.749651 13.656965 4.879914
50 C 6.561147 12.971906 5.494867
51 C 6.018615 11.813163 4.932724
52 H 6.451410 11.384991 4.032312
53 C 6.873355 18.305274 1.846233
54 H 7.191836 18.686701 2.812885
55 C 6.890934 16.575863 0.154899
56 H 7.224179 15.604167 -0.200264
57 C 5.995741 13.513665 6.653059
58 H 6.409389 14.414687 7.098466
59 C 12.767705 12.893823 7.271581
60 H 12.449867 13.861798 7.650176
61 C 13.620813 15.959872 0.769576
62 H 13.187385 15.058351 0.344389
63 C 13.645319 17.685431 2.464754
64 H 13.232314 18.133811 3.364595
65 C 12.748494 11.197173 5.547402
66 H 12.414616 10.839175 4.576965
67 C 4.347796 11.736482 6.684887
68 H 3.489619 11.258567 7.147018
69 C 15.292430 17.710992 0.686696
70 H 16.150598 18.171237 0.206950
71 C 5.604479 18.597737 -0.198159
72 H 4.943598 19.197022 -0.816648
73 C 14.035747 10.849736 7.569742
74 H 14.696619 10.232782 8.170616
75 H 2.973148 13.313897 9.768916
76 H 16.669301 20.799213 2.253939
77 H 4.547349 21.908744 1.146773
78 H 15.095100 12.204366 10.876082
79 H 15.043633 7.555275 6.138175
80 H 16.600875 16.057533 -2.391085
81 H 3.037095 8.654242 5.041551
82 H 4.594337 17.156500 -3.487709
83 H 9.495207 17.258187 5.444466
84 C 9.889831 17.738916 6.508672
85 C 10.754645 16.778135 7.072742
86 C 12.218138 16.783509 6.942786
87 H 10.351344 18.659276 6.147343
88 H 8.923913 17.868321 6.997852
89 H 10.314245 15.984478 7.673453
90 H 12.572664 17.503766 6.201591
91 H 12.561307 15.772955 6.684443
92 H 12.671836 17.013486 7.920119

(2a) $CH_3CH_2CH_2$
E = -3675.3200784 Ha
ATOM X Y Z
1 Cu 9.823630 13.884998 2.847832
2 Rh 9.818640 15.643647 4.607869
3 O 4.828605 9.449493 3.876568
4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.078571 12.861491 4.034557
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.575608 15.080566 1.829322
15 O 11.390139 14.850513 2.051841
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.258996 13.098134 3.827112
19 O 8.166043 14.710522 5.434573
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.471768 16.458649 3.664154
23 O 8.575020 16.752839 3.376543
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.039822 14.394066 5.717060
27 C 4.375664 9.962471 4.883679

28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916
40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.412756 13.292691 5.189949
44 C 12.331441 12.443747 6.021900
45 C 8.222961 16.229555 2.264341
46 C 7.308809 17.054003 1.399805
47 C 11.889075 15.893594 2.595963
48 C 13.079103 16.525844 1.926839
49 C 7.752573 13.641870 4.867275
50 C 6.561147 12.971906 5.494867
51 C 6.018615 11.813163 4.932724
52 H 6.451410 11.384991 4.032312
53 C 6.873355 18.305274 1.846233
54 H 7.191836 18.686701 2.812885
55 C 6.890934 16.575863 0.154899
56 H 7.224179 15.604167 -0.200264
57 C 5.995741 13.513665 6.653059
58 H 6.409389 14.414687 7.098466
59 C 12.767705 12.893823 7.271581
60 H 12.449867 13.861798 7.650176
61 C 13.620813 15.959872 0.769576
62 H 13.187385 15.058351 0.344389
63 C 13.645319 17.685431 2.464754
64 H 13.232314 18.133811 3.364595
65 C 12.748494 11.197173 5.547402
66 H 12.414616 10.839175 4.576965
67 C 4.347796 11.736482 6.684887
68 H 3.489619 11.258567 7.147018
69 C 15.292430 17.710992 0.686696
70 H 16.150598 18.171237 0.206950
71 C 5.604479 18.597737 -0.198159
72 H 4.943598 19.197022 -0.816648
73 C 14.035747 10.849736 7.569742
74 H 14.696619 10.232782 8.170616
75 H 2.973148 13.313897 9.768916
76 H 16.669301 20.799213 2.253939
77 H 4.547349 21.908744 1.146773
78 H 15.095100 12.204366 10.876082
79 H 15.043633 7.555275 6.138175
80 H 16.600875 16.057533 -2.391085
81 H 3.037095 8.654242 5.041551
82 H 4.594337 17.156500 -3.487709
83 C 9.780348 17.160622 6.005498
84 C 10.639550 16.932300 7.214747
85 C 12.142488 17.007776 6.978844
86 H 10.098525 18.022429 5.406851
87 H 8.712615 17.210682 6.242570
88 H 10.375395 15.983690 7.701452
89 H 12.403429 17.910092 6.412848
90 H 12.491726 16.139249 6.412714
91 H 12.676427 17.030989 7.934553
92 H 10.349200 17.724093 7.928295

(2b) CH_3CHCH_3

E = -3675.3242131 Ha

ATOM X Y Z
1 Cu 9.805947 13.771817 2.774174
2 Rh 9.813784 15.547260 4.502260
3 O 4.519181 8.979544 3.760932
4 O 5.710624 21.300221 2.694047
5 O 5.749651 15.639729 -2.887340
6 O 4.465860 14.580066 9.401731
7 O 13.935609 13.726388 10.263299
8 O 15.089811 14.786810 -2.025997
9 O 15.141946 20.437600 3.565290
10 O 13.900360 8.136441 4.610642
11 O 11.165752 12.651568 4.130252
12 O 2.687840 12.662797 9.437989
13 O 16.918763 20.470305 1.645350
14 O 8.443309 15.136564 1.628889
15 O 11.572892 14.857230 1.907753

16 O 4.348385 21.624831 0.482645
17 O 15.312882 11.525061 10.583350
18 O 8.056565 12.931915 3.851801
19 O 8.058618 14.553301 5.425251
20 O 15.287846 7.785032 6.801620
21 O 4.374452 17.835046 -3.249582
22 O 11.530447 16.455439 3.501529
23 O 8.476086 16.726800 3.230488
24 O 16.884418 16.689065 -2.094675
25 O 2.724258 8.914017 5.663859
26 O 11.171939 14.275784 5.699854
27 C 3.917688 9.571990 5.012539
28 C 4.519371 10.849951 5.624994
29 C 5.261784 20.786972 1.346891
30 C 5.734351 19.406992 0.853415
31 C 5.289670 16.991011 -2.394994
32 C 5.749352 17.507897 -1.018885
33 C 3.881027 13.327857 8.794126
34 C 4.499674 12.728682 7.517390
35 C 14.389831 12.381193 9.749020
36 C 13.910676 11.880700 8.373503
37 C 15.691419 16.039212 -1.434882
38 C 15.089231 16.654335 -0.157941
39 C 15.726684 19.827320 2.313958
40 C 15.107496 18.549747 1.717344
41 C 14.365571 8.633854 5.958562
42 C 13.898894 10.006936 6.476078
43 C 11.533217 13.125338 5.251322
44 C 12.491700 12.249303 6.144484
45 C 8.095057 16.267250 2.092742
46 C 7.138989 17.170008 1.233082
47 C 12.027585 15.913410 2.447375
48 C 13.273701 16.612361 1.796602
49 C 7.582769 13.481410 4.896572
50 C 6.335093 12.803965 5.582597
51 C 5.736653 11.525524 4.964759
52 H 6.194350 11.079329 4.020694
53 C 6.665196 18.549084 1.731082
54 H 7.004358 18.935004 2.748879
55 C 6.681177 16.649656 -0.142368
56 H 7.033843 15.630921 -0.512942
57 C 5.716164 13.404563 6.858589
58 H 6.159452 14.350008 7.315945
59 C 12.969733 12.751105 7.520061
60 H 12.625842 13.766797 7.906962
61 C 13.872524 15.994643 0.518992
62 H 13.415574 15.049655 0.074312
63 C 13.891102 17.890995 2.394755
64 H 13.447780 18.349427 3.339736
65 C 12.957853 10.877226 5.621153
66 H 12.606867 10.506139 4.601920
67 C 3.901582 11.451650 6.900236
68 H 3.000603 10.951128 7.387471
69 C 15.705982 17.930949 0.441301
70 H 16.607071 18.417558 -0.059683
71 C 5.276157 18.885628 -0.520512
72 H 4.587081 19.520472 -1.169921
73 C 14.374909 10.509149 7.851298
74 H 15.070963 9.864679 8.483639
75 H 2.381962 13.237788 10.336859
76 H 17.225167 21.370061 2.218639
77 H 4.108822 22.574315 1.005338
78 H 15.535430 12.043033 11.539508
79 H 15.500615 6.831478 6.274824
80 H 17.191377 16.090558 -2.977625
81 H 2.418606 8.028719 5.068179
82 H 4.129798 17.287487 -4.183596
83 C 8.752009 17.989088 5.788187
84 C 9.842407 16.991112 6.034691
85 C 11.219178 17.577610 6.132913
86 H 8.964554 18.609790 4.911150
87 H 7.772574 17.518833 5.664384
88 H 9.615551 16.304952 6.860242
89 H 11.443057 18.220893 5.275602
90 H 11.995158 16.812308 6.222492
91 H 11.257860 18.204087 7.038672
92 H 8.699395 18.658076 6.662603

(3a) $CH_3CH_2CH_2$+ CO
E = -3788.6461413 Ha
ATOM X Y Z
1 Cu 9.820406 13.878759 2.846939
2 Rh 9.827259 15.648571 4.598004
3 O 4.828605 9.449493 3.876568

4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.045162 12.838960 4.056760
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.599595 15.097061 1.814847
15 O 11.418545 14.823860 2.066394
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.231449 13.110330 3.805650
19 O 8.202722 14.681415 5.455558
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.424765 16.497540 3.611085
23 O 8.542546 16.738337 3.393915
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.102188 14.430765 5.682652
27 C 4.375664 9.962471 4.883679
28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916
40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.423377 13.298097 5.185842
44 C 12.331441 12.443747 6.021900
45 C 8.220362 16.230421 2.265850
46 C 7.308809 17.054003 1.399805
47 C 11.882777 15.895945 2.580701
48 C 13.079103 16.525844 1.926839
49 C 7.755505 13.637405 4.867092
50 C 6.561147 12.971906 5.494867
51 C 6.018615 11.813163 4.932724
52 H 6.451410 11.384991 4.032312
53 C 6.873355 18.305274 1.846233
54 H 7.191836 18.686701 2.812885
55 C 6.890934 16.575863 0.154899
56 H 7.224179 15.604167 -0.200264
57 C 5.995741 13.513665 6.653059
58 H 6.409389 14.414687 7.098466
59 C 12.767705 12.893823 7.271581
60 H 12.449867 13.861798 7.650176
61 C 13.620813 15.959872 0.769576
62 H 13.187385 15.058351 0.344389
63 C 13.645319 17.685431 2.464754
64 H 13.232314 18.133811 3.364595
65 C 12.748494 11.197173 5.547402
66 H 12.414616 10.839175 4.576965
67 C 4.347796 11.736482 6.684887
68 H 3.489619 11.258567 7.147018
69 C 15.292430 17.710992 0.686696
70 H 16.150598 18.171237 0.206950
71 C 5.604479 18.597737 -0.198159
72 H 4.943598 19.197022 -0.816648
73 C 14.035747 10.849736 7.569742
74 H 14.696619 10.232782 8.170616
75 H 2.973148 13.313897 9.768916
76 H 16.669301 20.799213 2.253939
77 H 4.547349 21.908744 1.146773
78 H 15.095100 12.204366 10.876082
79 H 15.043633 7.555275 6.138175
80 H 16.600875 16.057533 -2.391085
81 H 3.037095 8.654242 5.041551
82 H 4.594337 17.156500 -3.487709
83 C 9.822079 17.139578 6.029461
84 C 10.967996 17.092016 6.998161
85 C 12.352396 17.355571 6.420687
86 H 9.818592 18.046182 5.412527
87 H 8.855589 16.981206 6.518062

88 H 10.961638 16.143530 7.549828
89 H 12.359074 18.263631 5.805152
90 H 12.678352 16.523231 5.790189
91 H 13.080229 17.481394 7.228861
92 H 10.740902 17.870530 7.748542
93 C 9.061625 14.344811 8.537823
94 O 9.368655 13.246085 8.534904

(3b) CH_3CHCH_3+ CO
E = -3788.6690519 Ha

ATOM X Y Z
1 Cu 9.779372 13.862555 2.623676
2 Rh 9.804313 15.634846 4.390004
3 O 4.998016 9.275002 3.965585
4 O 5.758669 20.729823 2.803755
5 O 6.104064 16.064049 -2.689321
6 O 5.128244 14.363093 9.081507
7 O 13.337783 13.610584 9.757296
8 O 15.175309 14.619621 -1.469758
9 O 14.653733 20.107018 3.188919
10 O 13.557673 8.579573 4.589567
11 O 11.014319 12.827034 3.841169
12 O 3.670208 12.629249 9.145447
13 O 16.298048 19.996082 1.635485
14 O 8.537876 15.095054 1.607924
15 O 11.366051 14.791278 1.819464
16 O 4.739329 21.129960 0.819427
17 O 14.493878 11.676510 10.000243
18 O 8.214936 13.087165 3.622175
19 O 8.212569 14.670020 5.264627
20 O 14.636319 8.333922 6.568301
21 O 4.913235 17.990097 -2.808364
22 O 11.408774 16.444538 3.390322
23 O 8.532477 16.720579 3.207104
24 O 16.655844 16.336928 -1.440346
25 O 3.605931 9.227752 5.754091
26 O 11.071250 14.427043 5.464445
27 C 4.602940 9.779887 5.000988
28 C 5.127843 11.042894 5.586781
29 C 5.505465 20.380143 1.664493
30 C 5.976154 19.114882 1.039392
31 C 5.726802 17.098228 -2.168377
32 C 6.085173 17.539079 -0.794061
33 C 4.682551 13.347290 8.577559
34 C 5.161914 12.750349 7.302162
35 C 13.709222 12.544928 9.297551
36 C 13.375985 12.042187 7.938562
37 C 15.546048 15.677666 -0.993599
38 C 14.867574 16.395019 0.119419
39 C 15.180170 19.521500 2.259614
40 C 14.699436 18.238434 1.679790
41 C 13.860656 9.025529 5.681823
42 C 13.442305 10.353477 6.204970
43 C 11.373460 13.284423 4.972819
44 C 12.226212 12.414774 5.839293
45 C 8.185466 16.222878 2.081292
46 C 7.277162 17.082805 1.262921
47 C 11.849410 15.841778 2.352490
48 C 13.063287 16.452715 1.731018
49 C 7.786264 13.600167 4.705687
50 C 6.679182 12.894075 5.419406
51 C 6.152938 11.706995 4.906538
52 H 6.538607 11.293226 3.978735
53 C 6.804957 18.284928 1.797219
54 H 7.081752 18.577694 2.806647
55 C 6.911386 16.707893 -0.030403
56 H 7.267844 15.771176 -0.450641
57 C 6.185376 13.410945 6.619269
58 H 6.597804 14.328384 7.028781
59 C 12.588461 12.850847 7.116223
60 H 12.250205 13.818104 7.477952
61 C 13.716933 15.822151 0.671045
62 H 13.340781 14.882326 0.275658
63 C 13.557031 17.658365 2.235431
64 H 13.058305 18.144124 3.070119
65 C 12.649422 11.163834 5.386716
66 H 12.363593 10.815212 4.397678
67 C 4.631744 11.563208 6.786514
68 H 3.833641 11.049439 7.312397
69 C 15.358815 17.603835 0.622404
70 H 16.252049 18.046631 0.194384
71 C 5.618705 18.745479 -0.261372
72 H 4.977465 19.389162 -0.854591
73 C 13.811372 10.794626 7.479940

74 H 14.425173 10.165170 8.115988
75 H 3.438126 13.111320 9.964113
76 H 16.517427 20.829789 2.097370
77 H 4.488725 21.923906 1.332792
78 H 14.643898 12.105672 10.866162
79 H 14.850443 7.490284 6.122455
80 H 17.014874 15.780858 -2.160092
81 H 3.340299 8.416737 5.276452
82 H 4.741748 17.600180 -3.688568
83 C 8.585324 17.826818 5.943635
84 C 9.826151 16.981326 5.981549
85 C 11.120923 17.742308 5.983634
86 H 8.609112 18.551217 5.123427
87 H 7.678970 17.221017 5.857887
88 H 9.784942 16.253245 6.797736
89 H 11.190170 18.432797 5.136912
90 H 11.986716 17.074968 5.970269
91 H 11.169618 18.338256 6.908361
92 H 8.523224 18.385892 6.889903
93 C 8.996731 15.438646 9.021598
94 O 9.004122 14.301353 9.105033

TS-2a
E = -3788.6307232 Ha
Imaginary Frequency = -257.81 cm^{-1}

ATOM X Y Z
1 Cu 9.810314 13.976849 2.966282
2 Rh 9.908487 15.908908 4.750145
3 O 4.828605 9.449493 3.876568
4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.122605 12.986968 4.055480
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.524013 15.098095 1.964646
15 O 11.326463 14.896493 1.929054
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.315950 12.978018 3.885087
19 O 7.967925 14.812508 5.162660
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.566184 16.337855 3.667890
23 O 8.699317 16.924558 3.333267
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.097358 14.468941 5.795723
27 C 4.375664 9.962471 4.883679
28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916
40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.442600 13.370030 5.222907
44 C 12.331441 12.443747 6.021900
45 C 8.253787 16.291228 2.305250
46 C 7.308809 17.054003 1.399805
47 C 11.892032 15.849155 2.532682
48 C 13.079103 16.525844 1.926839
49 C 7.705835 13.627852 4.793480
50 C 6.561147 12.971906 5.494867
51 C 6.018615 11.813163 4.932724
52 H 6.451410 11.384991 4.032312
53 C 6.873355 18.305274 1.846233
54 H 7.191836 18.686701 2.812885
55 C 6.890934 16.575863 0.154899
56 H 7.224179 15.604167 -0.200264
57 C 5.995741 13.513665 6.653059
58 H 6.409389 14.414687 7.098466

59 C 12.767705 12.893823 7.271581
60 H 12.449867 13.861798 7.650176
61 C 13.620813 15.959872 0.769576
62 H 13.187385 15.058351 0.344389
63 C 13.645319 17.685431 2.464754
64 H 13.232314 18.133811 3.364595
65 C 12.748494 11.197173 5.547402
66 H 12.414616 10.839175 4.576965
67 C 4.347796 11.736482 6.684887
68 H 3.489619 11.258567 7.147018
69 C 15.292430 17.710992 0.686696
70 H 16.150598 18.171237 0.206950
71 C 5.604479 18.597737 -0.198159
72 H 4.943598 19.197022 -0.816648
73 C 14.035747 10.849736 7.569742
74 H 14.696619 10.232782 8.170616
75 H 2.973148 13.313897 9.768916
76 H 16.669301 20.799213 2.253939
77 H 4.547349 21.908744 1.146773
78 H 15.095100 12.204366 10.876082
79 H 15.043633 7.555275 6.138175
80 H 16.600875 16.057533 -2.391085
81 H 3.037095 8.654242 5.041551
82 H 4.594337 17.156500 -3.487709
83 C 10.558683 17.791746 5.473000
84 C 11.608376 17.757808 6.548244
85 C 12.993475 17.271604 6.146931
86 H 10.906492 18.261617 4.551012
87 H 9.624988 18.248577 5.806611
88 H 11.262421 17.193042 7.422486
89 H 13.390563 17.859010 5.311731
90 H 12.971549 16.221111 5.846908
91 H 13.678531 17.376455 6.993062
92 H 11.691491 18.804463 6.890277
93 C 8.953182 16.062855 6.939648
94 O 8.927940 15.613552 7.991509

TS-2b
E = -3788.6463179 Ha
Imaginary Frequency = -220.24 cm^{-1}
ATOM X Y Z
1 Cu 9.601981 13.825926 3.043582
2 Rh 9.731625 15.883107 4.716833
3 O 5.025881 8.918361 4.168600
4 O 6.477435 21.102801 2.189268
5 O 4.920312 15.202791 -1.665485
6 O 4.978841 14.032476 9.260445
7 O 14.710961 14.877963 9.207820
8 O 14.455468 14.544019 -1.842985
9 O 14.213839 20.023194 2.846395
10 O 13.765861 9.013041 5.109718
11 O 10.977848 13.073039 4.327098
12 O 3.581391 12.249558 9.326362
13 O 15.737922 19.940482 1.169819
14 O 8.287696 14.991673 2.070752
15 O 11.092914 14.521398 1.955452
16 O 5.105826 21.166062 0.386074
17 O 15.916961 12.983524 9.510612
18 O 8.218398 12.758158 3.887968
19 O 8.089223 14.417379 5.421801
20 O 15.308761 9.098041 6.768036
21 O 4.065111 17.239848 -2.170809
22 O 11.132866 16.337761 3.326631
23 O 8.278462 16.737060 3.550643
24 O 15.889252 16.295642 -1.954646
25 O 3.623371 8.843675 5.947393
26 O 11.180571 14.842032 5.758683
27 C 4.617299 9.414155 5.203044
28 C 5.119451 10.681843 5.797848
29 C 5.922895 20.524074 1.272059
30 C 6.048978 19.071205 0.983878
31 C 4.834258 16.393281 -1.424567
32 C 5.532616 17.089359 -0.310034
33 C 4.578604 12.994467 8.763816
34 C 5.097249 12.397540 7.504723
35 C 14.957887 13.728808 8.886857
36 C 14.271435 12.983243 7.798018
37 C 14.853274 15.603990 -1.395660
38 C 14.286701 16.291251 -0.204034
39 C 14.691338 19.441019 1.888522
40 C 14.213167 18.131867 1.369052
41 C 14.302070 9.629388 6.012427
42 C 13.955243 11.017309 6.420355
43 C 11.485485 13.677408 5.322505

44 C 12.573001 12.974699 6.072281
45 C 7.932915 16.145613 2.471262
46 C 7.026214 16.938065 1.585849
47 C 11.540778 15.641179 2.332339
48 C 12.665251 16.282645 1.589114
49 C 7.732741 13.303318 4.936736
50 C 6.641331 12.559569 5.644431
51 C 6.144243 11.360123 5.130772
52 H 6.547747 10.950052 4.208942
53 C 6.868156 18.306185 1.817830
54 H 7.392573 18.781993 2.643881
55 C 6.363372 16.329357 0.519199
56 H 6.490025 15.266560 0.329038
57 C 6.118006 13.073413 6.832180
58 H 6.501345 14.005375 7.237299
59 C 13.243940 13.630474 7.106833
60 H 12.975035 14.649137 7.373301
61 C 13.228042 15.671216 0.468427
62 H 12.850640 14.715642 0.113293
63 C 13.158857 17.510405 2.038759
64 H 12.716423 17.985186 2.912793
65 C 12.929940 11.669227 5.729192
66 H 12.416764 11.158071 4.918929
67 C 4.596681 11.198455 6.987709
68 H 3.799947 10.673819 7.504694
69 C 14.781873 17.518861 0.247353
70 H 15.605667 17.996816 -0.272823
71 C 5.376433 18.460023 -0.079708
72 H 4.735621 19.050750 -0.726287
73 C 14.625512 11.673580 7.457258
74 H 15.424766 11.169988 7.991089
75 H 3.322549 12.734252 10.135317
76 H 15.961931 20.793127 1.593243
77 H 5.097281 22.101017 0.672644
78 H 16.294586 13.569582 10.196390
79 H 15.449367 8.197125 6.414541
80 H 16.176252 15.758800 -2.720121
81 H 3.374125 8.031134 5.463666
82 H 3.660432 16.679720 -2.862805
83 C 10.163017 18.863983 4.231653
84 C 10.346939 17.828888 5.312404
85 C 11.757430 17.776996 5.833622
86 H 10.868828 18.716175 3.407852
87 H 9.145466 18.891248 3.835203
88 H 9.610751 17.962306 6.109838
89 H 12.460571 17.539902 5.026655
90 H 11.888974 17.054142 6.641905
91 H 12.025426 18.774786 6.212619
92 H 10.383595 19.846204 4.675742
93 C 8.936182 15.892535 7.375841
94 O 8.946930 15.358751 8.383404

(4a) $CH_3CH_2CH_2CO$

E = -3788.6780047 Ha

ATOM X Y Z
1 Cu 9.791101 13.662870 2.777452
2 Rh 9.792063 15.443165 4.506464
3 O 4.419645 8.852055 3.704412
4 O 5.731472 21.279328 2.765097
5 O 5.767746 15.664711 -2.862734
6 O 4.514723 14.509054 9.288723
7 O 13.907937 13.669571 10.153051
8 O 15.063530 14.816513 -1.986709
9 O 15.103384 20.437459 3.634145
10 O 13.965626 8.003744 4.578460
11 O 11.164293 12.532337 4.054459
12 O 2.698445 12.627473 9.373559
13 O 16.878490 20.484862 1.714578
14 O 8.430882 15.109271 1.664387
15 O 11.584376 14.824961 1.925980
16 O 4.387522 21.630438 0.549993
17 O 15.302869 11.488639 10.526363
18 O 8.051917 12.794403 3.769142
19 O 8.034844 14.401857 5.358934
20 O 15.330449 7.692459 6.787551
21 O 4.396860 17.864267 -3.215364
22 O 11.511846 16.397313 3.542569
23 O 8.462175 16.684259 3.284139
24 O 16.863113 16.714033 -2.046367
25 O 2.650868 8.833793 5.631030
26 O 11.167389 14.135854 5.646635
27 C 3.844579 9.468232 4.957049
28 C 4.472656 10.742590 5.552276
29 C 5.286586 20.777585 1.412610

30 C 5.749425 19.396986 0.910089
31 C 5.307507 17.013249 -2.363627
32 C 5.762656 17.518064 -0.982416
33 C 3.896926 13.259360 8.707229
34 C 4.493125 12.631618 7.434519
35 C 14.380033 12.319468 9.668362
36 C 13.918376 11.792212 8.297799
37 C 15.670770 16.063116 -1.388581
38 C 15.068034 16.674296 -0.110972
39 C 15.693160 19.830732 2.384162
40 C 15.078330 18.553562 1.781202
41 C 14.412882 8.523989 5.922887
42 C 13.932901 9.901019 6.417792
43 C 11.535250 12.997038 5.179531
44 C 12.505904 12.127197 6.060552
45 C 8.085134 16.235127 2.136346
46 C 7.138831 17.146967 1.271520
47 C 12.019185 15.878482 2.478886
48 C 13.253487 16.607306 1.841210
49 C 7.568580 13.337773 4.815352
50 C 6.319896 12.666814 5.492528
51 C 5.697220 11.396906 4.878689
52 H 6.141757 10.941442 3.933165
53 C 6.667382 18.521644 1.785158
54 H 6.999776 18.891846 2.810598
55 C 6.685881 16.646863 -0.112015
56 H 7.031733 15.628586 -0.490640
57 C 5.716629 13.279778 6.768170
58 H 6.178725 14.218767 7.220677
59 C 12.972292 12.641245 7.433449
60 H 12.614397 13.655995 7.811219
61 C 13.851633 16.008856 0.555606
62 H 13.395159 15.069521 0.098466
63 C 13.864487 17.883030 2.454205
64 H 13.418548 18.330284 3.402715
65 C 12.989412 10.756741 5.546543
66 H 12.646828 10.374233 4.529344
67 C 3.870920 11.361157 6.828709
68 H 2.965442 10.877854 7.324017
69 C 15.676724 17.950853 0.496815
70 H 16.569293 18.450971 -0.004635
71 C 5.295372 18.893190 -0.472462
72 H 4.614052 19.539388 -1.119155
73 C 14.398269 10.420274 7.791330
74 H 15.097650 9.788916 8.432488
75 H 2.424846 13.216247 10.273901
76 H 17.170545 21.392638 2.282701
77 H 4.154200 22.577152 1.080463
78 H 15.509708 12.025887 11.475347
79 H 15.558490 6.735219 6.274066
80 H 17.171363 16.115699 -2.928778
81 H 2.347482 7.923437 5.073167
82 H 4.127168 17.308151 -4.137363
83 C 10.314420 18.140343 5.652434
84 C 11.542258 18.520208 6.491525
85 C 12.750128 17.625078 6.253638
86 H 10.538701 18.198584 4.586286
87 H 9.479798 18.820042 5.871567
88 H 11.266299 18.511276 7.552180
89 H 13.050055 17.645183 5.201266
90 H 12.533853 16.581513 6.513081
91 H 13.595397 17.961670 6.861610
92 H 11.791426 19.554031 6.223753
93 O 9.490649 16.379035 7.110976
94 C 9.819888 16.756741 6.028511

(4b) CH_3CHCH_3CO
E = -3788.7122717 Ha
ATOM X Y Z
1 Cu 9.813787 13.771323 2.830256
2 Rh 9.813021 15.558945 4.604209
3 O 4.827363 9.362181 3.891782
4 O 6.702251 21.018371 2.371328
5 O 5.852283 15.658835 -2.384083
6 O 4.902875 14.338706 9.117477
7 O 13.581846 13.541651 9.882478
8 O 14.891164 14.925876 -1.620596
9 O 14.319807 20.228511 3.240919
10 O 13.554440 8.518567 4.701229
11 O 11.040473 12.771679 4.046185
12 O 3.471046 12.582165 9.136523
13 O 15.850899 20.295240 1.570753
14 O 8.612086 14.960239 1.754672
15 O 11.392778 14.696342 1.981607

16 O 5.440157 21.259416 0.504144
17 O 14.664614 11.562741 10.106121
18 O 8.233300 13.017555 3.800231
19 O 8.180919 14.603431 5.440130
20 O 14.670854 8.239635 6.653605
21 O 4.891821 17.691761 -2.671920
22 O 11.425931 16.322015 3.579886
23 O 8.543608 16.587362 3.353040
24 O 16.224975 16.758734 -1.674469
25 O 3.399813 9.297485 5.650644
26 O 11.082935 14.348869 5.694960
27 C 4.429006 9.843382 4.937295
28 C 4.983439 11.064386 5.579541
29 C 6.229107 20.541349 1.354826
30 C 6.438586 19.142182 0.897328
31 C 5.645776 16.788427 -1.978765
32 C 6.168304 17.341921 -0.699947
33 C 4.490453 13.316844 8.599545
34 C 5.013804 12.729795 7.336777
35 C 13.892300 12.457875 9.421714
36 C 13.490840 11.956427 8.080271
37 C 15.222452 15.997100 -1.145824
38 C 14.602334 16.623092 0.053510
39 C 14.828609 19.713027 2.260761
40 C 14.421790 18.403678 1.684616
41 C 13.884453 8.949444 5.791631
42 C 13.491023 10.275804 6.337862
43 C 11.398683 13.220320 5.184129
44 C 12.273713 12.345457 6.023313
45 C 8.262340 16.096428 2.206244
46 C 7.443016 16.980255 1.324283
47 C 11.839479 15.762967 2.505623
48 C 12.954440 16.481461 1.819259
49 C 7.760427 13.545978 4.860412
50 C 6.601705 12.863863 5.513809
51 C 6.051037 11.711435 4.949854
52 H 6.450884 11.309666 4.022784
53 C 7.201377 18.300895 1.710572
54 H 7.614580 18.680164 2.642222
55 C 6.937298 16.504488 0.113789
56 H 7.135820 15.482538 -0.198370
57 C 6.080516 13.374520 6.705475
58 H 6.508578 14.270266 7.147733
59 C 12.680092 12.774342 7.289135
60 H 12.361382 13.742974 7.664970
61 C 13.560435 15.938167 0.685931
62 H 13.227040 14.981284 0.292866
63 C 13.384579 17.714337 2.316291
64 H 12.910850 18.144801 3.196155
65 C 12.681256 11.097008 5.548163
66 H 12.366704 10.756121 4.565295
67 C 4.467171 11.570705 6.776432
68 H 3.639466 11.068799 7.266765
69 C 15.035955 17.855992 0.552898
70 H 15.846255 18.385168 0.061949
71 C 5.915162 18.660898 -0.307255
72 H 5.316560 19.309324 -0.938848
73 C 13.898974 10.705975 7.604316
74 H 14.526088 10.068961 8.219428
75 H 3.209008 13.061847 9.947487
76 H 16.032138 21.137759 2.033134
77 H 5.373592 22.150936 0.900562
78 H 14.864622 11.994167 10.960614
79 H 14.862293 7.397423 6.194904
80 H 16.554340 16.256566 -2.446344
81 H 3.120061 8.511452 5.140578
82 H 4.606110 17.222850 -3.481206
83 C 9.976052 19.014207 4.325484
84 C 10.369233 18.421010 5.671823
85 C 11.891790 18.437588 5.856087
86 H 10.452890 18.483610 3.498456
87 H 8.895217 19.014450 4.167124
88 H 9.929325 19.040224 6.464002
89 H 12.381395 17.821100 5.098988
90 H 12.183875 18.089689 6.850256
91 H 12.233541 19.469094 5.726624
92 H 10.325594 20.051414 4.314871
93 C 9.846950 17.016150 6.007775
94 O 9.501164 16.679252 7.103001

(5a) $CH_3CH_2CH_2CO + H_2$
E = -3789.8876808 Ha
ATOM X Y Z
1 Cu 13.173318 18.885315 5.737555

2	Rh	13.159579	20.652642	7.492243
3	O	8.179418	14.472021	6.780144
4	O	9.264318	25.891709	5.550213
5	O	9.325069	20.727060	0.505239
6	O	8.102052	19.545954	11.916121
7	O	17.079976	18.724198	12.736125
8	O	18.160004	19.918392	1.312183
9	O	18.242241	25.069953	6.370217
10	O	17.014354	13.663353	7.587088
11	O	14.395910	17.867230	6.961207
12	O	6.606580	17.844743	11.875328
13	O	19.736880	25.023200	4.668428
14	O	11.955970	20.120578	4.717105
15	O	14.771019	19.844995	4.962289
16	O	8.116175	26.086851	3.607044
17	O	18.227286	16.781091	12.936712
18	O	11.584901	18.132635	6.709724
19	O	11.542255	19.706997	8.356089
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.772828	21.505838	6.516936
23	O	11.881237	21.756280	6.302035
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.449326	19.459949	8.586009
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605
32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.775541	18.326293	8.091692
44	C	15.682254	17.466275	8.925476
45	C	11.567661	21.250916	5.170552
46	C	10.659622	22.076531	4.303381
47	C	15.234742	20.912284	5.481143
48	C	16.429917	21.548372	4.830414
49	C	11.103022	18.659342	7.770075
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887
53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	C	13.060783	23.509396	8.322098
84	C	14.101892	24.478979	8.880691
85	C	15.469342	24.270836	8.245306

86	H	13.103638	23.498726	7.231603
87	H	12.036613	23.792114	8.601842
88	H	14.153907	24.388320	9.970288
89	H	15.404238	24.416554	7.162001
90	H	15.842702	23.254124	8.409650
91	H	16.209522	24.976794	8.628313
92	H	13.750269	25.490653	8.648872
93	O	13.338425	21.813353	10.033462
94	C	13.209583	22.107220	8.881108
95	H	10.194182	22.729466	8.920190
96	H	10.371313	22.196436	8.421999

(5b) $CH_3CHCH_3CO + H_2$

E = -3788.6704895 Ha

ATOM	X	Y	Z
1	Cu	8.164977	14.422678	2.547865
2	Rh	8.164375	16.201128	4.283453
3	O	2.879644	9.633697	3.528402
4	O	4.071087	21.954374	2.461517
5	O	4.110114	16.293882	-3.119870
6	O	2.826323	15.234219	9.169201
7	O	12.296071	14.380541	10.030769
8	O	13.450273	15.440963	-2.258527
9	O	13.502409	21.091753	3.332760
10	O	12.260822	8.790594	4.378112
11	O	9.530526	13.308672	3.898843
12	O	1.048302	13.316950	9.205459
13	O	15.279225	21.124458	1.412820
14	O	6.817227	15.803064	1.380777
15	O	9.950334	15.502986	1.657448
16	O	2.708847	22.278984	0.250115
17	O	13.673344	12.179214	10.350820
18	O	6.407547	13.588337	3.612405
19	O	6.409978	15.198929	5.197893
20	O	13.648308	8.439185	6.569090
21	O	2.734915	18.489198	-3.482112
22	O	9.894899	17.080150	3.270525
23	O	6.789912	17.351903	3.024181
24	O	15.244880	17.343217	-2.327205
25	O	1.084720	9.568170	5.431329
26	O	9.533357	14.927680	5.474710
27	C	2.278151	10.226143	4.780009
28	C	2.879833	11.504104	5.392464
29	C	3.622247	21.441125	1.114361
30	C	4.094814	20.061145	0.620885
31	C	3.650133	17.645164	-2.627524
32	C	4.109815	18.162050	-1.251415
33	C	2.241489	13.982010	8.561596
34	C	2.860137	13.382835	7.284860
35	C	12.750293	13.035346	9.516490
36	C	12.271139	12.534853	8.140973
37	C	14.051881	16.693365	-1.667412
38	C	13.449693	17.308488	-0.390471
39	C	14.087146	20.481473	2.081428
40	C	13.467958	19.203900	1.484814
41	C	12.726034	9.288007	5.726032
42	C	12.259356	10.661089	6.243548
43	C	9.894737	13.779696	5.020290
44	C	10.852163	12.903456	5.911954
45	C	6.444310	16.914645	1.863469
46	C	5.499452	17.824161	1.000552
47	C	10.395637	16.550695	2.207501
48	C	11.634163	17.266514	1.564072
49	C	5.936466	14.132996	4.660901
50	C	4.695556	13.458118	5.350067
51	C	4.097116	12.179677	4.732229
52	H	4.554812	11.733482	3.788164
53	C	5.025659	19.203237	1.498552
54	H	5.364821	19.589157	2.516349
55	C	5.041640	17.303808	-0.374898
56	H	5.394305	16.285073	-0.745472
57	C	4.076626	14.058716	6.626059
58	H	4.519914	15.004161	7.083415
59	C	11.330196	13.405258	7.287531
60	H	10.986304	14.420950	7.674432
61	C	12.232987	16.648796	0.286462
62	H	11.776037	15.703807	-0.158218
63	C	12.251564	18.545148	2.162225
64	H	11.808243	19.003580	3.107206
65	C	11.318316	11.531379	5.388623
66	H	10.967330	11.160292	4.369390
67	C	2.262045	12.105803	6.667707
68	H	1.361066	11.605280	7.154941
69	C	14.066444	18.585102	0.208771
70	H	14.967534	19.071710	-0.292213

71	C	3.636620	19.539781	-0.753042
72	H	2.947544	20.174625	-1.402451
73	C	12.735371	11.163302	7.618768
74	H	13.431425	10.518832	8.251109
75	H	0.742425	13.891941	10.104330
76	H	15.585629	22.024213	1.986109
77	H	2.469284	23.228468	0.772808
78	H	13.895892	12.697186	11.306978
79	H	13.861078	7.485631	6.042294
80	H	15.551840	16.744711	-3.210155
81	H	0.779068	8.682871	4.835649
82	H	2.490260	17.941640	-4.416126
83	C	8.076745	19.722101	4.052353
84	C	8.552335	19.133224	5.369084
85	C	10.071781	19.309565	5.531949
86	H	8.561286	19.244241	3.197809
87	H	6.992764	19.641809	3.938874
88	H	8.064280	19.677447	6.188400
89	H	10.606501	18.792235	4.732251
90	H	10.423018	18.945100	6.500713
91	H	10.284845	20.379601	5.460050
92	H	8.350774	20.781412	4.060700
93	C	8.194448	17.679956	5.688041
94	O	7.955773	17.261430	6.782143
95	H	5.379328	18.767435	5.435701
96	H	5.575874	18.512135	4.756767

TS-3a

E = -3789.8202588Ha

Imaginary Frequency = -840.13 cm^{-1}

ATOM	X	Y	Z
1	Cu	13.173318	18.885315	5.737555
2	Rh	13.159579	20.652642	7.492243
3	O	8.179418	14.472021	6.780144
4	O	9.264318	25.891709	5.550213
5	O	9.325069	20.727060	0.505239
6	O	8.102052	19.545954	11.916121
7	O	17.079976	18.724198	12.736125
8	O	18.160004	19.918392	1.312183
9	O	18.242241	25.069953	6.370217
10	O	17.014354	13.663353	7.587088
11	O	14.395910	17.867230	6.961207
12	O	6.606580	17.844743	11.875328
13	O	19.736880	25.023200	4.668428
14	O	11.955970	20.120578	4.717105
15	O	14.771019	19.844995	4.962289
16	O	8.116175	26.086851	3.607044
17	O	18.227286	16.781091	12.936712
18	O	11.584901	18.132635	6.709724
19	O	11.542255	19.706997	8.356089
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.772828	21.505838	6.516936
23	O	11.881237	21.756280	6.302035
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.449326	19.459949	8.586009
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605
32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.775541	18.326293	8.091692
44	C	15.682254	17.466275	8.925476
45	C	11.567661	21.250916	5.170552
46	C	10.659622	22.076531	4.303381
47	C	15.234742	20.912284	5.481143
48	C	16.429917	21.548372	4.830414
49	C	11.103022	18.659342	7.770075
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887

53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	C	16.108002	22.713591	8.900267
84	C	17.566393	22.217052	8.893097
85	C	17.678984	20.748043	8.522992
86	H	15.667004	22.576382	7.903378
87	H	16.039119	23.783179	9.143837
88	H	18.037879	22.417321	9.860053
89	H	17.189593	20.554085	7.564147
90	H	17.207930	20.106461	9.275336
91	H	18.729377	20.456691	8.443084
92	H	18.057530	22.842704	8.138423
93	O	15.214011	21.452610	10.883414
94	C	15.253901	22.024207	9.867062
95	H	12.201126	22.411954	8.889060
96	H	12.940411	22.323995	9.058672

TS-3b

E = -3788.6574151 Ha

Imaginary Frequency = -2661.56 cm^{-1}

ATOM	X	Y	Z
1	Cu	8.164977	14.422678	2.547865
2	Rh	8.164375	16.201128	4.283453
3	O	2.879644	9.633697	3.528402
4	O	4.071087	21.954374	2.461517
5	O	4.110114	16.293882	-3.119870
6	O	2.826323	15.234219	9.169201
7	O	12.296071	14.380541	10.030769
8	O	13.450273	15.440963	-2.258527
9	O	13.502409	21.091753	3.332760
10	O	12.260822	8.790594	4.378112
11	O	9.530526	13.308672	3.898843
12	O	1.048302	13.316950	9.205459
13	O	15.279225	21.124458	1.412820
14	O	6.817227	15.803064	1.380777
15	O	9.950334	15.502986	1.657448
16	O	2.708847	22.278984	0.250115
17	O	13.673344	12.179214	10.350820
18	O	6.407547	13.588337	3.612405
19	O	6.409978	15.198929	5.197893
20	O	13.648308	8.439185	6.569090
21	O	2.734915	18.489198	-3.482112
22	O	9.894899	17.080150	3.270525
23	O	6.789912	17.351903	3.024181
24	O	15.244880	17.343217	-2.327205
25	O	1.084720	9.568170	5.431329
26	O	9.533357	14.927680	5.474710
27	C	2.278151	10.226143	4.780009
28	C	2.879833	11.504104	5.392464
29	C	3.622247	21.441125	1.114361
30	C	4.094814	20.061145	0.620885
31	C	3.650133	17.645164	-2.627524
32	C	4.109815	18.162050	-1.251415
33	C	2.241489	13.982010	8.561596

34 C 2.860137 13.382835 7.284860
35 C 12.750293 13.035346 9.516490
36 C 12.271139 12.534853 8.140973
37 C 14.051881 16.693365 -1.667412
38 C 13.449693 17.308488 -0.390471
39 C 14.087146 20.481473 2.081428
40 C 13.467958 19.203900 1.484814
41 C 12.726034 9.288007 5.726032
42 C 12.259356 10.661089 6.243548
43 C 9.894737 13.779696 5.020290
44 C 10.852163 12.903456 5.911954
45 C 6.444310 16.914645 1.863469
46 C 5.499452 17.824161 1.000552
47 C 10.395637 16.550695 2.207501
48 C 11.634163 17.266514 1.564072
49 C 5.936466 14.132996 4.660901
50 C 4.695556 13.458118 5.350067
51 C 4.097116 12.179677 4.732229
52 H 4.554812 11.733482 3.788164
53 C 5.025659 19.203237 1.498552
54 H 5.364821 19.589157 2.516349
55 C 5.041640 17.303808 -0.374898
56 H 5.394305 16.285073 -0.745472
57 C 4.076626 14.058716 6.626059
58 H 4.519914 15.004161 7.083415
59 C 11.330196 13.405258 7.287531
60 H 10.986304 14.420950 7.674432
61 C 12.232987 16.648796 0.286462
62 H 11.776037 15.703807 -0.158218
63 C 12.251564 18.545148 2.162225
64 H 11.808243 19.003580 3.107206
65 C 11.318316 11.531379 5.388623
66 H 10.967330 11.160292 4.369390
67 C 2.262045 12.105803 6.667707
68 H 1.361066 11.605280 7.154941
69 C 14.066444 18.585102 0.208771
70 H 14.967534 19.071710 -0.292213
71 C 3.636620 19.539781 -0.753042
72 H 2.947544 20.174625 -1.402451
73 C 12.735371 11.163302 7.618768
74 H 13.431425 10.518832 8.251109
75 H 0.742425 13.891941 10.104330
76 H 15.585629 22.024213 1.986109
77 H 2.469284 23.228468 0.772808
78 H 13.895892 12.697186 11.306978
79 H 13.861078 7.485631 6.042294
80 H 15.551840 16.744711 -3.210155
81 H 0.779068 8.682871 4.835649
82 H 2.490260 17.941640 -4.416126
83 C 7.893950 20.162145 5.173224
84 C 9.393523 20.430238 5.106837
85 C 9.876159 20.488856 3.651397
86 H 7.669120 19.177114 4.742034
87 H 7.518727 20.183428 6.200651
88 H 9.657058 21.366706 5.610374
89 H 9.704020 19.530622 3.150954
90 H 10.940409 20.739303 3.592692
91 H 9.304938 21.260344 3.125168
92 H 7.355170 20.914226 4.588493
93 C 10.129993 19.304845 5.796191
94 O 11.121648 19.405927 6.484737
95 H 9.665732 18.296884 5.596944
96 H 8.196743 17.363580 5.303226

(6a) n-pro + cat.

E = -3789.8600966 Ha

ATOM X Y Z
1 Cu 13.173318 18.885315 5.737555
2 Rh 13.159579 20.652642 7.492243
3 O 8.179418 14.472021 6.780144
4 O 9.264318 25.891709 5.550213
5 O 9.325069 20.727060 0.505239
6 O 8.102052 19.545954 11.916121
7 O 17.079976 18.724198 12.736125
8 O 18.160004 19.918392 1.312183
9 O 18.242241 25.069953 6.370217
10 O 17.014354 13.663353 7.587088
11 O 14.395910 17.867230 6.961207
12 O 6.606580 17.844743 11.875328
13 O 19.736880 25.023200 4.668428
14 O 11.955970 20.120578 4.717105
15 O 14.771019 19.844995 4.962289
16 O 8.116175 26.086851 3.607044

17	O	18.227286	16.781091	12.936712
18	O	11.584901	18.132635	6.709724
19	O	11.542255	19.706997	8.356089
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.772828	21.505838	6.516936
23	O	11.881237	21.756280	6.302035
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.449326	19.459949	8.586009
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605
32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.775541	18.326293	8.091692
44	C	15.682254	17.466275	8.925476
45	C	11.567661	21.250916	5.170552
46	C	10.659622	22.076531	4.303381
47	C	15.234742	20.912284	5.481143
48	C	16.429917	21.548372	4.830414
49	C	11.103022	18.659342	7.770075
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887
53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	H	13.195740	21.729676	8.598371
84	C	16.242867	22.915846	9.017736
85	C	17.747763	22.719670	8.936362
86	C	18.116030	21.331392	8.423767
87	H	15.764853	22.687749	8.054089
88	H	15.980768	23.966929	9.224452
89	H	18.205185	22.892457	9.917957
90	H	17.638005	21.148104	7.454039
91	H	17.787688	20.551428	9.119252
92	H	19.199250	21.243624	8.290740
93	H	18.134103	23.480911	8.249593
94	O	16.030457	21.482237	10.960454
95	C	15.522348	22.100281	10.046636
96	H	14.408782	22.086570	9.899378

Figure 9:
(1) H+propene

E = -3709.5769929 Ha

ATOM	X	Y	Z
1	Cu	14.167391	18.876345	5.725265
2	Ir	14.168272	20.658679	7.495109
3	O	9.179418	14.472021	6.780144
4	O	10.264318	25.891709	5.550213
5	O	10.325069	20.727060	0.505239
6	O	9.102052	19.545954	11.916121
7	O	18.079976	18.724198	12.736125
8	O	19.160004	19.918392	1.312183
9	O	19.242241	25.069953	6.370217
10	O	18.014354	13.663353	7.587088
11	O	15.415019	17.869045	6.954017
12	O	7.606580	17.844743	11.875328
13	O	20.736880	25.023200	4.668428
14	O	12.924330	20.104626	4.713724
15	O	15.750584	19.870448	4.953031
16	O	9.116175	26.086851	3.607044
17	O	19.227286	16.781091	12.936712
18	O	12.586557	18.100157	6.714838
19	O	12.534861	19.710909	8.330694
20	O	19.193058	13.415094	9.505913
21	O	9.147161	22.645674	0.251626
22	O	15.810209	21.495587	6.553054
23	O	12.907715	21.759748	6.284235
24	O	20.690185	21.589132	1.305915
25	O	7.650033	14.471635	8.451624
26	O	15.434252	19.449799	8.599574
27	C	8.726478	14.984999	7.787255
28	C	9.263642	16.216816	8.429122
29	C	9.938090	25.425276	4.473884
30	C	10.372971	24.099535	3.951886
31	C	9.976333	21.808976	0.941605
32	C	10.390256	22.367923	2.258479
33	C	8.676419	18.536787	11.384250
34	C	9.241030	17.919346	10.151702
35	C	18.405468	17.646280	12.272858
36	C	17.969704	17.120405	10.948941
37	C	19.613670	20.926864	1.821837
38	C	19.077400	21.572782	3.051925
39	C	19.667139	24.534769	5.362492
40	C	19.101645	23.300593	4.749125
41	C	18.363815	14.102886	8.667487
42	C	17.950785	15.421675	9.222567
43	C	15.775831	18.319781	8.088399
44	C	16.682254	17.466275	8.925476
45	C	12.564775	21.242266	5.158415
46	C	11.659622	22.076531	4.303381
47	C	16.242536	20.914280	5.490647
48	C	17.429917	21.548372	4.830414
49	C	12.102885	18.642907	7.760036
50	C	10.911960	17.994434	8.398443
51	C	10.369428	16.835691	7.836300
52	H	10.802223	16.407519	6.935887
53	C	11.224168	23.327802	4.749809
54	H	11.542649	23.709229	5.716460
55	C	11.241747	21.598391	3.058475
56	H	11.574992	20.626695	2.703312
57	C	10.346555	18.536193	9.556635
58	H	10.760203	19.437215	10.002041
59	C	17.118519	17.916351	10.175156
60	H	16.800681	18.884326	10.553752
61	C	17.971627	20.982400	3.673152
62	H	17.538199	20.080879	3.247965
63	C	17.996133	22.707959	5.368330
64	H	17.583127	23.156339	6.268171
65	C	17.099308	16.219700	8.450978
66	H	16.765430	15.861703	7.480541
67	C	8.698610	16.759010	9.588463
68	H	7.840433	16.281095	10.050594
69	C	19.643243	22.733520	3.590272
70	H	20.501412	23.193765	3.110526
71	C	9.955292	23.620265	2.705417
72	H	9.294412	24.219550	2.086928
73	C	18.386561	15.872264	10.473318
74	H	19.047433	15.255310	11.074192
75	H	7.323961	18.336425	12.672492
76	H	21.020114	25.821741	5.157515
77	H	8.898162	26.931272	4.050349
78	H	19.445913	17.226894	13.779658
79	H	19.394446	12.577803	9.041751
80	H	20.951689	21.080061	0.512491
81	H	7.387908	13.676770	7.945126

82 H 8.945151 22.179028 -0.584134
83 H 14.141039 21.741996 8.634610
84 C 13.728488 23.248498 10.021859
85 C 14.984755 22.936902 10.378840
86 C 16.204934 23.502478 9.741569
87 H 12.869040 22.770279 10.481181
88 H 13.533878 23.992235 9.251624
89 H 15.138883 22.167121 11.136086
90 H 16.723813 22.718693 9.174786
91 H 16.910478 23.873048 10.494674
92 H 15.955934 24.315652 9.053162

TS-1a
E = -3709.5601485 Ha
Imaginary Frequency = -968.46 cm^{-1}

ATOM X Y Z
1 Cu 14.167260 18.978454 5.826843
2 Ir 14.182387 20.748481 7.630910
3 O 9.183053 14.470670 6.775152
4 O 10.258017 25.895004 5.537593
5 O 10.330623 20.718546 0.508913
6 O 9.095054 19.541716 11.909226
7 O 18.072532 18.711954 12.726525
8 O 19.143374 19.907975 1.314914
9 O 19.245205 25.077670 6.349441
10 O 18.022171 13.648441 7.583630
11 O 15.428227 17.831887 6.943900
12 O 7.603808 17.834937 11.867893
13 O 20.743631 25.013398 4.649441
14 O 12.909563 20.117901 4.708781
15 O 15.751169 19.894161 4.969052
16 O 9.111331 26.082496 3.590768
17 O 19.225814 16.771410 12.924302
18 O 12.583730 18.109168 6.730804
19 O 12.507848 19.717389 8.365909
20 O 19.198244 13.403531 9.503672
21 O 9.152899 22.635282 0.250805
22 O 15.817594 21.525020 6.578153
23 O 12.911915 21.750098 6.310422
24 O 20.678669 21.571885 1.302881
25 O 7.652289 14.468238 8.443877
26 O 15.482198 19.422193 8.563106
27 C 8.730655 14.983206 7.782866
28 C 9.267005 16.209806 8.426086
29 C 9.933185 25.423451 4.458870
30 C 10.367994 24.101016 3.945666
31 C 9.982590 21.801007 0.944528
32 C 10.392395 22.361941 2.259935
33 C 8.673177 18.527456 11.375621
34 C 9.237324 17.912764 10.148745
35 C 18.404918 17.634287 12.256057
36 C 17.973836 17.110591 10.936540
37 C 19.599702 20.915585 1.823327
38 C 19.068973 21.564983 3.050942
39 C 19.671858 24.531170 5.344116
40 C 19.101515 23.302299 4.738068
41 C 18.369366 14.089811 8.664087
42 C 17.958124 15.407607 9.214573
43 C 15.797373 18.281541 8.059978
44 C 16.711018 17.450682 8.906549
45 C 12.567163 21.239672 5.170867
46 C 11.657753 22.080155 4.313314
47 C 16.232804 20.930427 5.507712
48 C 17.423721 21.556511 4.834095
49 C 12.100346 18.647904 7.769091
50 C 10.900792 17.995064 8.392468
51 C 10.368381 16.831309 7.835164
52 H 10.807835 16.407702 6.935940
53 C 11.217111 23.332678 4.748804
54 H 11.533708 23.710874 5.715196
55 C 11.241170 21.599693 3.066133
56 H 11.576851 20.626834 2.718735
57 C 10.337174 18.531798 9.552882
58 H 10.753434 19.432533 9.989452
59 C 17.135186 17.906330 10.158031
60 H 16.814512 18.873834 10.521688
61 C 17.964126 20.982865 3.677784
62 H 17.522420 20.084924 3.257544
63 C 17.998115 22.714411 5.362976
64 H 17.580451 23.165044 6.256903
65 C 17.115264 16.201906 8.440881
66 H 16.775931 15.848556 7.468466
67 C 8.699893 16.749982 9.584668
68 H 7.840455 16.270085 10.046568

69 C 19.639674 22.726824 3.581760
70 H 20.499863 23.182189 3.096191
71 C 9.954003 23.615153 2.700687
72 H 9.293772 24.212694 2.076484
73 C 18.393983 15.862672 10.462399
74 H 19.050537 15.242590 11.070062
75 H 7.321691 18.326151 12.663248
76 H 21.028390 25.812267 5.133919
77 H 8.891968 26.925560 4.031778
78 H 19.441924 17.214643 13.769069
79 H 19.399609 12.567779 9.038928
80 H 20.934609 21.061114 0.509973
81 H 7.394302 13.674424 7.936904
82 H 8.952699 22.165260 -0.581613
83 H 14.237909 21.155730 9.188668
84 C 14.236053 23.099444 8.353415
85 C 14.728446 22.628417 9.564306
86 C 16.188608 22.476849 9.848021
87 H 13.187859 23.357160 8.247702
88 H 14.919163 23.442957 7.582146
89 H 14.036643 22.563378 10.405278
90 H 16.400027 21.513007 10.322832
91 H 16.521009 23.263046 10.537393
92 H 16.770326 22.544575 8.924430

TS-1b
E = -3709.5660271 Ha
Imaginary Frequency = -291.25 cm^{-1}

ATOM X Y Z
1 Cu 13.720623 18.880904 5.796977
2 Ir 13.699532 20.689852 7.526815
3 O 8.891963 14.231900 7.085899
4 O 10.216924 26.019027 5.311144
5 O 9.709042 20.631359 0.536930
6 O 8.883521 19.449442 12.072920
7 O 17.681160 19.036928 12.772879
8 O 18.570330 20.112664 1.120513
9 O 18.495921 25.196043 6.239922
10 O 17.274215 13.543819 8.111728
11 O 15.025862 17.877490 7.068618
12 O 7.469575 17.681582 12.167599
13 O 19.902859 25.305683 4.467033
14 O 12.432404 20.039527 4.672514
15 O 15.308044 19.820619 4.887300
16 O 9.055691 26.225887 3.376530
17 O 18.675869 17.041320 13.175657
18 O 12.148729 17.989051 6.752951
19 O 12.076918 19.663914 8.305840
20 O 18.441202 13.399447 10.049535
21 O 8.708563 22.638126 0.207223
22 O 15.336803 21.445328 6.489968
23 O 12.489947 21.732351 6.205825
24 O 19.989050 21.880235 1.080918
25 O 7.490061 14.206862 8.866311
26 O 14.919148 19.470865 8.698968
27 C 8.490497 14.752048 8.111146
28 C 9.007705 16.024623 8.682334
29 C 9.830675 25.532590 4.262373
30 C 10.135811 24.154209 3.798681
31 C 9.473887 21.761810 0.924077
32 C 9.967585 22.345818 2.200051
33 C 8.476772 18.404672 11.594857
34 C 8.996894 17.775491 10.352907
35 C 17.921906 17.894082 12.422556
36 C 17.447629 17.274426 11.157363
37 C 18.975352 21.143593 1.625585
38 C 18.444033 21.742407 2.879945
39 C 18.910549 24.719244 5.196777
40 C 18.413840 23.460453 4.582809
41 C 17.651907 14.057848 9.148819
42 C 17.319991 15.440537 9.584906
43 C 15.304710 18.339932 8.207268
44 C 16.169525 17.520885 9.112534
45 C 12.129063 21.189276 5.090874
46 C 11.259515 22.049597 4.228245
47 C 15.749848 20.880476 5.404170
48 C 16.869355 21.596057 4.715410
49 C 11.683809 18.549987 7.781231
50 C 10.559374 17.876527 8.503242
51 C 10.045293 16.675491 8.009225
52 H 10.453136 16.244013 7.099163
53 C 10.936454 23.351642 4.615877
54 H 11.308800 23.748405 5.555806
55 C 10.773481 21.549135 3.018624

56 H 11.023386 20.537162 2.711085
57 C 10.032288 18.424183 9.674607
58 H 10.425455 19.357785 10.066195
59 C 16.636168 18.044412 10.319660
60 H 16.370949 19.055548 10.615108
61 C 17.405333 21.075050 3.535901
62 H 17.014217 20.148339 3.124604
63 C 17.372690 22.791498 5.230252
64 H 16.956035 23.214514 6.139469
65 C 16.516750 16.218837 8.746405
66 H 16.160215 15.806691 7.806252
67 C 8.485241 16.571396 9.858782
68 H 7.680023 16.066046 10.381747
69 C 18.950389 22.937330 3.401906
70 H 19.758877 23.453288 2.894331
71 C 9.649450 23.651668 2.587469
72 H 9.026695 24.271911 1.951164
73 C 17.787879 15.967433 10.793116
74 H 18.413964 15.364654 11.442800
75 H 7.211538 18.184919 12.965273
76 H 20.149176 26.111853 4.962838
77 H 8.923257 27.105497 3.782738
78 H 18.928259 17.550623 13.971433
79 H 18.589951 12.513715 9.662501
80 H 20.254293 21.396106 0.273651
81 H 7.230589 13.389745 8.395823
82 H 8.444905 22.149965 -0.598048
83 H 12.977553 21.849425 8.592571
84 C 13.504677 22.528613 9.541409
85 C 14.895366 22.386604 9.375556
86 C 15.747193 23.370751 8.690392
87 H 13.077110 23.504121 9.304385
88 H 13.037060 21.998168 10.369987
89 H 15.386198 21.538956 9.849523
90 H 16.457186 23.808741 9.407538
91 H 16.356587 22.873590 7.925513
92 H 15.173482 24.172676 8.219584

(2a) $CH_3CH_2CH_2$
E = -3709.6187358 Ha
ATOM X Y Z
1 Cu 9.822582 13.848052 2.811932
2 Ir 9.818944 15.619891 4.585503
3 O 4.828605 9.449493 3.876568
4 O 5.913504 20.869181 2.646637
5 O 5.974255 15.704532 -2.398336
6 O 4.751239 14.523426 9.012546
7 O 13.729162 13.701670 9.832550
8 O 14.809191 14.895864 -1.591392
9 O 14.891428 20.047425 3.466641
10 O 13.663540 8.640825 4.683512
11 O 11.078891 12.832416 4.038944
12 O 3.255767 12.822215 8.971752
13 O 16.386067 20.000672 1.764852
14 O 8.573483 15.084208 1.802092
15 O 11.413059 14.839132 2.037355
16 O 4.765362 21.064323 0.703468
17 O 14.876472 11.758563 10.033136
18 O 8.235919 13.081429 3.815788
19 O 8.178361 14.693775 5.426463
20 O 14.842244 8.392566 6.602337
21 O 4.796347 17.623146 -2.651950
22 O 11.461984 16.449567 3.650723
23 O 8.574722 16.736956 3.372481
24 O 16.339371 16.566604 -1.597661
25 O 3.299220 9.449107 5.548048
26 O 11.041469 14.390046 5.700396
27 C 4.375664 9.962471 4.883679
28 C 4.912828 11.194288 5.525546
29 C 5.587276 20.402748 1.570308
30 C 6.022158 19.077007 1.048310
31 C 5.625519 16.786448 -1.961971
32 C 6.039443 17.345395 -0.645096
33 C 4.325606 13.514259 8.480674
34 C 4.890217 12.896819 7.248126
35 C 14.054654 12.623752 9.369282
36 C 13.618891 12.097877 8.045365
37 C 15.262856 15.904336 -1.081739
38 C 14.726586 16.550254 0.148349
39 C 15.316325 19.512241 2.458916
40 C 14.750832 18.278065 1.845549
41 C 14.013001 9.080358 5.763911
42 C 13.599972 10.399147 6.318991
43 C 11.415732 13.275422 5.180706

44	C	12.331441	12.443747	6.021900
45	C	8.220096	16.220591	2.247640
46	C	7.308809	17.054003	1.399805
47	C	11.894680	15.882424	2.579198
48	C	13.079103	16.525844	1.926839
49	C	7.747733	13.623200	4.856691
50	C	6.561147	12.971906	5.494867
51	C	6.018615	11.813163	4.932724
52	H	6.451410	11.384991	4.032312
53	C	6.873355	18.305274	1.846233
54	H	7.191836	18.686701	2.812885
55	C	6.890934	16.575863	0.154899
56	H	7.224179	15.604167	-0.200264
57	C	5.995741	13.513665	6.653059
58	H	6.409389	14.414687	7.098466
59	C	12.767705	12.893823	7.271581
60	H	12.449867	13.861798	7.650176
61	C	13.620813	15.959872	0.769576
62	H	13.187385	15.058351	0.344389
63	C	13.645319	17.685431	2.464754
64	H	13.232314	18.133811	3.364595
65	C	12.748494	11.197173	5.547402
66	H	12.414616	10.839175	4.576965
67	C	4.347796	11.736482	6.684887
68	H	3.489619	11.258567	7.147018
69	C	15.292430	17.710992	0.686696
70	H	16.150598	18.171237	0.206950
71	C	5.604479	18.597737	-0.198159
72	H	4.943598	19.197022	-0.816648
73	C	14.035747	10.849736	7.569742
74	H	14.696619	10.232782	8.170616
75	H	2.973148	13.313897	9.768916
76	H	16.669301	20.799213	2.253939
77	H	4.547349	21.908744	1.146773
78	H	15.095100	12.204366	10.876082
79	H	15.043633	7.555275	6.138175
80	H	16.600875	16.057533	-2.391085
81	H	3.037095	8.654242	5.041551
82	H	4.594337	17.156500	-3.487709
83	C	9.785321	17.142476	6.004837
84	C	10.653956	16.933408	7.220915
85	C	12.155136	17.011678	6.976997
86	H	10.087099	18.033711	5.439257
87	H	8.724879	17.210092	6.273144
88	H	10.399998	15.989134	7.719290
89	H	12.407209	17.906356	6.396117
90	H	12.508123	16.136624	6.424109
91	H	12.693329	17.054182	7.928859
92	H	10.366858	17.731271	7.925425

(2b) CH_3CHCH_3

E = -3709.6260936 Ha

ATOM	X	Y	Z
1	Cu	13.167586	18.881495	5.738513
2	Ir	13.174828	20.666684	7.494038
3	O	8.179418	14.472021	6.780144
4	O	9.264318	25.891709	5.550213
5	O	9.325069	20.727060	0.505239
6	O	8.102052	19.545954	11.916121
7	O	17.079976	18.724198	12.736125
8	O	18.160004	19.918392	1.312183
9	O	18.242241	25.069953	6.370217
10	O	17.014354	13.663353	7.587088
11	O	14.416494	17.864279	6.956612
12	O	6.606580	17.844743	11.875328
13	O	19.736880	25.023200	4.668428
14	O	11.923284	20.100106	4.714892
15	O	14.752148	19.862576	4.948521
16	O	8.116175	26.086851	3.607044
17	O	18.227286	16.781091	12.936712
18	O	11.584858	18.104810	6.720411
19	O	11.533765	19.719190	8.328898
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.809101	21.496539	6.538014
23	O	11.919426	21.766622	6.271022
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.432351	19.447756	8.596099
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605

32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.775513	18.316388	8.088380
44	C	15.682254	17.466275	8.925476
45	C	11.570327	21.243113	5.151963
46	C	10.659622	22.076531	4.303381
47	C	15.240050	20.912731	5.479302
48	C	16.429917	21.548372	4.830414
49	C	11.098435	18.650384	7.759380
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887
53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	C	12.055390	23.024994	8.941250
84	C	13.163475	22.012321	9.105918
85	C	14.530317	22.634869	9.274564
86	H	12.236740	23.684558	8.085496
87	H	11.080018	22.546909	8.816802
88	H	12.944239	21.333112	9.939625
89	H	14.772292	23.305302	8.442666
90	H	15.317098	21.880035	9.359388
91	H	14.533101	23.232364	10.198587
92	H	12.013397	23.651518	9.844759

(3a) $CH_3CH_2CH_2$+ CO

E = -3822.9500781 Ha

ATOM	X	Y	Z
1	Cu	9.823093	13.861657	2.824660
2	Ir	9.818672	15.629605	4.594973
3	O	4.828605	9.449493	3.876568
4	O	5.913504	20.869181	2.646637
5	O	5.974255	15.704532	-2.398336
6	O	4.751239	14.523426	9.012546
7	O	13.729162	13.701670	9.832550
8	O	14.809191	14.895864	-1.591392
9	O	14.891428	20.047425	3.466641
10	O	13.663540	8.640825	4.683512
11	O	11.076805	12.842544	4.038602
12	O	3.255767	12.822215	8.971752
13	O	16.386067	20.000672	1.764852
14	O	8.577893	15.085645	1.811993
15	O	11.405463	14.843309	2.042200
16	O	4.765362	21.064323	0.703468
17	O	14.876472	11.758563	10.033136
18	O	8.242557	13.087296	3.818683
19	O	8.178874	14.694184	5.435097

20	O	14.842244	8.392566	6.602337
21	O	4.796347	17.623146	-2.651950
22	O	11.459760	16.460109	3.649111
23	O	8.562329	16.738532	3.381886
24	O	16.339371	16.566604	-1.597661
25	O	3.299220	9.449107	5.548048
26	O	11.055328	14.399240	5.701529
27	C	4.375664	9.962471	4.883679
28	C	4.912828	11.194288	5.525546
29	C	5.587276	20.402748	1.570308
30	C	6.022158	19.077007	1.048310
31	C	5.625519	16.786448	-1.961971
32	C	6.039443	17.345395	-0.645096
33	C	4.325606	13.514259	8.480674
34	C	4.890217	12.896819	7.248126
35	C	14.054654	12.623752	9.369282
36	C	13.618891	12.097877	8.045365
37	C	15.262856	15.904336	-1.081739
38	C	14.726586	16.550254	0.148349
39	C	15.316325	19.512241	2.458916
40	C	14.750832	18.278065	1.845549
41	C	14.013001	9.080358	5.763911
42	C	13.599972	10.399147	6.318991
43	C	11.420213	13.283444	5.181675
44	C	12.331441	12.443747	6.021900
45	C	8.217144	16.223349	2.254889
46	C	7.308809	17.054003	1.399805
47	C	11.891944	15.887830	2.581699
48	C	13.079103	16.525844	1.926839
49	C	7.749945	13.626557	4.860955
50	C	6.561147	12.971906	5.494867
51	C	6.018615	11.813163	4.932724
52	H	6.451410	11.384991	4.032312
53	C	6.873355	18.305274	1.846233
54	H	7.191836	18.686701	2.812885
55	C	6.890934	16.575863	0.154899
56	H	7.224179	15.604167	-0.200264
57	C	5.995741	13.513665	6.653059
58	H	6.409389	14.414687	7.098466
59	C	12.767705	12.893823	7.271581
60	H	12.449867	13.861798	7.650176
61	C	13.620813	15.959872	0.769576
62	H	13.187385	15.058351	0.344389
63	C	13.645319	17.685431	2.464754
64	H	13.232314	18.133811	3.364595
65	C	12.748494	11.197173	5.547402
66	H	12.414616	10.839175	4.576965
67	C	4.347796	11.736482	6.684887
68	H	3.489619	11.258567	7.147018
69	C	15.292430	17.710992	0.686696
70	H	16.150598	18.171237	0.206950
71	C	5.604479	18.597737	-0.198159
72	H	4.943598	19.197022	-0.816648
73	C	14.035747	10.849736	7.569742
74	H	14.696619	10.232782	8.170616
75	H	2.973148	13.313897	9.768916
76	H	16.669301	20.799213	2.253939
77	H	4.547349	21.908744	1.146773
78	H	15.095100	12.204366	10.876082
79	H	15.043633	7.555275	6.138175
80	H	16.600875	16.057533	-2.391085
81	H	3.037095	8.654242	5.041551
82	H	4.594337	17.156500	-3.487709
83	C	9.787303	17.133776	6.034617
84	C	10.680086	16.915620	7.232515
85	C	12.171850	17.061468	6.967852
86	H	10.067389	18.039278	5.482816
87	H	8.731628	17.182661	6.324053
88	H	10.468724	15.944136	7.696627
89	H	12.395079	18.039816	6.526668
90	H	12.525956	16.290812	6.277462
91	H	12.733847	16.966267	7.902192
92	H	10.374981	17.673345	7.972911
93	C	10.201393	19.639684	2.885439
94	O	11.004775	19.881041	3.658078

(3b) CH_3CHCH_3+ CO

E = -3822.9508277 Ha

ATOM	X	Y	Z
1	Cu	13.173344	18.879047	5.721987
2	Ir	13.173291	20.653706	7.490597
3	O	8.179418	14.472021	6.780144
4	O	9.264318	25.891709	5.550213
5	O	9.325069	20.727060	0.505239

6	O	8.102052	19.545954	11.916121
7	O	17.079976	18.724198	12.736125
8	O	18.160004	19.918392	1.312183
9	O	18.242241	25.069953	6.370217
10	O	17.014354	13.663353	7.587088
11	O	14.412555	17.852861	6.957956
12	O	6.606580	17.844743	11.875328
13	O	19.736880	25.023200	4.668428
14	O	11.929056	20.108712	4.702509
15	O	14.767637	19.856297	4.944400
16	O	8.116175	26.086851	3.607044
17	O	18.227286	16.781091	12.936712
18	O	11.577001	18.108711	6.713110
19	O	11.536970	19.712946	8.332840
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.799298	21.490957	6.532239
23	O	11.911868	21.755905	6.277824
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.437929	19.446527	8.587581
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605
32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.775834	18.310278	8.084940
44	C	15.682254	17.466275	8.925476
45	C	11.569070	21.242128	5.150390
46	C	10.659622	22.076531	4.303381
47	C	15.242764	20.908122	5.476629
48	C	16.429917	21.548372	4.830414
49	C	11.098557	18.646171	7.758487
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887
53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	C	12.112003	23.059094	8.918323
84	C	13.203633	22.028947	9.076072
85	C	14.581556	22.627749	9.234933
86	H	12.291989	23.708537	8.055194
87	H	11.126234	22.597704	8.813279
88	H	12.980854	21.363380	9.917844
89	H	14.830513	23.294496	8.402826

90	H	15.355569	21.858924	9.313716
91	H	14.600274	23.222778	10.160389
92	H	12.096231	23.692438	9.818161
93	C	12.603813	19.632009	12.029985
94	O	12.395218	20.617054	12.565962

TS-3a

E = -3821.7012798 Ha

Imaginary Frequency = -360.61 cm^{-1}

ATOM	X	Y	Z
1	Cu	9.769112	13.772878	2.657327
2	Ir	9.817012	15.578108	4.365350
3	O	4.570278	9.042607	3.800551
4	O	5.677176	21.242198	2.556661
5	O	5.682793	15.583488	-3.025506
6	O	4.513393	14.683453	9.400989
7	O	13.880352	13.886045	10.255965
8	O	15.152673	14.726391	-2.111436
9	O	15.151462	20.392675	3.463234
10	O	13.844190	8.246685	4.653841
11	O	11.173179	12.676844	4.089256
12	O	2.753807	12.749039	9.469315
13	O	16.963477	20.418794	1.577379
14	O	8.410894	15.111658	1.505247
15	O	11.574211	14.852662	1.784753
16	O	4.293010	21.576659	0.362611
17	O	15.232526	11.675415	10.609925
18	O	8.023202	12.970412	3.799012
19	O	8.097435	14.623991	5.337316
20	O	15.218414	7.896252	6.851680
21	O	4.304214	17.777875	-3.380590
22	O	11.540390	16.449666	3.384106
23	O	8.461432	16.722921	3.090318
24	O	16.953819	16.622698	-2.166291
25	O	2.784414	8.972665	5.710344
26	O	11.149755	14.373635	5.578870
27	C	3.970541	9.636187	5.052655
28	C	4.563287	10.923829	5.653519
29	C	5.214745	20.734929	1.211637
30	C	5.686475	19.359169	0.707523
31	C	5.223251	16.933655	-2.529968
32	C	5.692656	17.453832	-1.158546
33	C	3.933293	13.421665	8.808101
34	C	4.543965	12.819413	7.529041
35	C	14.328026	12.533104	9.757432
36	C	13.862261	12.025632	8.380074
37	C	15.752489	15.977936	-1.517123
38	C	15.134881	16.603846	-0.253156
39	C	15.756042	19.781512	2.221707
40	C	15.137320	18.510541	1.611550
41	C	14.306013	8.747192	6.001529
42	C	13.850274	10.128640	6.505392
43	C	11.525298	13.197259	5.184790
44	C	12.470525	12.379330	6.131392
45	C	8.066268	16.246329	1.953051
46	C	7.102641	17.131757	1.082705
47	C	12.036447	15.902186	2.319346
48	C	13.284870	16.593242	1.667724
49	C	7.587031	13.540139	4.841431
50	C	6.358907	12.894310	5.574854
51	C	5.768229	11.603702	4.978095
52	H	6.222344	11.152410	4.034826
53	C	6.627666	18.509257	1.576962
54	H	6.975350	18.900864	2.589585
55	C	6.634465	16.600273	-0.285787
56	H	6.984563	15.579156	-0.652434
57	C	5.746366	13.503149	6.850449
58	H	6.183989	14.458175	7.293246
59	C	12.939878	12.896678	7.504947
60	H	12.604277	13.922167	7.873813
61	C	13.902354	15.956606	0.408295
62	H	13.447553	15.009748	-0.034674
63	C	13.901821	17.869827	2.266793
64	H	13.443647	18.339884	3.198886
65	C	12.925118	10.995757	5.633394
66	H	12.576512	10.613224	4.617645
67	C	3.951194	11.531211	6.929008
68	H	3.059835	11.026766	7.429712
69	C	15.751905	17.880285	0.348607
70	H	16.663765	18.358167	-0.141086
71	C	5.219233	18.832832	-0.661451
72	H	4.522580	19.463385	-1.307082
73	C	14.318782	10.642877	7.878886
74	H	15.003401	9.999984	8.525120

75	H	2.448358	13.332729	10.362285
76	H	17.246626	21.329888	2.144049
77	H	4.076260	22.530148	0.886563
78	H	15.457312	12.204223	11.560263
79	H	15.476810	6.966947	6.301762
80	H	17.217577	16.068499	-3.093895
81	H	2.441082	8.122616	5.083537
82	H	4.094250	17.251486	-4.334298
83	C	9.765269	16.192871	6.634290
84	C	11.058217	16.557973	7.281845
85	C	11.756035	17.841507	6.872829
86	H	8.981247	16.946751	6.694078
87	H	9.398212	15.216793	6.934421
88	H	11.751421	15.715127	7.229181
89	H	11.090619	18.708723	6.929085
90	H	12.151688	17.760640	5.853718
91	H	12.605177	18.026784	7.536293
92	H	10.765470	16.633877	8.345661
93	C	9.895229	17.781072	4.638521
94	O	9.942817	18.863590	4.271842

TS-3b

E = -3821.7030663 Ha

Imaginary Frequency = -236.88 cm^{-1}

ATOM	X	Y	Z
1	Cu	13.174668	18.696682	5.624998
2	Ir	13.131409	20.396478	7.439520
3	O	7.834440	13.902768	6.557337
4	O	9.117107	26.270812	5.745127
5	O	9.127757	20.706237	0.064788
6	O	7.785047	19.457355	12.244398
7	O	17.318000	18.599039	13.105438
8	O	18.427048	19.863812	0.904223
9	O	18.398261	25.424222	6.586750
10	O	17.284272	13.025535	7.432416
11	O	14.538246	17.541864	6.987197
12	O	5.981935	17.562608	12.254468
13	O	20.165122	25.531039	4.661623
14	O	11.825461	20.118606	4.494929
15	O	14.948654	19.808618	4.821046
16	O	7.770017	26.651983	3.536317
17	O	18.716872	16.410603	13.415648
18	O	11.383269	17.831230	6.701342
19	O	11.414269	19.406927	8.320867
20	O	18.686828	12.671028	9.611003
21	O	7.772843	22.918294	-0.271188
22	O	14.844491	21.355178	6.464817
23	O	11.757701	21.558035	6.233621
24	O	20.189460	21.796884	0.855504
25	O	6.022677	13.831842	8.442578
26	O	14.504299	19.135853	8.588731
27	C	7.226197	14.488538	7.809081
28	C	7.833383	15.754874	8.441487
29	C	8.669888	25.787170	4.386255
30	C	9.129988	24.411711	3.867208
31	C	8.677835	22.054667	0.574184
32	C	9.134295	22.545592	1.960303
33	C	7.191221	18.213455	11.627579
34	C	7.815169	17.613789	10.354315
35	C	17.785030	17.260021	12.585424
36	C	17.297833	16.754273	11.214933
37	C	19.009634	21.118711	1.509359
38	C	18.405895	21.703168	2.798967
39	C	18.988644	24.851173	5.320495
40	C	18.396839	23.568567	4.705930
41	C	17.752273	13.518408	8.780854
42	C	17.281462	14.886909	9.309010
43	C	14.890568	17.993182	8.117317
44	C	15.856639	17.121002	9.001928
45	C	11.435652	21.193175	5.035186
46	C	10.506267	22.152801	4.212907
47	C	15.371798	20.853563	5.391912
48	C	16.605019	21.592852	4.761239
49	C	10.919452	18.350862	7.759394
50	C	9.672018	17.687360	8.441969
51	C	9.062530	16.427094	7.799077
52	H	9.520270	15.992052	6.849429
53	C	10.045821	23.527320	4.734110
54	H	10.384694	23.890624	5.760143
55	C	10.054104	21.663916	2.824598
56	H	10.400327	20.648771	2.436648
57	C	9.045036	18.282095	9.715742
58	H	9.490786	19.220460	10.184786
59	C	16.341906	17.618674	10.375213

60	H	15.994100	18.630286	10.769435
61	C	17.205540	21.009902	3.469080
62	H	16.761697	20.066738	3.008623
63	C	17.198829	22.872929	5.378650
64	H	16.748259	23.307882	6.331860
65	C	16.328816	15.756287	8.465139
66	H	15.973389	15.389528	7.445533
67	C	7.207631	16.350906	9.716700
68	H	6.294213	15.857891	10.187421
69	C	19.000083	22.983301	3.415570
70	H	19.885383	23.499312	2.915151
71	C	8.672316	23.919483	2.481203
72	H	7.992338	24.572269	1.840661
73	C	17.769362	15.388571	10.681624
74	H	18.480059	14.749325	11.302063
75	H	5.682605	18.132469	13.158742
76	H	20.554596	26.327225	5.329838
77	H	7.561003	27.603435	4.068449
78	H	18.745477	16.800012	14.454669
79	H	18.886934	11.715024	9.083651
80	H	20.577854	21.156189	0.036595
81	H	5.774052	12.902118	7.889512
82	H	7.450623	22.350138	-1.168621
83	C	13.520931	23.742184	6.719213
84	C	13.424228	22.943683	7.962554
85	C	14.611681	23.019282	8.847011
86	H	14.531190	23.754819	6.305780
87	H	12.787072	23.460428	5.965790
88	H	12.436937	22.927822	8.414567
89	H	14.900000	24.079885	8.918879
90	H	15.463902	22.511828	8.379509
91	H	14.455263	22.623617	9.850496
92	H	13.266677	24.769020	7.035606
93	C	12.870471	20.828440	9.681315
94	O	12.890845	20.333529	10.714775

(4a) $CH_3CH_2CH_2CO$

E = -3822.9961231 Ha

ATOM	X	Y	Z
1 Cu	9.813816	13.878451	2.853373
2 Ir	9.820762	15.658691	4.624638
3 O	4.828605	9.449493	3.876568
4 O	5.913504	20.869181	2.646637
5 O	5.974255	15.704532	-2.398336
6 O	4.751239	14.523426	9.012546
7 O	13.729162	13.701670	9.832550
8 O	14.809191	14.895864	-1.591392
9 O	14.891428	20.047425	3.466641
10 O	13.663540	8.640825	4.683512
11 O	11.071383	12.853936	4.044060
12 O	3.255767	12.822215	8.971752
13 O	16.386067	20.000672	1.764852
14 O	8.566214	15.082242	1.827907
15 O	11.400070	14.842892	2.045164
16 O	4.765362	21.064323	0.703468
17 O	14.876472	11.758563	10.033136
18 O	8.242238	13.082374	3.817205
19 O	8.164626	14.700367	5.423833
20 O	14.842244	8.392566	6.602337
21 O	4.796347	17.623146	-2.651950
22 O	11.468559	16.463495	3.646742
23 O	8.570519	16.755812	3.377897
24 O	16.339371	16.566604	-1.597661
25 O	3.299220	9.449107	5.548048
26 O	11.076869	14.416165	5.705735
27 C	4.375664	9.962471	4.883679
28 C	4.912828	11.194288	5.525546
29 C	5.587276	20.402748	1.570308
30 C	6.022158	19.077007	1.048310
31 C	5.625519	16.786448	-1.961971
32 C	6.039443	17.345395	-0.645096
33 C	4.325606	13.514259	8.480674
34 C	4.890217	12.896819	7.248126
35 C	14.054654	12.623752	9.369282
36 C	13.618891	12.097877	8.045365
37 C	15.262856	15.904336	-1.081739
38 C	14.726586	16.550254	0.148349
39 C	15.316325	19.512241	2.458916
40 C	14.750832	18.278065	1.845549
41 C	14.013001	9.080358	5.763911
42 C	13.599972	10.399147	6.318991
43 C	11.424180	13.294496	5.185606
44 C	12.331441	12.443747	6.021900
45 C	8.217658	16.226473	2.259561
46 C	7.308809	17.054003	1.399805

47	C	11.893189	15.885096	2.581239
48	C	13.079103	16.525844	1.926839
49	C	7.745300	13.629451	4.855001
50	C	6.561147	12.971906	5.494867
51	C	6.018615	11.813163	4.932724
52	H	6.451410	11.384991	4.032312
53	C	6.873355	18.305274	1.846233
54	H	7.191836	18.686701	2.812885
55	C	6.890934	16.575863	0.154899
56	H	7.224179	15.604167	-0.200264
57	C	5.995741	13.513665	6.653059
58	H	6.409389	14.414687	7.098466
59	C	12.767705	12.893823	7.271581
60	H	12.449867	13.861798	7.650176
61	C	13.620813	15.959872	0.769576
62	H	13.187385	15.058351	0.344389
63	C	13.645319	17.685431	2.464754
64	H	13.232314	18.133811	3.364595
65	C	12.748494	11.197173	5.547402
66	H	12.414616	10.839175	4.576965
67	C	4.347796	11.736482	6.684887
68	H	3.489619	11.258567	7.147018
69	C	15.292430	17.710992	0.686696
70	H	16.150598	18.171237	0.206950
71	C	5.604479	18.597737	-0.198159
72	H	4.943598	19.197022	-0.816648
73	C	14.035747	10.849736	7.569742
74	H	14.696619	10.232782	8.170616
75	H	2.973148	13.313897	9.768916
76	H	16.669301	20.799213	2.253939
77	H	4.547349	21.908744	1.146773
78	H	15.095100	12.204366	10.876082
79	H	15.043633	7.555275	6.138175
80	H	16.600875	16.057533	-2.391085
81	H	3.037095	8.654242	5.041551
82	H	4.594337	17.156500	-3.487709
83	C	10.372340	18.392581	5.742054
84	C	11.612757	18.725851	6.582252
85	C	12.791402	17.797524	6.325074
86	H	10.604115	18.452321	4.677596
87	H	9.571032	19.108177	5.965432
88	H	11.338922	18.704960	7.641924
89	H	13.096731	17.834820	5.275231
90	H	12.539807	16.757188	6.563080
91	H	13.646651	18.089642	6.940423
92	H	11.896941	19.755183	6.335271
93	O	9.476556	16.703862	7.215094
94	C	9.831788	17.019474	6.110340

(4b) CH_3CHCH_3CO

E = -3823.0002279 Ha

ATOM	X	Y	Z
1	Cu	9.810881	13.771992	2.834195
2	Ir	9.813588	15.567426	4.608950
3	O	4.808370	9.413811	3.868280
4	O	6.686186	21.012375	2.356627
5	O	5.821246	15.623652	-2.362948
6	O	4.924965	14.306896	9.171818
7	O	13.353322	13.423122	9.997946
8	O	14.812450	14.952912	-1.679896
9	O	14.397713	20.168619	3.289780
10	O	13.804025	8.676554	4.581716
11	O	11.056506	12.791683	4.046099
12	O	3.491225	12.551127	9.168904
13	O	15.928301	20.228326	1.618753
14	O	8.588479	14.943974	1.767386
15	O	11.374353	14.701326	1.969984
16	O	5.421320	21.242668	0.489609
17	O	14.504467	11.479128	10.186031
18	O	8.245756	13.024708	3.831797
19	O	8.176824	14.628680	5.455896
20	O	14.809140	8.324897	6.582690
21	O	4.858417	17.654225	-2.660860
22	O	11.436266	16.314190	3.584496
23	O	8.555159	16.596291	3.343945
24	O	16.185124	16.757387	-1.713546
25	O	3.374881	9.338414	5.621799
26	O	11.068028	14.353494	5.712681
27	C	4.410916	9.884298	4.918929
28	C	4.974672	11.091388	5.579384
29	C	6.211616	20.529898	1.343745
30	C	6.420622	19.127932	0.893417
31	C	5.615635	16.755999	-1.965040

32	C	6.143950	17.318649	-0.692573
33	C	4.508044	13.294879	8.639136
34	C	5.023437	12.728534	7.362916
35	C	13.727191	12.373926	9.506654
36	C	13.403873	11.916616	8.128359
37	C	15.173573	16.006231	-1.187513
38	C	14.581309	16.620260	0.032010
39	C	14.891932	19.659770	2.299159
40	C	14.451416	18.371740	1.698827
41	C	14.043143	9.050431	5.715928
42	C	13.554619	10.323009	6.312761
43	C	11.399357	13.227855	5.193084
44	C	12.268155	12.355684	6.034903
45	C	8.252886	16.089692	2.204338
46	C	7.428996	16.969195	1.327591
47	C	11.837759	15.758009	2.498648
48	C	12.954184	16.471828	1.816613
49	C	7.762335	13.558797	4.883740
50	C	6.605795	12.880436	5.537098
51	C	6.045357	11.739866	4.957725
52	H	6.439272	11.349273	4.023459
53	C	7.188156	18.292419	1.707870
54	H	7.606729	18.679148	2.634153
55	C	6.917134	16.486521	0.122083
56	H	7.113752	15.462883	-0.185497
57	C	6.091664	13.377359	6.738207
58	H	6.525878	14.263757	7.193486
59	C	12.599284	12.740418	7.337081
60	H	12.229618	13.679179	7.740919
61	C	13.537462	15.939979	0.665659
62	H	13.184833	14.995858	0.259069
63	C	13.409371	17.689418	2.329715
64	H	12.952927	18.113396	3.221634
65	C	12.745992	11.146425	5.525040
66	H	12.491079	10.839893	4.514148
67	C	4.465483	11.583407	6.784982
68	H	3.635593	11.080181	7.270242
69	C	15.041313	17.836340	0.548389
70	H	15.855031	18.360763	0.057932
71	C	5.891937	18.639661	-0.306263
72	H	5.290114	19.284454	-0.938519
73	C	13.882418	10.705613	7.617477
74	H	14.507775	10.065934	8.231651
75	H	3.233931	13.016172	9.989849
76	H	16.133874	21.055240	2.098773
77	H	5.354953	22.136619	0.880585
78	H	14.648639	11.878772	11.066921
79	H	15.070857	7.522900	6.087987
80	H	16.493604	16.264327	-2.499806
81	H	3.089627	8.561810	5.100381
82	H	4.569247	17.180170	-3.465903
83	C	10.015079	19.022986	4.275817
84	C	10.395724	18.450859	5.635743
85	C	11.917379	18.466598	5.827901
86	H	10.494415	18.477632	3.459370
87	H	8.935020	19.025218	4.110088
88	H	9.957081	19.091070	6.411259
89	H	12.408771	17.813659	5.102552
90	H	12.198819	18.156313	6.837450
91	H	12.273085	19.487394	5.656569
92	H	10.368282	20.058801	4.247022
93	C	9.867024	17.049774	5.992398
94	O	9.532397	16.757322	7.112255

TS-3a

E = -3824.0971804 Ha

Imaginary Frequency = -1000.71 cm^{-1}

ATOM	X	Y	Z
1	Cu	13.173318	18.885315	5.737555
2	Ir	13.159579	20.652642	7.492243
3	O	8.179418	14.472021	6.780144
4	O	9.264318	25.891709	5.550213
5	O	9.325069	20.727060	0.505239
6	O	8.102052	19.545954	11.916121
7	O	17.079976	18.724198	12.736125
8	O	18.160004	19.918392	1.312183
9	O	18.242241	25.069953	6.370217
10	O	17.014354	13.663353	7.587088
11	O	14.395910	17.867230	6.961207
12	O	6.606580	17.844743	11.875328
13	O	19.736880	25.023200	4.668428
14	O	11.955970	20.120578	4.717105
15	O	14.771019	19.844995	4.962289
16	O	8.116175	26.086851	3.607044
17	O	18.227286	16.781091	12.936712

18	O	11.584901	18.132635	6.709724
19	O	11.542255	19.706997	8.356089
20	O	18.193058	13.415094	9.505913
21	O	8.147161	22.645674	0.251626
22	O	14.772828	21.505838	6.516936
23	O	11.881237	21.756280	6.302035
24	O	19.690185	21.589132	1.305915
25	O	6.650033	14.471635	8.451624
26	O	14.449326	19.459949	8.586009
27	C	7.726478	14.984999	7.787255
28	C	8.263642	16.216816	8.429122
29	C	8.938090	25.425276	4.473884
30	C	9.372971	24.099535	3.951886
31	C	8.976333	21.808976	0.941605
32	C	9.390256	22.367923	2.258479
33	C	7.676419	18.536787	11.384250
34	C	8.241030	17.919346	10.151702
35	C	17.405468	17.646280	12.272858
36	C	16.969704	17.120405	10.948941
37	C	18.613670	20.926864	1.821837
38	C	18.077400	21.572782	3.051925
39	C	18.667139	24.534769	5.362492
40	C	18.101645	23.300593	4.749125
41	C	17.363815	14.102886	8.667487
42	C	16.950785	15.421675	9.222567
43	C	14.775541	18.326293	8.091692
44	C	15.682254	17.466275	8.925476
45	C	11.567661	21.250916	5.170552
46	C	10.659622	22.076531	4.303381
47	C	15.234742	20.912284	5.481143
48	C	16.429917	21.548372	4.830414
49	C	11.103022	18.659342	7.770075
50	C	9.911960	17.994434	8.398443
51	C	9.369428	16.835691	7.836300
52	H	9.802223	16.407519	6.935887
53	C	10.224168	23.327802	4.749809
54	H	10.542649	23.709229	5.716460
55	C	10.241747	21.598391	3.058475
56	H	10.574992	20.626695	2.703312
57	C	9.346555	18.536193	9.556635
58	H	9.760203	19.437215	10.002041
59	C	16.118519	17.916351	10.175156
60	H	15.800681	18.884326	10.553752
61	C	16.971627	20.982400	3.673152
62	H	16.538199	20.080879	3.247965
63	C	16.996133	22.707959	5.368330
64	H	16.583127	23.156339	6.268171
65	C	16.099308	16.219700	8.450978
66	H	15.765430	15.861703	7.480541
67	C	7.698610	16.759010	9.588463
68	H	6.840433	16.281095	10.050594
69	C	18.643243	22.733520	3.590272
70	H	19.501412	23.193765	3.110526
71	C	8.955292	23.620265	2.705417
72	H	8.294412	24.219550	2.086928
73	C	17.386561	15.872264	10.473318
74	H	18.047433	15.255310	11.074192
75	H	6.323961	18.336425	12.672492
76	H	20.020114	25.821741	5.157515
77	H	7.898162	26.931272	4.050349
78	H	18.445913	17.226894	13.779658
79	H	18.394446	12.577803	9.041751
80	H	19.951689	21.080061	0.512491
81	H	6.387908	13.676770	7.945126
82	H	7.945151	22.179028	-0.584134
83	C	14.849105	23.146889	8.934818
84	C	16.307990	22.950032	9.357823
85	C	16.943788	21.638110	8.923022
86	H	14.748815	23.204713	7.850302
87	H	14.472808	24.088069	9.356167
88	H	16.380649	23.054042	10.445453
89	H	16.907279	21.529442	7.836115
90	H	16.434969	20.777493	9.368101
91	H	17.990474	21.618249	9.238673
92	H	16.856017	23.787025	8.909458
93	O	13.890291	21.461010	10.476974
94	C	13.943114	22.078014	9.462308
95	H	12.578074	22.715344	9.083948
96	H	12.539019	22.057272	8.451152

TS-3b

E = -3822.9513068 Ha

Imaginary Frequency = -6661982.52 cm^{-1}

ATOM	X	Y	Z
1	Cu	8.164977	14.422678	2.547865

2	Ir	8.164375	16.201128	4.283453
3	O	2.879644	9.633697	3.528402
4	O	4.071087	21.954374	2.461517
5	O	4.110114	16.293882	-3.119870
6	O	2.826323	15.234219	9.169201
7	O	12.296071	14.380541	10.030769
8	O	13.450273	15.440963	-2.258527
9	O	13.502409	21.091753	3.332760
10	O	12.260822	8.790594	4.378112
11	O	9.530526	13.308672	3.898843
12	O	1.048302	13.316950	9.205459
13	O	15.279225	21.124458	1.412820
14	O	6.817227	15.803064	1.380777
15	O	9.950334	15.502986	1.657448
16	O	2.708847	22.278984	0.250115
17	O	13.673344	12.179214	10.350820
18	O	6.407547	13.588337	3.612405
19	O	6.409978	15.198929	5.197893
20	O	13.648308	8.439185	6.569090
21	O	2.734915	18.489198	-3.482112
22	O	9.894899	17.080150	3.270525
23	O	6.789912	17.351903	3.024181
24	O	15.244880	17.343217	-2.327205
25	O	1.084720	9.568170	5.431329
26	O	9.533357	14.927680	5.474710
27	C	2.278151	10.226143	4.780009
28	C	2.879833	11.504104	5.392464
29	C	3.622247	21.441125	1.114361
30	C	4.094814	20.061145	0.620885
31	C	3.650133	17.645164	-2.627524
32	C	4.109815	18.162050	-1.251415
33	C	2.241489	13.982010	8.561596
34	C	2.860137	13.382835	7.284860
35	C	12.750293	13.035346	9.516490
36	C	12.271139	12.534853	8.140973
37	C	14.051881	16.693365	-1.667412
38	C	13.449693	17.308488	-0.390471
39	C	14.087146	20.481473	2.081428
40	C	13.467958	19.203900	1.484814
41	C	12.726034	9.288007	5.726032
42	C	12.259356	10.661089	6.243548
43	C	9.894737	13.779696	5.020290
44	C	10.852163	12.903456	5.911954
45	C	6.444310	16.914645	1.863469
46	C	5.499452	17.824161	1.000552
47	C	10.395637	16.550695	2.207501
48	C	11.634163	17.266514	1.564072
49	C	5.936466	14.132996	4.660901
50	C	4.695556	13.458118	5.350067
51	C	4.097116	12.179677	4.732229
52	H	4.554812	11.733482	3.788164
53	C	5.025659	19.203237	1.498552
54	H	5.364821	19.589157	2.516349
55	C	5.041640	17.303808	-0.374898
56	H	5.394305	16.285073	-0.745472
57	C	4.076626	14.058716	6.626059
58	H	4.519914	15.004161	7.083415
59	C	11.330196	13.405258	7.287531
60	H	10.986304	14.420950	7.674432
61	C	12.232987	16.648796	0.286462
62	H	11.776037	15.703807	-0.158218
63	C	12.251564	18.545148	2.162225
64	H	11.808243	19.003580	3.107206
65	C	11.318316	11.531379	5.388623
66	H	10.967330	11.160292	4.369390
67	C	2.262045	12.105803	6.667707
68	H	1.361066	11.605280	7.154941
69	C	14.066444	18.585102	0.208771
70	H	14.967534	19.071710	-0.292213
71	C	3.636620	19.539781	-0.753042
72	H	2.947544	20.174625	-1.402451
73	C	12.735371	11.163302	7.618768
74	H	13.431425	10.518832	8.251109
75	H	0.742425	13.891941	10.104330
76	H	15.585629	22.024213	1.986109
77	H	2.469284	23.228468	0.772808
78	H	13.895892	12.697186	11.306978
79	H	13.861078	7.485631	6.042294
80	H	15.551840	16.744711	-3.210155
81	H	0.779068	8.682871	4.835649
82	H	2.490260	17.941640	-4.416126
83	C	8.218949	19.703557	5.567305
84	C	9.734782	19.836189	5.655441
85	C	10.341123	20.448811	4.403398

86	H	7.931982	19.217544	4.628749
87	H	7.824372	19.096273	6.390886
88	H	9.962715	20.483125	6.520335
89	H	10.047759	19.851360	3.533109
90	H	11.432693	20.488136	4.444110
91	H	9.963107	21.464766	4.261418
92	H	7.746721	20.688804	5.605536
93	C	10.382597	18.522731	6.037615
94	O	11.520331	18.192870	5.773271
95	H	8.174411	17.321964	5.381989
96	H	9.717460	17.840854	6.624327

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