



Supporting Information

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On the Reaction Mechanism of the Rhodium-Catalyzed Arylation of Fullerene (C₆₀) with Organoboron Compounds in the Presence of Water

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open_201500093_sm_miscellaneous_information.pdf

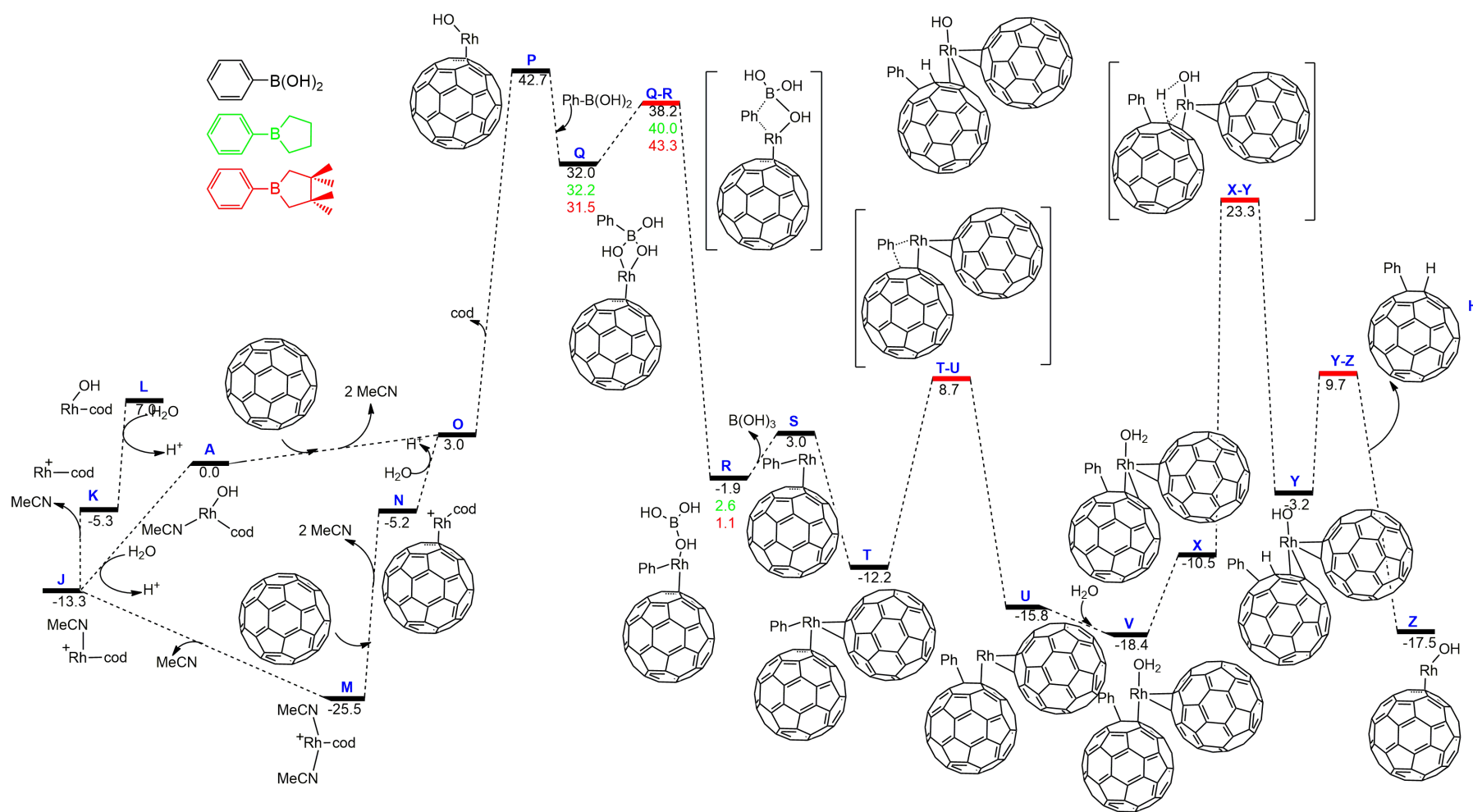


Figure S1. Alternative reaction pathways for the addition of phenyl groups or its derivatives to fullerene (C₆₀) catalyzed by rhodium in water (energies in kcal/mol).

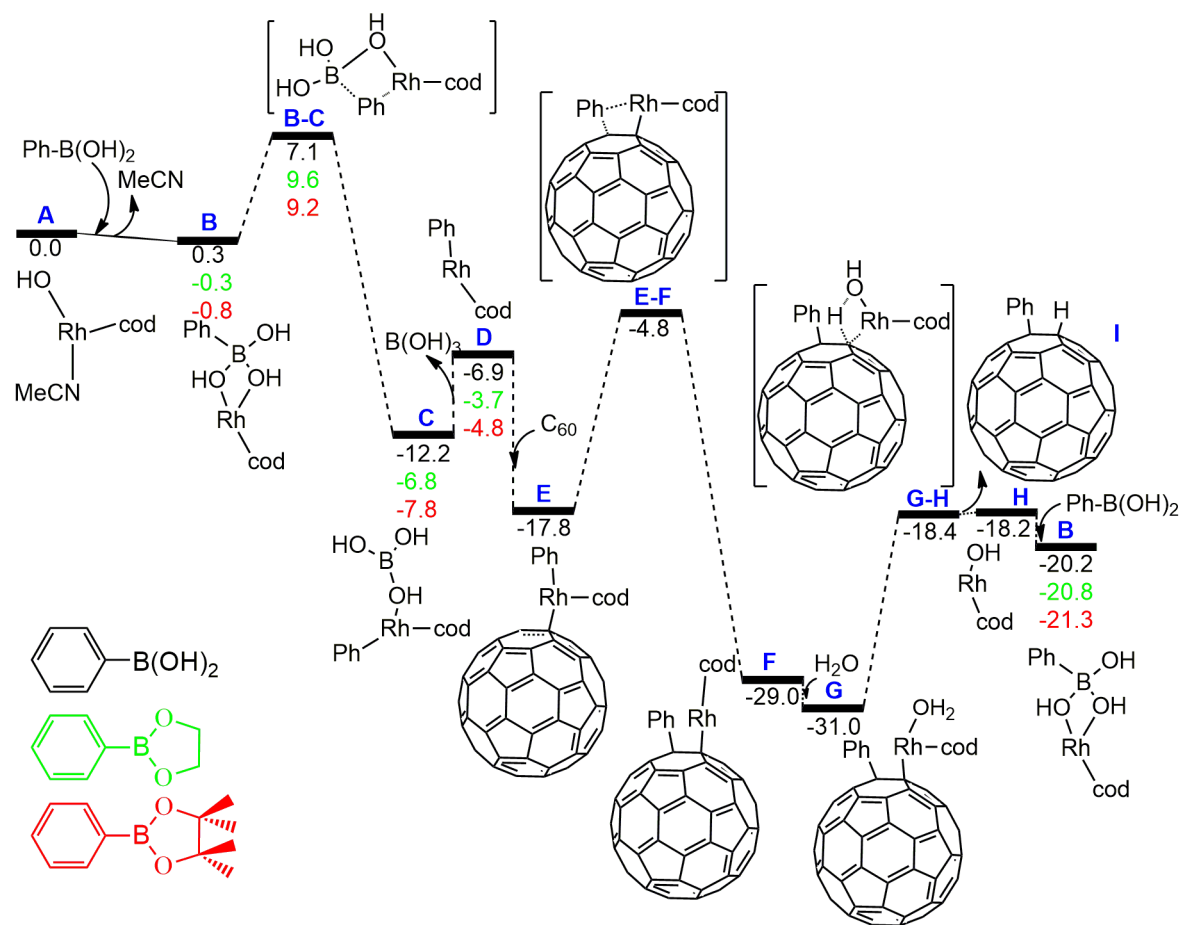


Figure S2. Reaction profile for the catalyzed by rhodium addition to fullerene (C_{60}) of phenylboronic acid (black), 2-phenyl-1,3,2-dioxaborinane (green) and the 4,4,5,5-tetramethyl-2-phenyl-1,3,2-dioxaborolane (red) in water (Gibbs energies in kcal/mol).

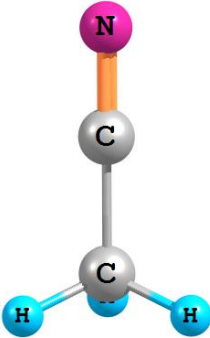
Index by labels of the structures analyzed in this manuscript

1. MeCN
2. A
3. H₂O
4. Ph-B(OH)₂
5. Ph-B(O-C₂H₄-O)
6. Ph-B(O-C₂(Me)₂H₄-O)
7. B
8. B-C
9. C
10. C₆₀
11. D
12. B-(OH)₃
13. B(OH)-(O-C₂H₄-O)
14. B(OH)-(O-C₂(Me)₂H₄-O)
15. E
16. E-F
17. F
18. G
19. G-H
20. I
21. H = L
22. J
23. K
24. L
25. M
26. N
27. O
28. P
29. COD
30. Q
31. Q-R
32. R
33. S
34. T
35. T-U
36. U
37. V
38. X
39. X-Y
40. Y
41. Y-Z

Table S1. Coordinate data sets, absolute energies (a.u.), 3D view for DFT optimized complexes (main distances in Å).

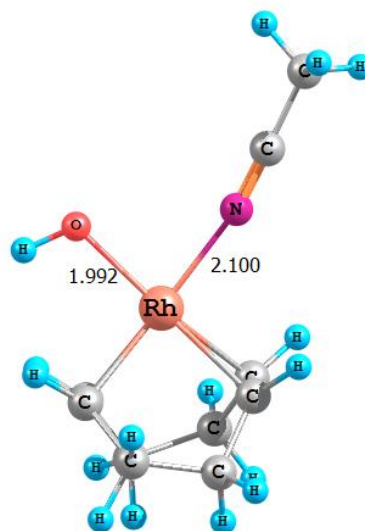
MeCN		
N	1.440817000	0.000001000 0.000110000
C	0.280592000	0.000001000 -0.000245000
C	-1.180966000	0.000001000 0.000053000
H	-1.561091000	-0.999857000 0.232534000
H	-1.561045000	0.701193000 0.749800000
H	-1.561343000	0.298644000 -0.981948000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -132.75149$
 $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -132.72986$
 $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -132.69818$
 $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -132.67655$



A

C	-0.539692000	1.597321000	0.546122000
C	-1.733569000	-0.951952000	0.760355000
C	-1.592273000	-1.238972000	-0.611651000
C	-0.633185000	1.408111000	-0.848088000
C	-2.153170000	-0.420631000	-1.761821000
C	-1.934868000	1.099519000	-1.586593000
C	-1.683581000	1.479158000	1.540333000
C	-2.546886000	0.215353000	1.318313000
H	-1.574296000	-1.776620000	1.454778000
H	-1.347038000	-2.266362000	-0.880896000
H	0.295547000	2.199581000	0.907478000
H	0.147183000	1.858862000	-1.460404000
H	-2.316261000	2.381806000	1.530125000
H	-2.997163000	-0.086570000	2.271012000
H	-3.221974000	-0.645410000	-1.911788000
H	-1.914675000	1.575068000	-2.574278000
H	-3.385098000	0.434921000	0.647406000
H	-1.239113000	1.428854000	2.541717000
H	-1.639702000	-0.751471000	-2.672339000
H	-2.782576000	1.549508000	-1.057345000
Rh	0.219854000	-0.358324000	0.090381000
N	2.207786000	0.302711000	-0.060202000
C	3.350803000	0.468845000	-0.111115000
C	4.796054000	0.649733000	-0.175087000
H	5.078522000	1.621017000	0.242655000
H	5.291613000	-0.141997000	0.395496000
H	5.133790000	0.599297000	-1.215077000
O	1.089454000	-2.123965000	0.396534000
H	0.429872000	-2.822089000	0.538849000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -631.24957$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -631.04877$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -630.99438$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -630.79358$ 

H₂O

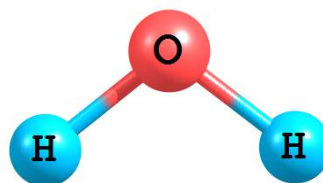
O	0.00000000	0.00000000	0.119449000
H	0.00000000	0.762631000	-0.477796000
H	0.00000000	-0.762631000	-0.477796000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -76.40702$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -76.40355$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -76.41483$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -76.41136$



Ph-B(OH)₂

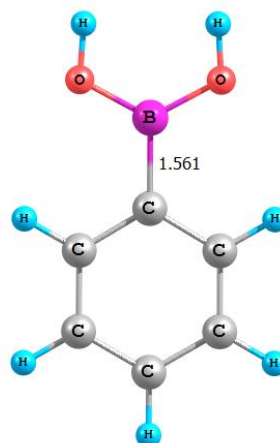
O	-2.384994000	1.212562000	-0.000461000
H	-3.350677000	1.153694000	-0.000732000
B	-1.734746000	-0.000164000	-0.000016000
O	-2.385517000	-1.212471000	0.000631000
H	-3.351158000	-1.152687000	-0.000097000
C	-0.173307000	-0.000010000	-0.000134000
C	0.551417000	-1.205540000	-0.000287000
C	0.551429000	1.205529000	0.000292000
C	1.946305000	-1.209390000	-0.000248000
H	0.009821000	-2.147634000	-0.000254000
C	1.946284000	1.209333000	0.000224000
H	0.009767000	2.147573000	0.000582000
C	2.646095000	-0.000045000	-0.000027000
H	2.488626000	-2.151703000	-0.000342000
H	2.488631000	2.151628000	0.000550000
H	3.733466000	-0.000045000	0.000097000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -408.25139$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -408.15927$

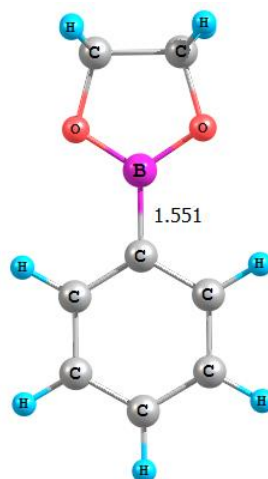
$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -408.11344$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -408.02132$



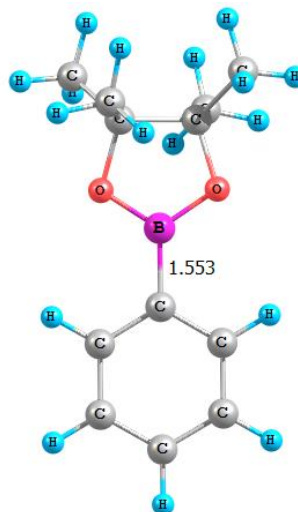
Ph-B(O-C₂H₄-O)

O	1.729523000	-1.148309000	0.014602000
B	0.972405000	0.000029000	0.000000000
O	1.729567000	1.148330000	-0.014603000
C	-0.578831000	0.000027000	0.000000000
C	-1.301045000	1.207139000	-0.002275000
C	-1.301003000	-1.207116000	0.002275000
C	-2.695713000	1.210175000	-0.002346000
H	-0.758666000	2.149096000	-0.003930000
C	-2.695668000	-1.210198000	0.002346000
H	-0.758587000	-2.149049000	0.003927000
C	-3.394481000	-0.000023000	0.000000000
H	-3.238776000	2.151883000	-0.004108000
H	-3.238704000	-2.151923000	0.004105000
H	-4.481761000	-0.000045000	0.000000000
C	3.113186000	-0.776352000	-0.022524000
H	3.563333000	-1.169932000	-0.940892000
H	3.628506000	-1.224175000	0.833833000
C	3.113218000	0.776318000	0.022524000
H	3.628553000	1.224127000	-0.833831000
H	3.563377000	1.169878000	0.940893000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -485.66200$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -485.53662$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -485.45987$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -485.33449$ 

Ph-B(O-C₂(Me)₂H₄-O)

O	-0.635303000	1.127179000	0.208913000
B	0.124418000	-0.000118000	-0.000100000
O	-0.635405000	-1.127273000	-0.208977000
C	1.677480000	0.000004000	-0.000064000
C	2.400060000	-1.196510000	-0.157613000
C	2.400066000	1.196534000	0.157602000
C	3.794831000	-1.199737000	-0.158897000
H	1.856898000	-2.130119000	-0.279875000
C	3.794787000	1.199732000	0.158932000
H	1.856833000	2.130095000	0.279913000
C	4.493663000	-0.000014000	-0.000001000
H	4.338019000	-2.133316000	-0.282466000
H	4.338042000	2.133267000	0.282550000
H	5.580984000	0.000050000	-0.000013000
C	-2.018865000	0.785783000	-0.082432000
C	-2.293154000	1.247905000	-1.520240000
H	-1.652647000	0.723085000	-2.236118000
H	-3.338266000	1.086977000	-1.805598000
H	-2.076267000	2.318001000	-1.596169000
C	-2.919178000	1.542971000	0.892650000
H	-2.649820000	1.340764000	1.931782000
H	-2.820063000	2.619983000	0.722418000
H	-3.970981000	1.272118000	0.744397000
C	-2.018954000	-0.785754000	0.082470000
C	-2.919378000	-1.542841000	-0.892587000
H	-2.820522000	-2.619862000	-0.722251000
H	-3.971125000	-1.271720000	-0.744420000
H	-2.649893000	-1.340720000	-1.931711000
C	-2.293121000	-1.247917000	1.520278000
H	-3.338091000	-1.086517000	1.805880000
H	-2.076739000	-2.318127000	1.596005000
H	-1.652204000	-0.723503000	2.236089000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -642.93018$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -642.69725$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -642.64812$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -642.41519$ 

B

C	-1.301328000	1.464444000	0.642962000
C	-2.043523000	-1.247960000	0.849595000
C	-2.084344000	-1.441813000	-0.551879000
C	-1.594986000	1.323553000	-0.721416000
C	-2.953427000	-0.676402000	-1.532421000
C	-2.936689000	0.846741000	-1.273586000
C	-2.223190000	1.107442000	1.796923000
C	-2.922275000	-0.260248000	1.612929000
H	-1.632163000	-2.065039000	1.441029000
H	-1.743739000	-2.411942000	-0.917843000
H	-0.492614000	2.146447000	0.901068000
H	-0.983751000	1.899247000	-1.411888000
H	-2.968142000	1.902440000	1.958748000
H	-3.159546000	-0.678794000	2.597200000
H	-3.985882000	-1.060364000	-1.522114000
H	-3.145477000	1.374884000	-2.210764000
H	-3.881032000	-0.138334000	1.097469000
H	-1.609907000	1.073324000	2.704644000
H	-2.564190000	-0.873126000	-2.538295000
H	-3.740302000	1.127723000	-0.584599000
Rh	-0.342593000	-0.330563000	-0.053846000
O	2.906085000	-1.768636000	1.327444000
H	2.954130000	-2.730318000	1.430959000
B	2.261310000	-1.472665000	0.083429000
O	2.838771000	-2.063294000	-1.115146000
H	3.802010000	-1.998577000	-1.062423000
O	0.807915000	-2.069178000	0.053933000
H	0.761856000	-2.612897000	-0.750920000
C	2.037741000	0.161224000	-0.013194000
C	1.774339000	0.789628000	-1.256430000
C	2.245380000	1.016899000	1.100059000
C	1.758712000	2.188602000	-1.390361000
H	1.681865000	0.169082000	-2.145706000
C	2.235953000	2.403539000	0.971759000
H	2.465971000	0.556396000	2.058762000
C	1.992892000	2.993935000	-0.278457000
H	1.587582000	2.639912000	-2.365203000
H	2.430341000	3.033439000	1.837029000
H	2.000220000	4.076538000	-0.379986000

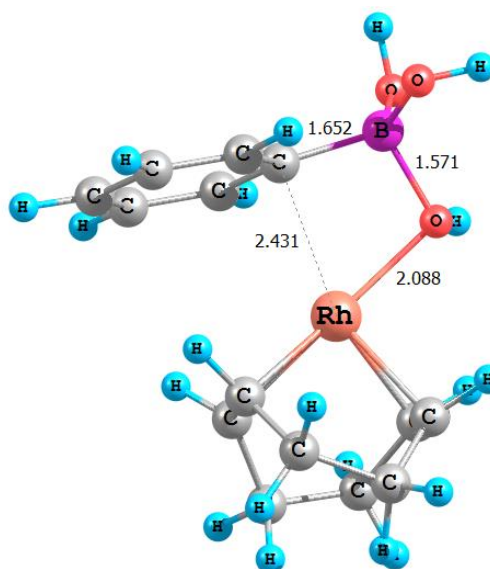
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.75241$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.47560$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.41611$$

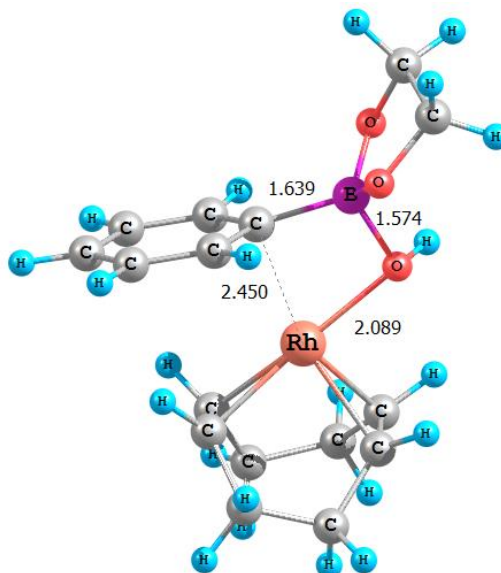
$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.13930$$

With Ph-B(OH)₂



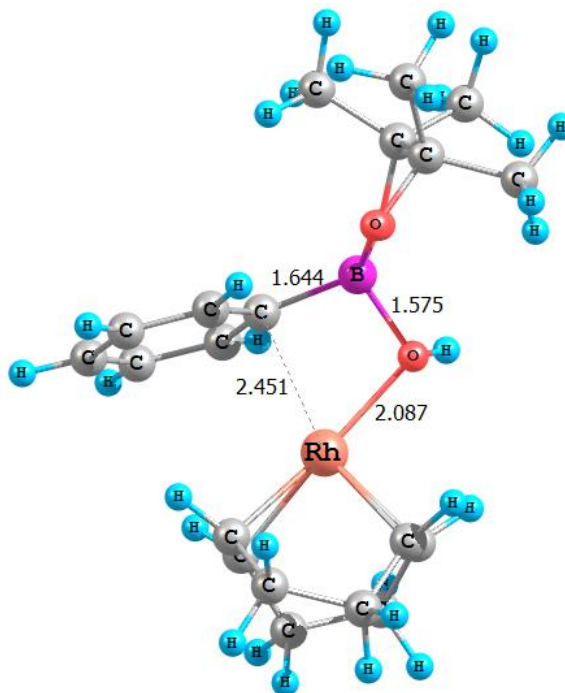
B

C	-2.051969000	1.137089000	0.568222000
C	-1.899467000	-1.654527000	0.934549000
C	-1.914585000	-1.933289000	-0.452408000
C	-2.323753000	0.831566000	-0.774358000
C	-3.008040000	-1.536450000	-1.427170000
C	-3.462817000	-0.071096000	-1.243499000
C	-2.789365000	0.580154000	1.774539000
C	-3.023506000	-0.947024000	1.687592000
H	-1.233517000	-2.262294000	1.545766000
H	-1.295008000	-2.766673000	-0.787666000
H	-1.485901000	2.048491000	0.758306000
H	-1.943379000	1.526360000	-1.519469000
H	-3.744596000	1.107615000	1.923231000
H	-3.089301000	-1.359267000	2.700432000
H	-3.867113000	-2.221534000	-1.349338000
H	-3.850717000	0.308709000	-2.195357000
H	-3.985176000	-1.163933000	1.210051000
H	-2.179171000	0.796861000	2.658759000
H	-2.607025000	-1.662974000	-2.439605000
H	-4.296092000	-0.013195000	-0.535283000
Rh	-0.599597000	-0.302920000	-0.083652000
O	3.102774000	-0.723502000	1.199171000
B	2.263549000	-0.580412000	0.039659000
O	3.044528000	-0.951916000	-1.132751000
O	1.047537000	-1.579234000	0.059349000
H	1.173529000	-2.176340000	-0.697025000
C	1.539949000	0.888782000	-0.028665000
C	1.022264000	1.393641000	-1.247803000
C	1.534534000	1.772242000	1.082185000
C	0.572073000	2.722423000	-1.364851000
H	1.083867000	0.777130000	-2.143128000
C	1.082035000	3.082956000	0.972017000
H	1.948235000	1.413715000	2.020752000
C	0.602221000	3.564432000	-0.258071000
H	0.222775000	3.094185000	-2.325463000
H	1.115273000	3.745644000	1.833845000
H	0.269726000	4.598801000	-0.346357000
C	4.373563000	-1.195978000	-0.696697000
H	4.810164000	-2.031381000	-1.259084000
H	5.001460000	-0.306062000	-0.865446000
C	4.229388000	-1.489180000	0.807577000
H	4.053536000	-2.564167000	0.981199000
H	5.108705000	-1.190471000	1.391821000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -984.15981$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.84821$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.76416$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.45256$ With Ph-B(O-C₂H₄-O)

B

C	-2.926072000	0.849870000	0.679971000
C	-2.336698000	-1.904127000	0.799738000
C	-2.346105000	-2.064434000	-0.605859000
C	-3.186899000	0.620148000	-0.679780000
C	-3.514258000	-1.762895000	-1.526999000
C	-4.184860000	-0.407509000	-1.209793000
C	-3.528166000	0.084924000	1.846679000
C	-3.535187000	-1.446169000	1.626415000
H	-1.568089000	-2.448609000	1.346711000
H	-1.614327000	-2.759287000	-1.021352000
H	-2.505567000	1.820703000	0.940737000
H	-2.944193000	1.427789000	-1.366251000
H	-4.544768000	0.447508000	2.065494000
H	-3.513568000	-1.950628000	2.598588000
H	-4.254551000	-2.578059000	-1.497626000
H	-4.652543000	-0.014477000	-2.119459000
H	-4.464878000	-1.762321000	1.141002000
H	-2.923757000	0.313091000	2.731966000
H	-3.126094000	-1.739416000	-2.552044000
H	-4.997407000	-0.540049000	-0.487667000
Rh	-1.288015000	-0.285269000	-0.117898000
O	2.426633000	-0.214323000	1.157903000
B	1.591106000	-0.129403000	-0.007741000
O	2.439125000	-0.301230000	-1.174369000
O	0.537035000	-1.297387000	-0.090657000
H	0.750071000	-1.798026000	-0.896098000
C	0.645720000	1.215278000	0.007897000
C	0.039343000	1.700210000	-1.178122000
C	0.517287000	2.024377000	1.166705000
C	-0.612952000	2.947322000	-1.218049000
H	0.184942000	1.152428000	-2.107957000
C	-0.134182000	3.253143000	1.132898000
H	0.994788000	1.683995000	2.081057000
C	-0.699060000	3.721530000	-0.065608000
H	-1.028345000	3.312558000	-2.154574000
H	-0.193078000	3.864213000	2.030817000
H	-1.188914000	4.691735000	-0.093744000
C	3.805958000	-0.262956000	-0.740592000
C	3.699199000	-0.737852000	0.762982000
C	4.634329000	-1.173504000	-1.650506000
H	4.628834000	-0.77584000	-2.672319000
H	5.677299000	-1.228064000	-1.315635000
H	4.226040000	-2.187050000	-1.681688000
C	3.671452000	-2.271626000	0.903432000
H	4.649785000	-2.722949000	0.700221000
H	3.381509000	-2.523740000	1.928849000
H	2.935067000	-2.719214000	0.229598000
C	4.768782000	-0.165320000	1.697702000
H	4.730585000	0.926431000	1.725309000
H	4.600002000	-0.531989000	2.716410000
H	5.775557000	-0.474080000	1.390488000
C	4.305980000	1.187205000	-0.868800000
H	5.372838000	1.281872000	-0.635163000
H	4.149762000	1.522911000	-1.899621000
H	3.744118000	1.853270000	-0.206836000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1141.42664$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1141.00838$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.95231$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.53405$ With Ph-B(O-C₂(Me)₂H₄-O)

B-C

C	1.126280000	-1.134138000	1.266407000
C	2.521449000	1.055225000	0.130125000
C	2.337036000	0.607803000	-1.188191000
C	1.169773000	-1.694699000	-0.022348000
C	2.785736000	-0.728759000	-1.751848000
C	2.452223000	-1.919794000	-0.822049000
C	2.311761000	-0.602498000	2.053125000
C	3.265264000	0.273957000	1.207034000
H	2.425054000	2.126483000	0.303783000
H	2.141386000	1.372248000	-1.942968000
H	0.258959000	-1.379197000	1.877605000
H	0.322459000	-2.312563000	-0.314576000
H	2.866614000	-1.430597000	2.522330000
H	3.787550000	0.976650000	1.866055000
H	3.862069000	-0.714558000	-1.985282000
H	2.341169000	-2.825878000	-1.428262000
H	4.044717000	-0.343218000	0.747749000
H	1.912849000	0.000449000	2.877786000
H	2.268190000	-0.869417000	-2.708216000
H	3.285835000	-2.116884000	-0.138996000
Rh	0.475543000	0.346491000	-0.140284000
O	-1.771042000	2.315892000	1.351363000
H	-0.897949000	2.316820000	1.767447000
B	-1.693729000	1.879478000	0.012793000
O	-2.761234000	2.221699000	-0.838083000
H	-3.578094000	2.294001000	-0.325496000
O	-0.398336000	2.204832000	-0.653672000
H	-0.563625000	2.362912000	-1.597701000
C	-1.705505000	-0.085972000	0.046440000
C	-2.048289000	-0.733599000	-1.166573000
C	-2.240916000	-0.651006000	1.226059000
C	-2.848801000	-1.876982000	-1.202015000
H	-1.698261000	-0.319667000	-2.111249000
C	-3.054673000	-1.784241000	1.206579000
H	-2.040649000	-0.160647000	2.175973000
C	-3.352128000	-2.406394000	-0.010160000
H	-3.091993000	-2.346997000	-2.152322000
H	-3.462661000	-2.181567000	2.133430000
H	-3.984787000	-3.290655000	-0.030532000

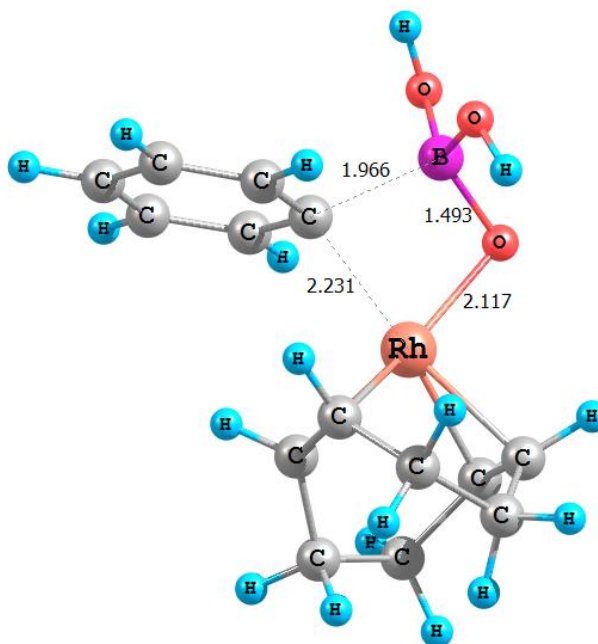
$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.73814$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.46343$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.40350$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.12879$

With Ph-B(OH)₂



B-C

C	-1.658966000	1.002222000	1.256681000
C	-2.552936000	-1.493576000	0.239974000
C	-2.538549000	-1.059415000	-1.092282000
C	-1.895110000	1.493617000	-0.040795000
C	-3.317145000	0.114932000	-1.659499000
C	-3.230343000	1.381872000	-0.775813000
C	-2.638635000	0.225928000	2.117791000
C	-3.403743000	-0.871154000	1.339976000
H	-2.181991000	-2.498288000	0.438964000
H	-2.200104000	-1.778523000	-1.841224000
H	-0.852361000	1.472497000	1.816970000
H	-1.240422000	2.292226000	-0.385271000
H	-3.347724000	0.909845000	2.611399000
H	-3.716230000	-1.654818000	2.039319000
H	-4.370080000	-0.159076000	-1.832177000
H	-3.366473000	2.267557000	-1.406778000
H	-4.326232000	-0.463932000	0.912237000
H	-2.060913000	-0.246414000	2.921215000
H	-2.895376000	0.340739000	-2.646127000
H	-4.053368000	1.399915000	-0.052886000
Rh	-0.738136000	-0.320427000	-0.146153000
O	2.161017000	-1.710807000	1.053552000
B	1.754923000	-1.294749000	-0.228204000
O	2.837867000	-1.296412000	-1.135985000
O	0.533040000	-1.920235000	-0.734878000
H	0.620628000	-2.039099000	-1.694513000
C	1.235891000	0.665488000	-0.055270000
C	1.458701000	1.424168000	-1.230161000
C	1.706726000	1.232554000	1.151444000
C	2.094525000	2.666869000	-1.205404000
H	1.141690000	1.024844000	-2.192392000
C	2.350921000	2.470119000	1.191228000
H	1.586421000	0.668549000	2.074118000
C	2.540612000	3.193908000	0.009875000
H	2.250801000	3.220381000	-2.128680000
H	2.708623000	2.870609000	2.137404000
H	3.042796000	4.158152000	0.035013000
C	4.007860000	-1.66041000	-0.402899000
H	4.314579000	-2.676509000	-0.689215000
H	4.828657000	-0.973612000	-0.638769000
C	3.579510000	-1.587916000	1.081548000
H	4.003329000	-2.393230000	1.690772000
H	3.863866000	-0.624259000	1.528641000

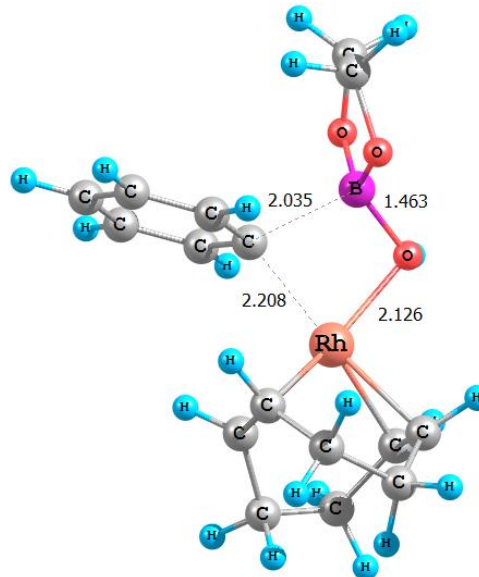
$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -984.14258$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.83135$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.74832$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.43709$

With Ph-B(O-C₂H₄-O)



B-C

C	-2.484455000	0.539399000	1.383294000
C	-2.779003000	-1.935652000	0.021080000
C	-2.920543000	-1.323248000	-1.234804000
C	-2.885986000	1.132548000	0.171613000
C	-3.980380000	-0.317797000	-1.628197000
C	-4.178346000	0.793512000	-0.570382000
C	-3.208101000	-0.568627000	2.126660000
C	-3.713338000	-1.700165000	1.200618000
H	-2.164070000	-2.833158000	0.074581000
H	-2.441495000	-1.833303000	-2.078648000
H	-1.798691000	1.114450000	2.003619000
H	-2.463596000	2.109788000	-0.055244000
H	-4.042125000	-0.158199000	2.718432000
H	-3.800752000	-2.625914000	1.780646000
H	-4.939251000	-0.815037000	-1.844592000
H	-4.552887000	1.695710000	-1.067291000
H	-4.721924000	-1.475663000	0.837781000
H	-2.499908000	-0.991431000	2.849259000
H	-3.656089000	0.143030000	-2.568803000
H	-4.953401000	0.503508000	0.147475000
Rh	-1.321161000	-0.298501000	-0.200313000
O	1.833096000	-1.039320000	0.831070000
B	1.343363000	-0.620370000	-0.414235000
O	2.387970000	-0.313287000	-1.302669000
O	0.280006000	-1.424293000	-1.031079000
H	0.352870000	-1.344335000	-1.996531000
C	0.320398000	1.146289000	-0.012960000
C	0.337871000	2.029985000	-1.117716000
C	0.652697000	1.707984000	1.241206000
C	0.650624000	3.385400000	-0.984501000
H	0.114385000	1.648250000	-2.113135000
C	0.966463000	3.058963000	1.390971000
H	0.693456000	1.056075000	2.110765000
C	0.961315000	3.903775000	0.274740000
H	0.658245000	4.033863000	-1.857838000
H	1.221495000	3.456386000	2.371165000
H	1.208329000	4.956932000	0.386016000
C	3.628036000	-0.346479000	-0.560551000
C	3.255216000	-1.257504000	0.682990000
C	3.941838000	-0.869182000	1.992935000
H	3.600221000	-1.531508000	2.795692000
H	5.030847000	-0.968768000	1.912975000
H	3.705143000	0.158085000	2.279257000
C	3.457821000	-2.757674000	0.414334000
H	4.518530000	-3.025203000	0.348442000
H	3.010207000	-3.324622000	1.236951000
H	2.961863000	-3.064056000	-0.511864000
C	4.007327000	1.092784000	-0.180538000
H	4.982553000	1.131117000	0.317939000
H	4.066531000	1.692921000	-1.094289000
H	3.262305000	1.551804000	0.472569000
C	4.707969000	-0.926339000	-1.477784000
H	4.870183000	-0.248713000	-2.322795000
H	5.660374000	-1.034852000	-0.945460000
H	4.418980000	-1.900796000	-1.878428000

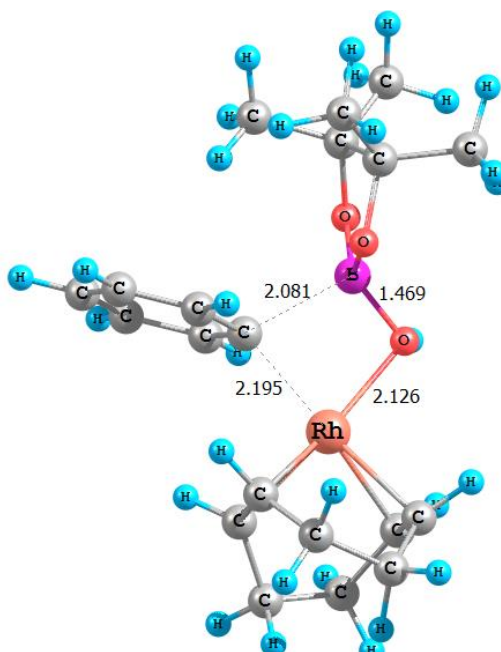
$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1141.40868$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.99038$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.93685$

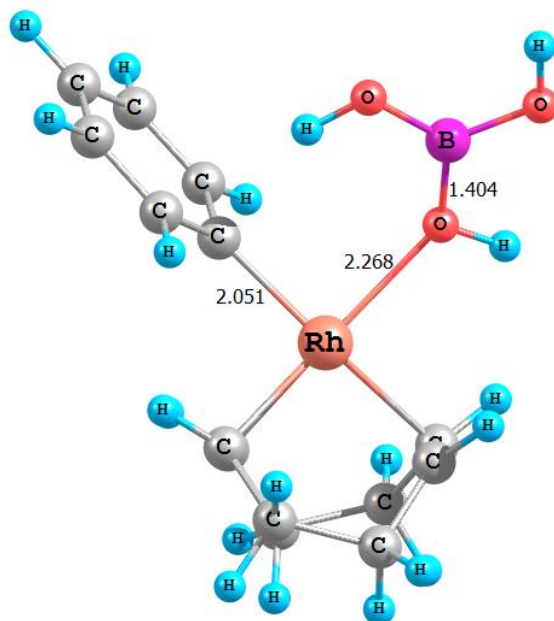
$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.51855$

With Ph-B(O-C₂(Me)₂H₄-O)



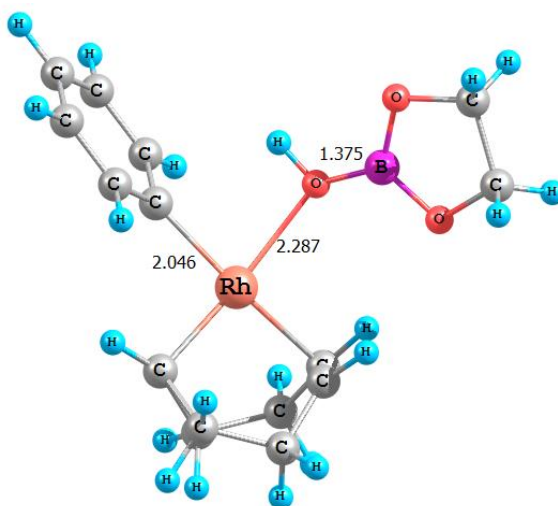
C

C	1.358057000	1.434590000	-1.041978000
C	2.405946000	-1.163987000	-0.439714000
C	2.326223000	-0.981824000	0.933873000
C	1.529417000	1.711847000	0.339137000
C	2.986730000	0.125345000	1.737490000
C	2.846652000	1.527339000	1.096357000
C	2.408747000	0.873312000	-1.983546000
C	3.226862000	-0.294170000	-1.380355000
H	2.091919000	-2.127310000	-0.841519000
H	1.998558000	-1.832442000	1.536932000
H	0.576659000	1.996878000	-1.552925000
H	0.853771000	2.448955000	0.770762000
H	3.087726000	1.670662000	-2.327392000
H	3.616344000	-0.915988000	-2.194818000
H	4.049163000	-0.103687000	1.917595000
H	2.913102000	2.282486000	1.888102000
H	4.104890000	0.091428000	-0.852085000
H	1.885452000	0.514007000	-2.878413000
H	2.507095000	0.140070000	2.723429000
H	3.690723000	1.724748000	0.425293000
Rh	0.456018000	-0.097792000	0.085562000
O	-2.707768000	-1.865896000	-0.707525000
H	-2.515270000	-0.907404000	-0.687718000
B	-1.778891000	-2.614903000	-0.079339000
O	-1.882090000	-3.974752000	0.033812000
H	-2.700321000	-4.293407000	-0.373799000
O	-0.633375000	-2.043843000	0.496748000
H	-0.068000000	-2.728913000	0.885299000
C	-1.345523000	0.880916000	0.049303000
C	-2.015618000	1.125068000	1.270653000
C	-2.015626000	1.292970000	-1.124326000
C	-3.267484000	1.744509000	1.317990000
H	-1.549352000	0.823966000	2.208011000
C	-3.277504000	1.904643000	-1.084362000
H	-1.549002000	1.133686000	-2.095651000
C	-3.906937000	2.136398000	0.138001000
H	-3.747522000	1.918751000	2.279071000
H	-3.762888000	2.199649000	-2.012571000
H	-4.883183000	2.613193000	0.173378000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.77413$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.49941$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.43451$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -906.15979$ With Ph-B(OH)₂

C

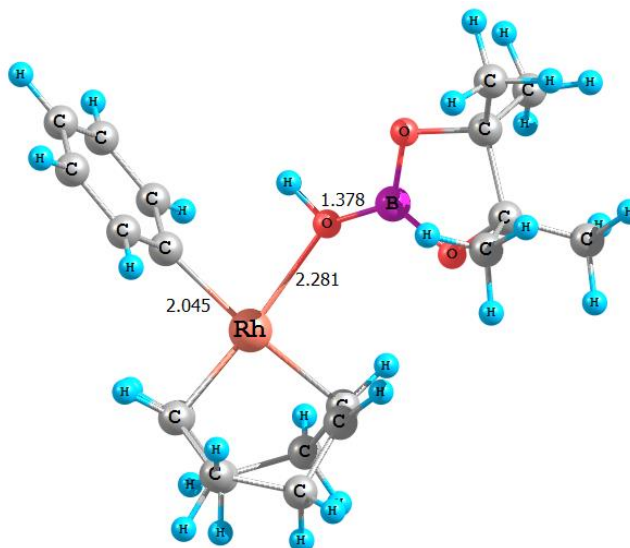
C	-2.264148000	-0.524425000	1.094415000
C	-0.239208000	-2.423579000	0.352907000
C	-0.438253000	-2.253508000	-1.007273000
C	-2.642436000	-0.559610000	-0.274488000
C	-1.742610000	-2.451155000	-1.759333000
C	-2.973708000	-1.837895000	-1.047585000
C	-2.070724000	-1.728598000	1.999718000
C	-1.302653000	-2.896602000	1.332799000
H	0.791634000	-2.469468000	0.699618000
H	0.451111000	-2.202647000	-1.636236000
H	-2.496020000	0.392474000	1.636335000
H	-3.107909000	0.343174000	-0.668130000
H	-3.040138000	-2.087222000	2.383459000
H	-0.826424000	-3.500635000	2.114429000
H	-1.918986000	-3.519862000	-1.961879000
H	-3.737936000	-1.612320000	-1.800570000
H	-2.003166000	-3.567093000	0.823931000
H	-1.505704000	-1.388158000	2.876786000
H	-1.628622000	-1.971558000	-2.738944000
H	-3.428369000	-2.572832000	-0.373200000
Rh	-0.566071000	-0.200022000	-0.098804000
O	3.077086000	-1.426143000	-0.175336000
B	2.808329000	-0.087163000	-0.269390000
O	3.859175000	0.736100000	0.037828000
O	1.574912000	0.377516000	-0.659318000
H	1.495893000	1.350282000	-0.664023000
C	-0.762748000	1.832869000	0.020933000
C	-0.684177000	2.599645000	-1.165518000
C	-0.824159000	2.558417000	1.231035000
C	-0.673363000	4.000700000	-1.146293000
H	-0.653600000	2.094415000	-2.131457000
C	-0.807384000	3.956613000	1.257552000
H	-0.880948000	2.022988000	2.177575000
C	-0.734042000	4.685697000	0.067873000
H	-0.622843000	4.553715000	-2.082491000
H	-0.852417000	4.478709000	2.211654000
H	-0.725381000	5.772714000	0.088049000
C	4.995062000	-0.108781000	0.285326000
C	4.415324000	-1.549106000	0.333502000
H	4.973737000	-2.253046000	-0.290078000
H	4.369257000	-1.945144000	1.354003000
H	5.468334000	0.190921000	1.224548000
H	5.716034000	0.023526000	-0.529077000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -984.17154$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.86445$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.77054$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -983.46345$ With Ph-B(O-C₂H₄-O)

C

C	-2.931582000	-0.851504000	1.079850000
C	-0.641301000	-2.404884000	0.302726000
C	-0.874225000	-2.251397000	-1.053930000
C	-3.308945000	-0.930487000	-0.287722000
C	-2.136891000	-2.642817000	-1.800682000
C	-3.443120000	-2.235299000	-1.076006000
C	-2.542842000	-2.018579000	1.970577000
C	-1.611715000	-3.048143000	1.282637000
H	0.385367000	-2.287694000	0.644343000
H	-0.009042000	-2.052821000	-1.686960000
H	-3.300957000	0.011653000	1.634167000
H	-3.914946000	-0.108166000	-0.666510000
H	-3.439555000	-2.526457000	2.362696000
H	-1.042329000	-3.582682000	2.052553000
H	-2.146458000	-3.724021000	-2.013420000
H	-4.237403000	-2.120996000	-1.823083000
H	-2.206608000	-3.810550000	0.768523000
H	-2.024987000	-1.601587000	2.843858000
H	-2.105971000	-2.142312000	-2.775926000
H	-3.776247000	-3.039116000	-0.409513000
Rh	-1.312704000	-0.254831000	-0.118226000
O	2.493617000	-0.899498000	-0.286325000
B	2.015641000	0.377520000	-0.383095000
O	2.941091000	1.358753000	-0.154582000
O	0.701250000	0.642201000	-0.702114000
H	0.484213000	1.592963000	-0.720765000
C	-1.817625000	1.720626000	0.042886000
C	-1.921913000	2.511774000	-1.124890000
C	-1.927309000	2.404689000	1.273627000
C	-2.126041000	3.896964000	-1.068302000
H	-1.864367000	2.035786000	-2.104264000
C	-2.126208000	3.787585000	1.337225000
H	-1.850646000	1.848190000	2.206585000
C	-2.228347000	4.541392000	0.165196000
H	-2.210606000	4.468825000	-1.990660000
H	-2.202546000	4.277924000	2.306134000
H	-2.387172000	5.615906000	0.213887000
C	4.240384000	0.693490000	-0.096224000
C	3.838840000	-0.793334000	0.272254000
C	5.100084000	1.410981000	0.941216000
H	6.064309000	0.904810000	1.064394000
H	5.295868000	2.435609000	0.609555000
H	4.603799000	1.460536000	1.912887000
C	4.864784000	0.826955000	-1.490729000
H	4.924920000	1.887716000	-1.752833000
H	5.875229000	0.406621000	-1.520996000
H	4.257488000	0.323935000	-2.250230000
C	4.707765000	-1.876218000	-0.362403000
H	5.742889000	-1.800238000	-0.010512000
H	4.326772000	-2.863005000	-0.080787000
H	4.703324000	-1.811874000	-1.452753000
C	3.710513000	-1.030083000	1.782325000
H	3.250980000	-2.008847000	1.951560000
H	4.687868000	-1.019956000	2.275721000
H	3.076796000	-0.272290000	2.254371000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1141.44151$
 $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1141.02763$
 $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.95983$
 $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -1140.54595$

 With Ph-B(O-C₂(Me)₂H₄-O)


C₆₀

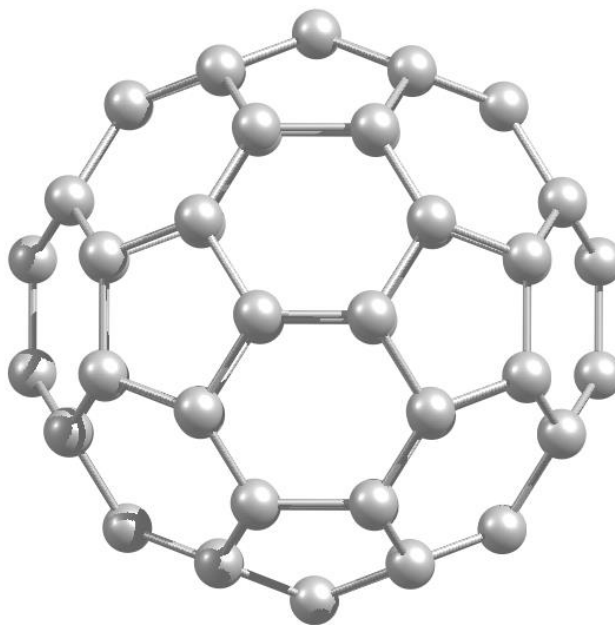
C	3.459098000	-0.327925000	0.726729000
C	3.187913000	1.027483000	1.175870000
C	2.928449000	-1.413717000	1.424603000
C	3.459098000	-0.327925000	-0.726729000
C	2.396623000	1.243315000	2.304990000
C	3.020489000	1.865222000	0.000000000
C	2.104155000	-1.188943000	2.600436000
C	2.375328000	-2.544483000	0.697868000
C	3.187913000	1.027483000	-1.175870000
C	2.928449000	-1.413717000	-1.424603000
C	1.843966000	0.112632000	3.032082000
C	1.405022000	2.306074000	2.305179000
C	2.068024000	2.885489000	0.000000000
C	1.041678000	-2.180820000	2.600414000
C	1.209331000	-3.018773000	1.424647000
C	2.375328000	-2.544483000	-0.697868000
C	2.396623000	1.243315000	-2.304990000
C	2.104155000	-1.188943000	-2.600436000
C	0.510126000	0.476253000	3.480910000
C	0.238865000	1.831545000	3.031553000
C	1.244057000	3.110542000	1.175960000
C	1.244057000	3.110542000	-1.175960000
C	-0.238869000	-1.831545000	3.031547000
C	0.089605000	-3.474267000	0.726802000
C	1.209331000	-3.018773000	-1.424647000
C	1.843966000	0.112632000	-3.032082000
C	1.405022000	2.306074000	-2.305179000
C	1.041678000	-2.180820000	-2.600414000
C	-0.510124000	-0.476256000	3.480905000
C	-1.041675000	2.180818000	2.600411000
C	-0.089607000	3.474266000	0.726801000
C	-1.405023000	-2.306083000	2.305186000
C	0.089605000	-3.474267000	-0.726802000
C	-1.244050000	-3.110537000	1.175956000
C	0.510126000	0.476253000	-3.480910000
C	0.238865000	1.831545000	-3.031553000
C	-0.238869000	-1.831545000	-3.031547000
C	-1.843966000	-0.112632000	3.032083000
C	-2.104161000	1.188942000	2.600432000
C	-1.209331000	3.018776000	1.424644000
C	-1.209331000	3.018776000	-1.424644000
C	-2.396633000	-1.243313000	2.304992000
C	-1.244050000	-3.110537000	-1.175956000
C	-2.068019000	-2.885489000	0.000000000
C	-0.510124000	-0.476256000	-3.480905000
C	-1.041675000	2.180818000	-2.600411000
C	-1.405023000	-2.306083000	-2.305186000
C	-2.928447000	1.413724000	1.424603000
C	-2.375329000	2.544483000	0.697871000
C	-2.375329000	2.544483000	-0.697871000
C	-3.187910000	-1.027483000	1.175873000
C	-3.020489000	-1.865221000	0.000000000
C	-1.843966000	-0.112632000	-3.032083000
C	-2.104161000	1.188942000	-2.600432000
C	-2.396633000	-1.243313000	-2.304992000
C	-3.459094000	0.327925000	0.726726000
C	-2.928447000	1.413724000	-1.424603000
C	-3.187910000	-1.027483000	-1.175873000
C	-3.459094000	0.327925000	-0.726726000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2286.12812$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2285.79613$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2284.98121$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2284.64922$



D

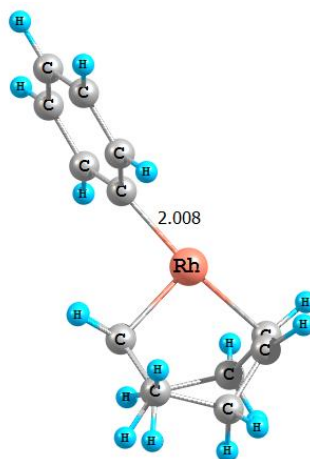
C	0.805383000	0.603332000	1.418426000
C	2.321543000	0.799568000	-1.026880000
C	2.203767000	-0.548977000	-1.324727000
C	0.915449000	-0.813880000	1.242866000
C	2.647520000	-1.703086000	-0.440655000
C	2.241092000	-1.553669000	1.048772000
C	1.953436000	1.596306000	1.382708000
C	2.968334000	1.351215000	0.235352000
H	2.175655000	1.509389000	-1.841885000
H	2.003585000	-0.816643000	-2.364560000
H	-0.053500000	0.953142000	1.992061000
H	0.120919000	-1.410708000	1.690970000
H	2.481597000	1.609673000	2.350321000
H	3.469805000	2.296585000	-0.001767000
H	3.735785000	-1.854701000	-0.516118000
H	2.159924000	-2.554087000	1.488736000
H	3.757037000	0.669744000	0.570866000
H	1.515051000	2.595025000	1.264891000
H	2.186472000	-2.613896000	-0.840290000
H	3.033076000	-1.044924000	1.610495000
Rh	0.208028000	0.080038000	-0.512707000
C	-1.739935000	0.000328000	-0.033766000
C	-2.428571000	-1.194355000	0.259920000
C	-2.513612000	1.168056000	-0.211424000
C	-3.825149000	-1.230302000	0.327861000
H	-1.871921000	-2.115413000	0.424382000
C	-3.909903000	1.135515000	-0.140017000
H	-2.022076000	2.121538000	-0.407330000
C	-4.570165000	-0.065876000	0.128842000
H	-4.331566000	-2.169346000	0.542217000
H	-4.480967000	2.050311000	-0.285220000
H	-5.655262000	-0.092445000	0.190365000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -654.27314$

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -654.04260$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -653.94643$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -653.71589$



B(OH)₃

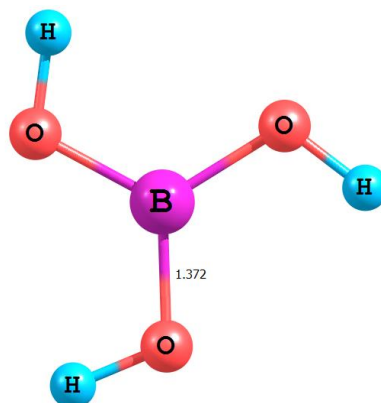
O	1.240295000	-0.586677000	-0.000173000
H	1.165651000	-1.551412000	0.001289000
B	-0.000061000	-0.000066000	-0.000042000
O	-0.111940000	1.367335000	-0.000075000
H	0.760918000	1.784790000	0.000090000
O	-1.128351000	-0.780619000	-0.000088000
H	-1.926298000	-0.233363000	0.000698000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -252.47085$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -252.44858$

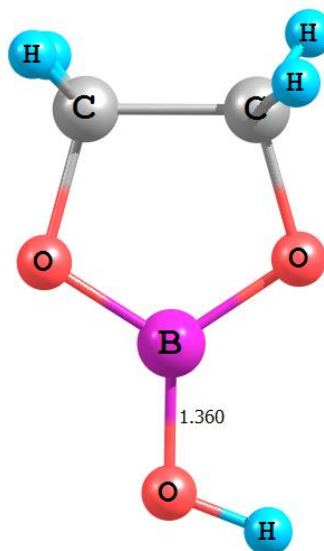
$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -252.45916$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -252.43689$



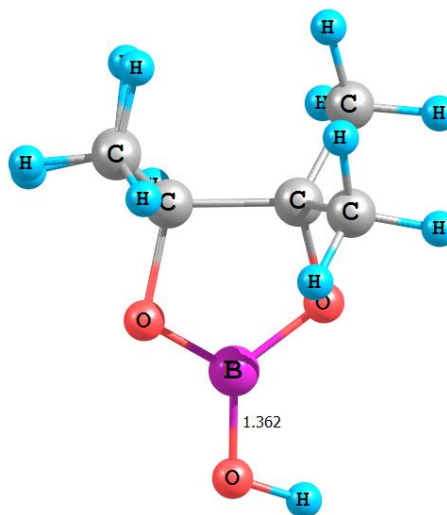
B(OH)-(O-C₂H₄-O)

O	-0.023906000	-1.167162000	0.064686000
B	0.766975000	-0.045518000	0.001210000
O	0.057443000	1.138453000	-0.062765000
O	2.124876000	-0.116984000	0.001604000
H	2.515005000	0.768061000	-0.019850000
C	-1.330156000	0.807181000	0.070818000
C	-1.381929000	-0.737626000	-0.072255000
H	-1.995438000	-1.213972000	0.699143000
H	-1.758426000	-1.048083000	-1.054819000
H	-1.905828000	1.325487000	-0.702594000
H	-1.684984000	1.144313000	1.052489000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -329.87133$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -329.81501$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -329.80040$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -329.74408$ 

B(OH)-(O-C₂(Me)₂H₄-O)

O	-0.802062000	-1.114604000	-0.418381000
B	-1.594531000	-0.068082000	-0.015653000
O	-0.884020000	1.040681000	0.399004000
O	-2.954775000	-0.138868000	-0.030183000
H	-3.340150000	0.705629000	0.243482000
C	0.506947000	0.800696000	0.046462000
C	0.559612000	-0.777819000	-0.044367000
C	1.393587000	1.421206000	1.124538000
H	2.451458000	1.210372000	0.929692000
H	1.261358000	2.508175000	1.128702000
H	1.140758000	1.047534000	2.119519000
C	0.749446000	1.493083000	-1.301573000
H	0.491479000	2.552767000	-1.208005000
H	1.796879000	1.420139000	-1.612644000
H	0.123626000	1.060202000	-2.088672000
C	1.503957000	-1.335625000	-1.108034000
H	2.542663000	-1.057449000	-0.895173000
H	1.441084000	-2.428575000	-1.115509000
H	1.243167000	-0.977868000	-2.106758000
C	0.831204000	-1.451746000	1.307948000
H	0.649131000	-2.526425000	1.210261000
H	1.866099000	-1.304389000	1.634773000
H	0.163529000	-1.066147000	2.085246000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -487.14028$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -486.97741$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -486.98941$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -486.82654$ 

E

C	-5.51099200	-0.53636900	1.34461100
C	-4.07491100	-2.67023900	-0.00587500
C	-4.44745400	-2.24283700	-1.25988500
C	-6.14387300	-0.32024800	0.09559900
C	-5.86383000	-2.05151400	-1.77131900
C	-6.82209400	-1.39712400	-0.75041200
C	-5.35600600	-1.86489100	2.05609900
C	-5.01710300	-3.05089700	1.12148300
H	-3.04056400	-2.96511700	0.12975800
H	-3.68403500	-2.26411300	-2.03693000
H	-5.46017300	0.32347900	2.01074300
H	-6.50826900	0.68980100	-0.08029800
H	-6.26861700	-2.09400400	2.63037300
H	-4.55023500	-3.84410700	1.71680800
H	-6.27392400	-3.01427800	-2.11590000
H	-7.65473100	-0.94150300	-1.29844900
H	-5.93476600	-3.48389300	0.71202800
H	-4.55368800	-1.75250100	2.79553500
H	-5.80959200	-1.41133600	-2.66014900
H	-7.27335700	-2.15805200	-0.10434600
Rh	-4.00028700	-0.26749300	-0.15022700
C	-4.15415000	1.75621200	0.03837500
C	-4.37718600	2.46262400	-1.16094000
C	-4.12019200	2.50795500	1.22567500
C	-4.53229900	3.85268900	-1.17686100
H	-4.42832900	1.92371500	-2.10743200
C	-4.27767200	3.89938000	1.21665600
H	-3.94791900	2.01241500	2.17914700
C	-4.48213000	4.57916500	0.01545000
H	-4.69630700	4.36586800	-2.12233400
H	-4.23730500	4.45058600	2.15416100
H	-4.60425000	5.65927200	0.00719700
C	4.09412500	1.02417500	2.58323100
C	3.09109400	2.07685000	2.59078200
C	1.79456700	1.80009000	3.02780700
C	1.44798900	0.46383700	3.48098300
C	2.41213500	-0.54593700	3.47650100
C	3.76143700	-0.25985800	3.01611000
C	4.92009300	1.20112100	1.39966000
C	4.42983900	2.36304300	0.67849000
C	3.29964500	2.90470700	1.41447500
C	2.20360800	3.42556000	0.72501300
C	0.65366800	2.34039000	2.30844000
C	0.09207000	0.17909300	3.04236000
C	-0.24980000	-1.10101600	2.61276600
C	0.75424800	-2.15171800	2.60727800
C	2.05777500	-1.88129900	3.02953900
C	3.18680300	-2.42197100	2.29220000
C	4.24116800	-1.42077000	2.28437800
C	5.03344100	-1.25110900	1.14815200
C	5.38167100	0.08638300	0.69704600
C	4.41922900	2.36439200	-0.71798300
C	4.89861200	1.20421600	-1.44884900
C	5.37027000	0.08786900	-0.75559500
C	5.01546600	-1.24914600	-1.20408700
C	4.80662300	-2.07627400	-0.02710000
C	3.79545100	-3.03744400	-0.02011000
C	2.96882600	-3.21349100	1.16262400
C	1.61235300	-3.48974400	0.72400800
C	0.52991200	-2.96993900	1.43107400
C	-0.40006700	1.34086100	2.31429600
C	-1.11583600	-1.27443700	-1.40519500
C	-1.66642700	-0.16169700	-0.71568100
C	-1.23149600	1.17569700	-1.15103200
C	-0.43747100	1.34711800	-2.28193000
C	0.04702800	0.18576300	-3.01429100
C	0.71551700	-2.14968800	-2.59981900
C	0.50804600	-2.97106800	-1.42205100
C	-0.62527700	-2.42327200	-0.68896100
C	-0.61235500	-2.41754800	0.71507400
C	-1.10389800	-1.27677200	1.44588500
C	-1.64170500	-0.16122800	0.76419200
C	-0.99245000	1.99034100	0.02139100
C	0.01237300	2.95883300	0.01405900
C	0.83645300	3.14242300	-1.16661800
C	0.61768700	2.34663800	-2.29097500
C	1.74778400	1.80700000	-3.02800400
C	1.39507400	0.47165400	-3.47723000
C	2.35836400	-0.53863700	-3.48749700
C	2.01176700	-1.87704100	-3.03977200
C	1.60161800	-3.49102600	-0.73298400
C	2.95101800	-3.21195800	-1.19067500
C	3.15268000	-2.41921900	-2.32261600
C	4.20603900	-1.41694700	-2.32834700
C	3.71504000	-0.25242300	-3.05001800
C	4.05337700	1.02908300	-2.61923300
C	3.05115600	2.08238600	-2.61027800
C	3.27808300	2.90802100	-1.43594400
C	2.19263300	3.42732900	-0.72910500
C	-1.21041200	1.17172100	1.19546000
C	0.85459500	3.13896800	1.18189700
C	-0.28795700	-1.09784400	-2.58679800

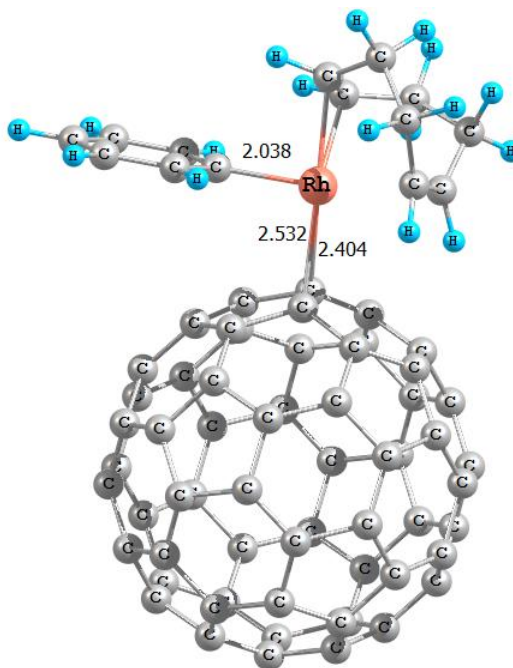
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2940.41188$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2939.82758$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.95319$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.36889$$

In [5,6] bond



E-F

C	-5.510992000	-0.536369000	1.344611000
C	-4.074911000	-2.670239000	-0.005875000
C	-4.447454000	-2.242837000	-1.259885000
C	-6.143873000	-0.320248000	0.095599000
C	-5.863830000	-2.051514000	-1.771319000
C	-6.822094000	-1.397124000	-0.750412000
C	-5.356006000	-1.864891000	2.056099000
C	-5.017103000	-3.050897000	1.121483000
H	-3.040564000	-2.965117000	0.129758000
H	-3.684035000	-2.264113000	-2.036930000
H	-5.460173000	0.323479000	2.010743000
H	-6.508269000	0.689801000	-0.080298000
H	-6.268617000	-2.094004000	2.630373000
H	-4.550235000	-3.844107000	1.716808000
H	-6.273924000	-3.014278000	-2.115900000
H	-7.654731000	-0.941503000	-1.298449000
H	-5.934766000	-3.483893000	0.712028000
H	-4.553688000	-1.752501000	2.795535000
H	-5.809592000	-1.411336000	-2.660149000
H	-7.273357000	-2.158052000	-0.104346000
Rh	-4.000287000	-0.267493000	-0.150227000
C	-4.154150000	1.756212000	0.038375000
C	-4.377186000	2.462624000	-1.160940000
C	-4.120192000	2.507955000	1.225675000
C	-4.532299000	3.852689000	-1.176861000
H	-4.428329000	1.923715000	-2.107432000
C	-4.277672000	3.899380000	1.216656000
H	-3.947919000	2.012415000	2.179147000
C	-4.482130000	4.579165000	0.015450000
H	-4.696307000	4.365868000	-2.122334000
H	-4.237305000	4.450586000	2.154161000
H	-4.604250000	5.659272000	0.007197000
C	4.094125000	1.024175000	2.583231000
C	3.091094000	2.076850000	2.590782000
C	1.794567000	1.800090000	3.027807000
C	1.447989000	0.463837000	3.480983000
C	2.412135000	-0.545937000	3.476501000
C	3.761437000	-0.259858000	3.016110000
C	4.920093000	1.201121000	1.399660000
C	4.429839000	2.630430000	0.678490000
C	3.299645000	2.904707000	1.414475000
C	2.203608000	3.425560000	0.725013000
C	0.653668000	2.340390000	2.308444000
C	0.092070000	0.179093000	3.042360000
C	-0.249800000	-1.101016000	2.612766000
C	0.754248000	-2.151718000	2.607278000
C	2.057775000	-1.881299000	3.029539000
C	3.186803000	-2.421971000	2.292200000
C	4.241168000	-1.420770000	2.284378000
C	5.033441000	-1.251109000	1.148152000
C	5.381671000	0.086383000	0.697046000
C	4.419229000	2.364392000	-0.717983000
C	4.898612000	1.204216000	-1.448849000
C	5.370270000	0.087869000	-0.755595000
C	5.015466000	-1.249146000	-1.204087000
C	4.806622000	-2.076274000	-0.027100000
C	3.795451000	-3.037744000	-0.020110000
C	2.968826000	-3.213491000	1.162624000
C	1.612353000	-3.489744000	0.724008000
C	0.529912000	-2.969939000	1.431074000
C	-0.400067000	1.340861000	2.314296000
C	-1.115836000	-1.274437000	-1.405195000
C	-1.666427000	-0.161697000	-0.715681000
C	-1.231496000	1.175697000	-1.151032000
C	-0.437471000	1.347118000	-2.281930000
C	0.047028000	0.185763000	-3.014291000
C	0.715517000	-2.149688000	-2.599819000
C	0.508046000	-2.971068000	-1.422051000
C	-0.625277000	-2.423272000	-0.688961000
C	-0.612355000	-2.417548000	0.715074000
C	-1.103898000	-1.276772000	1.445885000
C	-1.641705000	-0.161228000	0.764192000
C	-0.992450000	1.990341000	0.021391000
C	0.012373000	2.958833000	0.014059000
C	0.836453000	3.142423000	-1.166618000
C	0.617687000	2.346638000	-2.290975000
C	1.747784000	1.807000000	-3.028004000
C	1.395074000	0.471654000	-3.477230000
C	2.358364000	-0.538637000	-3.487497000
C	2.011767000	-1.877041000	-3.039772000
C	1.601618000	-3.491026000	-0.732984000
C	2.951018000	-3.211958000	-1.190675000
C	3.152680000	-2.419219000	-2.322616000
C	4.206039000	-1.416947000	-2.328347000
C	3.715040000	-0.252424000	-3.050018000
C	4.053377000	1.029083000	-2.619233000
C	3.051156000	2.082386000	-2.610278000
C	3.278083000	2.908021000	-1.435944000
C	2.192633000	3.427329000	-0.729105000
C	-1.210412000	1.171721000	1.195460000
C	0.854595000	3.138968000	1.181897000
C	-0.287957000	-1.097844000	-2.586798000

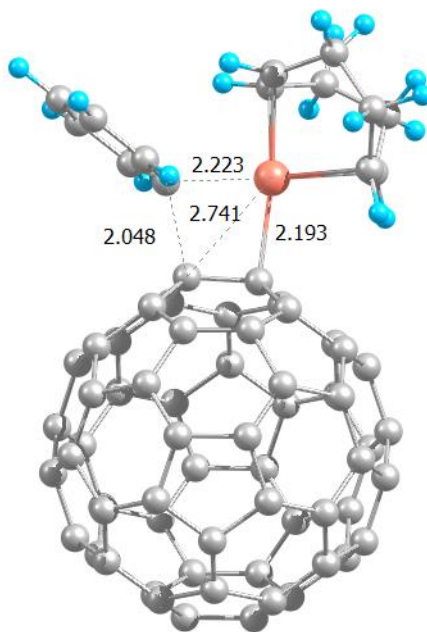
$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2940.38250$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2939.79685$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.92844$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.34279$

In [5,6] bond



E

C	-5.725768000	-0.400602000	1.108908000
C	-4.145926000	-2.671948000	0.271466000
C	-4.246948000	-2.349149000	-1.067926000
C	-6.082757000	-0.298768000	-0.243678000
C	-5.518208000	-2.174339000	-1.870878000
C	-6.631011000	-1.423284000	-1.112020000
C	-5.753689000	-1.650624000	1.962440000
C	-5.301100000	-2.928433000	1.222287000
H	-3.174991000	-2.999471000	0.628808000
H	-3.352287000	-2.475144000	-1.673637000
H	-5.739241000	0.523323000	1.682101000
H	-6.305400000	0.702554000	-0.601210000
H	-6.762857000	-1.793353000	2.381775000
H	-4.987663000	-3.672775000	1.962780000
H	-5.882172000	-3.154862000	-2.216579000
H	-7.328461000	-0.995672000	-1.841037000
H	-6.141175000	-3.376165000	0.683071000
H	-5.090431000	-1.480730000	2.818835000
H	-5.261945000	-1.609130000	-2.774755000
H	-7.220845000	-2.117894000	-0.505357000
Rh	-3.860973000	-0.321696000	-0.037507000
C	-4.092266000	1.750507000	0.017293000
C	-4.282293000	2.436415000	-1.195280000
C	-4.155959000	2.500740000	1.202678000
C	-4.538303000	3.812168000	-1.221324000
H	-4.230427000	1.895797000	-2.138872000
C	-4.412446000	3.877408000	1.181133000
H	-3.990664000	2.016459000	2.163283000
C	-4.606488000	4.539824000	-0.031415000
H	-4.682804000	4.313058000	-2.176398000
H	-4.454910000	4.429668000	2.117690000
H	-4.804319000	5.608399000	-0.050124000
C	3.312382000	0.830317000	-3.137740000
C	2.642224000	-0.423186000	-3.444442000
C	1.248487000	-0.484000000	-3.453292000
C	0.463426000	0.704106000	-3.161303000
C	1.108242000	1.909139000	-2.870356000
C	2.559783000	1.972354000	-2.855721000
C	4.493010000	0.525005000	-2.349756000
C	4.555958000	-0.917523000	-2.172019000
C	3.413317000	-1.503780000	-2.849168000
C	2.759812000	-2.604275000	-2.291588000
C	0.567085000	-1.628821000	-2.872855000
C	-0.704228000	0.299151000	-2.402171000
C	-1.187000000	1.103868000	-1.376302000
C	-0.506423000	2.342748000	-1.061495000
C	0.611661000	2.746548000	-1.797494000
C	1.754259000	3.335958000	-1.118092000
C	2.959769000	2.855410000	-1.772423000
C	4.095376000	2.561698000	-1.015344000
C	4.877146000	1.373117000	-1.309632000
C	5.000929000	-1.452576000	-0.961479000
C	5.399246000	-0.568674000	0.121515000
C	5.338137000	0.815021000	-0.048831000
C	4.840681000	1.659612000	1.024611000
C	4.073072000	2.738968000	0.427507000
C	2.916005000	3.202897000	1.055340000
C	1.733401000	3.506072000	0.266417000
C	0.568654000	3.093294000	1.031600000
C	-0.525098000	2.516910000	0.379290000
C	-0.636702000	-1.152190000	-2.222814000
C	-0.712365000	-0.593397000	2.345959000
C	-1.102269000	-1.438078000	1.313149000
C	-0.307092000	-2.610409000	1.014000000
C	0.827783000	-2.915114000	1.773307000
C	1.224988000	-2.038207000	2.854546000
C	1.138395000	0.359334000	3.437514000
C	0.369642000	1.439312000	2.841873000
C	-0.773365000	0.858774000	2.166898000
C	-1.211690000	1.386969000	0.961064000
C	-1.713198000	0.520409000	-0.124185000
C	-1.657135000	-0.902314000	0.048243000
C	-0.280488000	-2.785866000	-0.428040000
C	0.874665000	-3.261385000	-1.056855000
C	2.055632000	-3.569538000	-0.266732000
C	2.032475000	-3.399217000	1.117575000
C	3.176373000	-2.814349000	1.797210000
C	2.676781000	-1.971719000	2.870964000
C	3.317143000	-0.766762000	3.165673000
C	2.531895000	0.422230000	3.457753000
C	1.027396000	2.542414000	2.290194000
C	2.478235000	2.605120000	2.306578000
C	3.216354000	1.567441000	2.879691000
C	4.420151000	1.085850000	2.226056000
C	4.482494000	-0.356963000	2.402885000
C	4.963571000	-1.167087000	1.372700000
C	4.296948000	-2.420400000	1.063380000
C	4.320580000	-2.596973000	-0.379744000
C	3.222674000	-3.161787000	-1.031337000
C	-1.054784000	-1.721429000	-1.025836000
C	1.308467000	-2.669181000	-2.304976000
C	0.469451000	-0.894382000	3.129415000

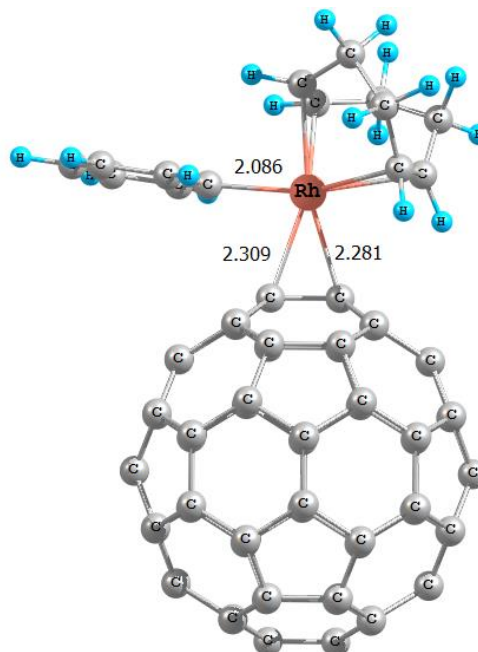
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2940.41791$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2939.83211$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.96673$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.38093$$

In [6,6] bond



E-F

C	-5.873718000	-0.147010000	0.949932000
C	-4.344353000	-2.528672000	0.475775000
C	-4.332001000	-2.354467000	-0.912453000
C	-6.088197000	-0.137787000	-0.428826000
C	-5.544096000	-2.215012000	-1.813588000
C	-6.649555000	-1.304059000	-1.232045000
C	-6.098813000	-1.316456000	1.888085000
C	-5.600000000	-2.668598000	1.327507000
H	-3.435043000	-2.917375000	0.928454000
H	-3.423932000	-2.646170000	-1.437707000
H	-5.820360000	0.820206000	1.444897000
H	-6.155867000	0.836275000	-0.907761000
H	-7.163741000	-1.390540000	2.160818000
H	-5.386154000	-3.341731000	2.165469000
H	-5.958073000	-3.207370000	-2.054089000
H	-7.253455000	-0.909594000	-2.057247000
H	-6.390198000	-3.155799000	0.746600000
H	-5.562066000	-1.098756000	2.819278000
H	-5.197781000	-1.792922000	-2.764773000
H	-7.336426000	-1.888082000	-0.610771000
Rh	-3.902348000	-0.401053000	-0.015623000
C	-3.602777000	1.773052000	0.012402000
C	-3.912273000	2.379691000	-1.221622000
C	-3.860566000	2.499842000	1.189148000
C	-4.531574000	3.629525000	-1.272154000
H	-3.669840000	1.868981000	-2.150667000
C	-4.472672000	3.754073000	1.140127000
C	-3.582113000	2.081167000	2.153342000
C	-4.814291000	4.321968000	-0.090427000
H	-4.778643000	4.070190000	-2.235065000
H	-4.673183000	4.292019000	2.063642000
H	-5.277523000	5.304083000	-0.129784000
C	3.440935000	1.378077000	-2.867417000
C	2.665119000	0.291067000	-3.444630000
C	1.271654000	0.359223000	-3.453187000
C	0.596657000	1.516106000	-2.893097000
C	1.342661000	2.564877000	-2.347162000
C	2.792666000	2.492943000	-2.331291000
C	4.579367000	0.798388000	-2.179503000
C	4.508544000	-0.647209000	-2.332328000
C	3.329723000	-0.960930000	-3.118695000
C	2.570614000	-2.094444000	-2.818931000
C	0.478941000	-0.820988000	-3.145424000
C	-0.609555000	1.057059000	-2.234413000
C	-1.032660000	1.654083000	-1.059124000
C	-0.247938000	2.716450000	-0.478685000
C	0.909189000	3.180239000	-1.112040000
C	2.090928000	3.497225000	-0.325096000
C	3.256829000	3.069759000	-1.080004000
C	4.350888000	2.510282000	-0.416962000
C	5.025395000	1.351889000	-0.977326000
C	4.888129000	-1.479131000	-1.277058000
C	5.348035000	-0.901215000	-0.025250000
C	5.417308000	0.485181000	0.121391000
C	4.981608000	1.106906000	1.360974000
C	4.323641000	2.358811000	1.028895000
C	3.203632000	2.772068000	1.753269000
C	2.064870000	3.351658000	1.061183000
C	0.856146000	2.883247000	1.721436000
C	-0.275379000	2.565077000	0.964079000
C	-0.688685000	-0.400594000	-2.403506000
C	-0.773081000	-0.880419000	2.181629000
C	-1.203935000	-1.415631000	0.975474000
C	-0.521719000	-2.562621000	0.419318000
C	0.567175000	-3.136731000	1.086479000
C	1.023801000	-2.570821000	2.336353000
C	1.143570000	-0.363542000	3.438552000
C	0.485004000	0.887271000	3.106378000
C	-0.693873000	0.579070000	2.321676000
C	-1.080087000	1.409396000	1.282779000
C	-1.713570000	0.883244000	0.030832000
C	-1.749495000	-0.585072000	-0.124897000
C	-0.495756000	-2.412437000	-1.022629000
C	0.619965000	-2.839543000	-1.753374000
C	1.756122000	-3.422798000	-1.058761000
C	1.730479000	-3.568341000	0.328899000
C	2.912751000	-3.258033000	1.115455000
C	2.474223000	-2.636884000	2.355261000
C	3.217369000	-1.593569000	2.911931000
C	2.536608000	-0.434060000	3.465710000
C	1.246646000	2.023180000	2.817055000
C	2.696852000	1.950410000	2.840251000
C	3.329090000	0.745673000	3.155536000
C	4.493980000	0.317204000	2.404306000
C	4.423630000	-1.128677000	2.251868000
C	4.844808000	-1.724933000	1.061561000
C	4.072958000	-2.810387000	0.481937000
C	4.099717000	-2.658313000	-0.964221000
C	2.965478000	-2.960633000	-1.719386000
C	-1.165712000	-1.174613000	-1.354773000
C	1.119911000	-2.028160000	-2.840514000
C	0.367723000	-1.450987000	2.862091000

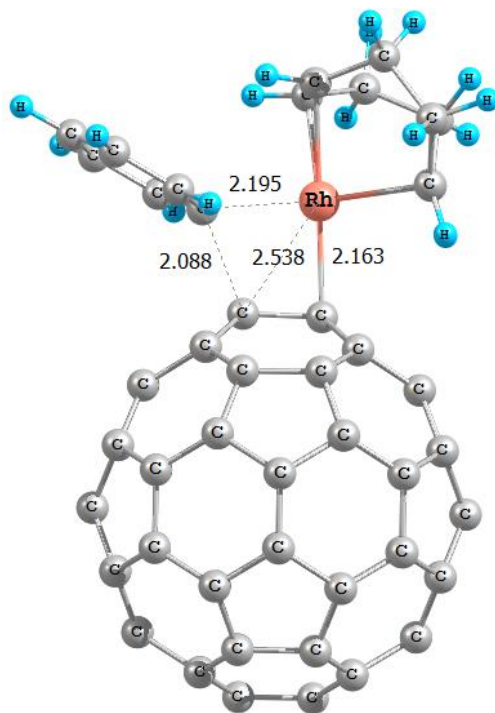
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2940.39991$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2939.81245$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.94794$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.36048$$

In [6,6] bond



F

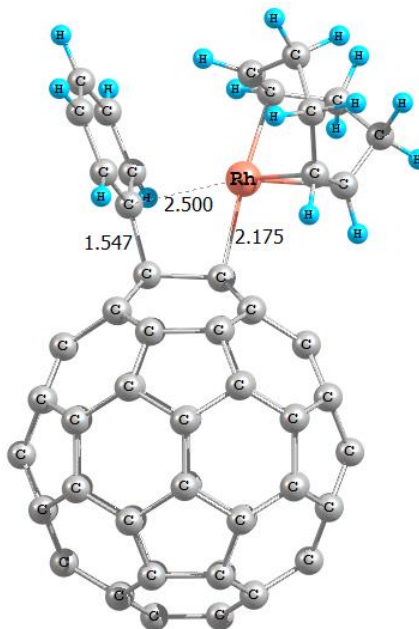
C	5.950018000	-0.519418000	-1.207449000
C	4.238520000	-2.396489000	0.087340000
C	4.350735000	-1.760941000	1.346215000
C	6.255424000	-0.066438000	0.073735000
C	5.635833000	-1.477682000	2.099338000
C	6.775284000	-0.945944000	1.201042000
C	6.015871000	-1.954581000	-1.697432000
C	5.415161000	-2.971666000	-0.700713000
H	3.276568000	-2.851115000	-0.138127000
H	3.471380000	-1.785911000	1.986738000
H	5.922252000	0.225482000	-2.002540000
H	6.406376000	1.003133000	0.199098000
H	7.052214000	-2.230582000	-1.948882000
H	5.072966000	-3.852117000	-1.255739000
H	5.964198000	-2.380468000	2.639299000
H	7.473084000	-0.365337000	1.815163000
H	6.185155000	-3.333133000	-0.010508000
H	5.451075000	-2.004893000	-2.635585000
H	5.406947000	-0.730074000	2.868161000
H	7.356814000	-1.776954000	0.789172000
H	4.022544000	-0.264201000	-0.148597000
Rh	3.074695000	2.041774000	0.035550000
C	3.646573000	2.666378000	1.165579000
C	3.779073000	2.102893000	-1.187361000
C	4.834177000	3.382151000	1.058362000
H	3.119275000	2.626236000	2.113528000
C	4.974351000	2.839339000	-1.289819000
H	3.319749000	1.707389000	-2.090178000
C	5.495968000	3.484846000	-0.175501000
H	5.238122000	3.883888000	1.933520000
H	5.474004000	2.913904000	-2.251923000
H	6.406460000	4.071727000	-0.258423000
C	-3.603231000	0.872722000	2.998782000
C	-2.687411000	-0.161943000	3.455290000
C	-1.313453000	0.080852000	3.463462000
C	-0.798154000	1.365733000	3.031014000
C	-1.680632000	2.365267000	2.606559000
C	-3.109458000	2.112495000	2.585999000
C	-4.608442000	0.229328000	2.255204000
C	-4.413892000	-1.204199000	2.254608000
C	-3.195869000	-1.447292000	3.003389000
C	-2.304186000	-2.438384000	2.585879000
C	-0.381918000	-0.950007000	3.032543000
C	0.448621000	1.140459000	2.330309000
C	0.788310000	1.915245000	1.240309000
C	-0.145975000	2.905876000	0.771678000
C	-1.346021000	3.156425000	1.447853000
C	-2.568801000	3.402667000	0.697190000
C	-3.660482000	2.753858000	1.402530000
C	-4.684141000	2.132315000	0.683715000
C	-5.197965000	0.844902000	1.118012000
C	-4.701896000	-1.962977000	1.117844000
C	-5.245786000	-1.319383000	-0.066236000
C	-5.491997000	0.055242000	-0.065988000
C	-5.154637000	0.853128000	-1.232846000
C	-4.657625000	2.137448000	-0.770544000
C	-3.608675000	2.764389000	-1.446556000
C	-2.544032000	3.408219000	-0.696134000
C	-1.294870000	3.165651000	-1.401427000
C	-0.122659000	2.908863000	-0.679982000
C	0.716200000	-0.314282000	2.345171000
C	0.804355000	-0.299136000	-2.248034000
C	1.323989000	-0.899462000	-1.106621000
C	0.774119000	-2.170494000	-0.680763000
C	-0.239316000	-2.807724000	-1.405654000
C	-0.775995000	-2.177662000	-2.588275000
C	-1.185092000	0.103683000	-3.437652000
C	-0.688499000	1.385323000	-2.976775000
C	0.528686000	1.152924000	-2.229925000
C	0.817131000	1.915057000	-1.118289000
C	1.662631000	1.410256000	0.072435000
C	1.861143000	-0.157315000	0.073215000
C	0.743566000	-2.173522000	0.765163000
C	-0.294662000	-2.818121000	1.449300000
C	-1.356181000	-3.466564000	0.697060000
C	-1.329378000	-3.460343000	-0.697718000
C	-2.549941000	-3.219061000	-1.447905000
C	-2.205868000	-2.419653000	-2.614168000
C	-3.083000000	-1.426338000	-3.058124000
C	-2.558629000	-0.138359000	-3.482110000
C	-1.585192000	2.382998000	-2.577919000
C	-3.013378000	2.130362000	-2.612163000
C	-3.490890000	0.893561000	-3.052804000
C	-4.582871000	0.245232000	-2.353695000
C	-4.328173000	-1.188546000	-2.353550000
C	-4.658170000	-1.955024000	-1.233472000
C	-3.749155000	-2.989392000	-0.771613000
C	-3.776796000	-2.994779000	0.683077000
C	-2.604298000	-3.230482000	1.402655000
C	1.267839000	-0.904487000	1.217296000
C	-0.874205000	-2.195118000	2.613465000
C	-0.268231000	-0.930002000	-2.980202000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2940.43664$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2939.84708$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.98851$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2938.39895$$



G

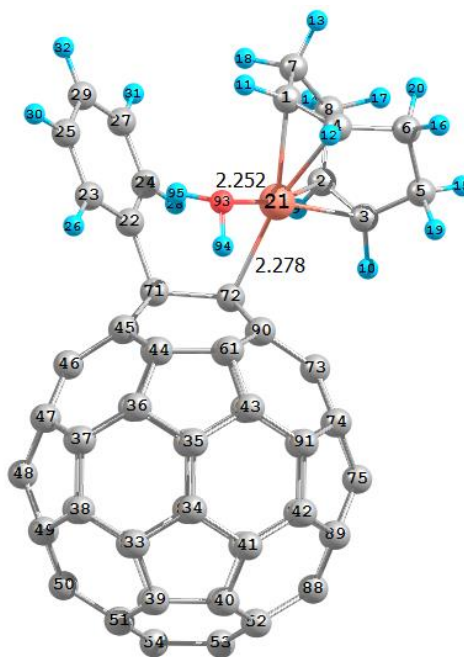
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C	-5.803262000	-1.428973000	-1.252590000
C	-4.848999000	-3.407232000	0.014939000
C	-6.071577000	-2.833343000	-0.733245000
C	-6.764267000	-0.216532000	0.829870000
C	-6.049110000	-1.118915000	1.864707000
H	-3.881769000	-0.914758000	2.317484000
H	-3.026624000	-2.664542000	0.962358000
H	-6.221888000	0.655554000	-1.126432000
H	-5.627637000	-1.333860000	-2.322375000
H	-7.832165000	-0.478050000	0.769359000
H	-6.156888000	-0.675064000	2.860718000
H	-5.158684000	-4.207105000	0.706631000
H	-6.323395000	-3.489664000	-1.573715000
H	-6.538314000	-2.098398000	1.920802000
H	-6.721175000	0.821936000	1.172596000
H	-4.172762000	-3.875594000	-0.710050000
H	-6.951078000	-2.825245000	-0.080209000
Rh	-3.984149000	-0.534679000	-0.346511000
C	-2.873916000	2.371599000	0.155729000
C	-3.236117000	3.297947000	-0.835342000
C	-3.699061000	2.256791000	1.286700000
C	-4.402184000	4.065264000	-0.714981000
H	-2.582004000	3.453447000	-1.689948000
C	-4.847599000	3.037224000	1.418355000
H	-3.419713000	1.572313000	2.081389000
C	-5.211836000	3.938045000	0.412471000
H	-4.659458000	4.775229000	-1.496632000
H	-5.456911000	2.947027000	2.313928000
H	-6.107160000	4.544379000	0.516948000
C	3.545714000	0.691776000	-3.086389000
C	2.571983000	-0.322726000	-3.461711000
C	1.206685000	-0.028614000	-3.413031000
C	0.764939000	1.286010000	-2.997910000
C	1.701174000	2.266954000	-2.653309000
C	3.118807000	1.962243000	-2.693594000
C	4.623974000	0.034843000	-2.373587000
C	4.317281000	-1.387057000	-2.310325000
C	3.055709000	-1.608393000	-2.992396000
C	2.146719000	-2.547725000	-2.495997000
C	0.256648000	-1.007194000	-2.906991000
C	-0.451340000	1.130856000	-2.227892000
C	-0.707724000	1.951450000	-1.148544000
C	0.283911000	2.920880000	-0.764435000
C	1.453818000	3.107810000	-1.508871000
C	2.720168000	3.335561000	-0.828644000
C	3.751584000	2.623950000	-1.563104000
C	4.786162000	1.988505000	-0.872770000
C	5.230469000	0.668367000	-1.285701000
C	4.632695000	-2.116285000	-1.162009000
C	5.256852000	-1.454290000	-0.029071000
C	5.535813000	-0.090841000	-0.089604000
C	5.303371000	0.757617000	1.062866000
C	4.830767000	2.043431000	0.579849000
C	3.839269000	2.731427000	1.282859000
C	2.763663000	3.389677000	0.563010000
C	1.542324000	3.218331000	1.336924000
C	0.327253000	2.981124000	0.684341000
C	-0.799571000	-0.307745000	-2.203847000
C	-0.638106000	-0.130453000	2.400692000
C	-1.230311000	-0.743236000	1.304605000
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C	0.276429000	-2.703625000	1.605293000
C	0.892049000	-2.054804000	2.735543000
C	1.421594000	0.236165000	3.480547000
C	0.948464000	1.519375000	3.001419000
C	-0.315086000	1.310804000	2.326501000
C	-0.629072000	2.041325000	1.202689000
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C	-1.813701000	-0.031381000	0.129352000
C	-0.786730000	-2.105711000	-0.534419000
C	0.188107000	-2.807121000	-1.244983000
C	1.259871000	-3.474291000	-0.524699000
C	1.303584000	-3.420695000	0.860920000
C	2.567978000	-3.202846000	1.550359000
C	2.311923000	-2.351941000	2.702968000
C	3.243353000	-1.377259000	3.067042000
C	2.786774000	-0.056919000	3.468760000
C	1.861988000	2.468017000	2.526316000
C	3.279775000	2.161243000	2.498920000
C	3.733985000	0.923060000	2.959138000
C	4.766596000	0.210371000	2.231493000
C	4.460355000	-1.210791000	2.294109000
C	4.705993000	-2.026866000	1.187296000
C	3.737812000	-3.041376000	0.807134000
C	3.691969000	-3.096160000	-0.646472000
C	2.477016000	-3.309041000	-1.299064000
C	-1.301239000	-0.833047000	-1.005133000
C	0.728247000	-2.252695000	-2.467068000
C	0.447905000	-0.776604000	3.103054000
O	-3.769971000	0.546549000	-2.310134000
H	-2.885691000	0.309984000	-2.663279000
H	-3.731489000	1.504248000	-2.118395000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3016.86342$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3016.25018$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3015.42067$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3014.80743$



G-H

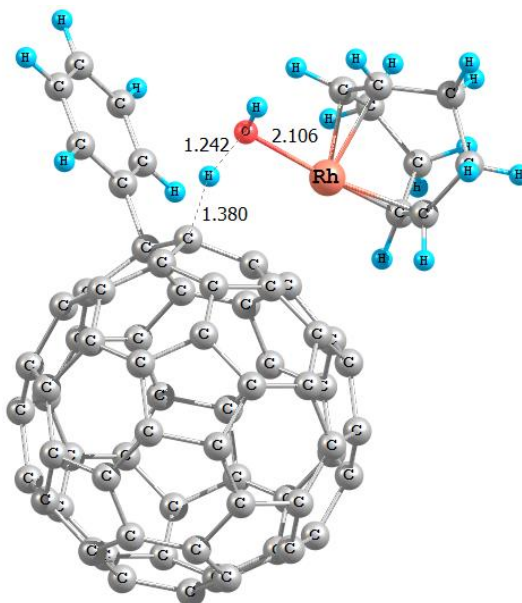
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C	-6.312032000	-0.632831000	1.555601000
C	-5.649444000	-1.963895000	1.975412000
H	-3.436627000	-2.091763000	1.961383000
H	-3.116551000	-3.285492000	-0.081204000
H	-6.028661000	0.839162000	-0.064878000
H	-6.089162000	-0.598049000	-1.967935000
H	-7.402762000	-0.679036000	1.701547000
H	-5.509703000	-1.967999000	3.061880000
H	-5.505032000	-4.447222000	-0.357801000
H	-6.912330000	-2.804199000	-1.907429000
H	-6.308057000	-2.810537000	1.754003000
H	-5.949814000	0.168564000	2.209498000
H	-4.749495000	-3.689943000	-1.751347000
H	-7.155435000	-2.718068000	-0.177221000
Rh	-3.962571000	-0.756163000	-0.329220000
C	-2.381805000	3.224127000	0.127540000
C	-2.529761000	4.186319000	-0.882065000
C	-3.290353000	3.226634000	1.190800000
C	-3.564909000	5.118112000	-0.834727000
H	-1.827367000	4.207312000	-1.711384000
C	-4.328928000	4.161100000	1.241406000
H	-3.190019000	2.493934000	1.986051000
C	-4.471263000	5.109385000	0.229340000
H	-3.660425000	5.856504000	-1.626692000
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C	2.994031000	2.542959000	-2.051770000
C	2.350133000	3.256374000	-0.966501000
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C	4.192154000	2.584722000	0.533193000
C	5.394711000	0.587627000	-0.273554000
C	5.152664000	-0.232844000	-1.450401000
C	4.425079000	0.567458000	-2.418966000
C	3.432227000	-0.018668000	-3.206892000
C	1.958621000	1.935745000	-2.873401000
C	0.919096000	3.096949000	-1.105280000
C	0.123554000	2.965988000	0.013154000
C	0.736596000	2.944754000	1.311572000
C	2.115262000	3.126899000	1.470304000
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C	4.133267000	1.990704000	1.861000000
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C	5.032838000	-1.395862000	1.150715000
C	4.197973000	-1.553357000	2.329339000
C	3.989409000	-0.238369000	2.910064000
C	2.752119000	0.089204000	3.469999000
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C	0.732737000	1.223630000	3.079261000
C	0.031763000	1.974599000	2.129413000
C	0.670667000	2.279920000	-2.312437000
C	-1.648922000	-0.802188000	0.299598000
C	-1.435689000	-0.195888000	-0.959143000
C	-0.798656000	-0.925471000	-2.043208000
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C	-0.112252000	0.039726000	-2.865018000
C	1.118632000	-0.292092000	-3.446079000
C	1.696236000	-1.601829000	-3.200691000
C	1.019014000	-2.537111000	-2.412636000
C	1.747169000	-3.335884000	-1.440933000
C	0.908515000	-3.487765000	-0.260357000
C	1.487031000	-3.480824000	1.012196000
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C	0.428663000	-0.176370000	3.228633000
C	1.672586000	-0.885765000	3.468088000
C	1.876350000	-2.148954000	2.909353000
C	3.162930000	-2.491707000	2.333814000
C	2.921490000	-3.312692000	1.156573000
C	3.724529000	-3.160550000	0.024596000
C	3.124881000	-3.173103000	-1.299698000
C	3.831122000	-2.202236000	-2.122658000
C	3.132595000	-1.434719000	-3.055980000
C	-0.354036000	1.346828000	-2.290338000
C	2.185258000	0.680987000	-3.456458000
C	-0.961691000	-2.085473000	0.534651000
O	-3.898639000	0.992507000	-1.500528000
H	-2.700180000	1.311229000	-1.562700000
H	-4.212743000	0.824181000	-2.405471000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3016.84619$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3016.23888$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3015.39418$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3014.78687$$



I

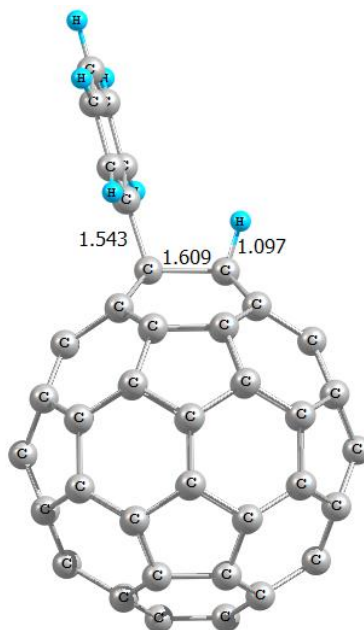
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C	1.903165000	-1.178113000	-2.091016000
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C	0.914506000	0.725151000	-3.033410000
C	2.565487000	1.175322000	0.706336000
C	2.565499000	-1.174938000	0.706958000
C	0.914509000	-0.726746000	-3.033026000
C	1.640255000	-2.284545000	-1.314879000
C	1.978232000	2.278588000	0.126523000
C	0.396210000	3.004832000	-1.471050000
C	-0.284146000	1.425005000	-3.218882000
C	2.097286000	0.725983000	1.989794000
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C	0.396225000	-3.005604000	-1.469460000
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C	1.105581000	-1.423470000	2.688481000
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C	-0.550513000	-2.595065000	-2.415481000
C	-1.531148000	-0.698006000	-3.391267000
C	-0.040542000	-3.448869000	-0.157541000
C	0.508725000	2.593148000	2.088096000
C	-1.398296000	3.469144000	0.160326000
C	-1.962680000	2.598413000	-2.080717000
C	-2.571388000	1.424246000	-2.685149000
C	0.066600000	0.697800000	3.400114000
C	0.508739000	-2.592045000	2.089470000
C	0.066604000	-0.696003000	3.400485000
C	-1.962596000	-2.599514000	-2.079341000
C	-2.571384000	-1.425673000	-2.684398000
C	-1.398279000	-3.469059000	0.162159000
C	-0.904361000	2.599746000	2.418704000
C	-1.840140000	3.027990000	1.474111000
C	-2.379457000	3.027294000	-0.818446000
C	-3.570888000	0.726802000	-2.003437000
C	-1.179494000	1.425692000	3.231479000
C	-0.904349000	-2.598474000	2.420081000
C	-1.179487000	-1.423989000	3.232236000
C	-2.379443000	-3.027730000	-0.816845000
C	-3.570887000	-0.727873000	-2.003055000
C	-1.840125000	-3.027214000	1.475710000
C	-3.085369000	2.304627000	1.305451000
C	-3.418817000	2.304345000	-0.111891000
C	-4.002973000	1.175423000	-0.691346000
C	-2.377764000	0.728096000	3.066899000
C	-2.377759000	-0.726485000	3.067283000
C	-3.418806000	-2.304415000	-0.1110675000
C	-4.002970000	-1.175802000	-0.690725000
C	-3.085356000	-2.303946000	1.305667000
C	-3.349984000	1.176329000	2.085274000
C	-4.271133000	0.000024000	0.120184000
C	-3.349977000	-1.175238000	2.085893000
C	-3.951330000	0.000383000	1.479078000
C	4.722229000	0.000012000	0.014591000
C	5.437318000	1.205181000	0.029007000
C	5.437319000	-1.205156000	0.029249000
C	6.832859000	1.205191000	0.058222000
H	4.902009000	2.150003000	0.025259000
C	6.832860000	-1.205158000	0.058461000
H	4.902010000	-2.149978000	0.025697000
C	7.536536000	0.000019000	0.074164000
H	7.368476000	2.150671000	0.073230000
H	7.368478000	-2.150634000	0.073658000
H	8.622694000	0.000022000	0.101277000
H	3.715755000	-0.000565000	-2.193765000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2518.37760$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2517.94917$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2517.11109$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2516.68266$$



H = L

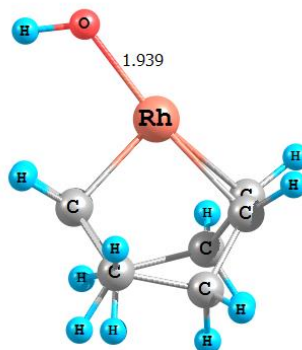
C	-0.900729000	-1.176670000	0.970867000
C	-0.147501000	-0.092466000	-1.505505000
C	0.003235000	1.230485000	-0.973159000
C	-0.983154000	0.155288000	1.420812000
C	-1.087485000	2.038151000	-0.291214000
C	-1.862965000	1.220657000	0.768928000
C	-1.626741000	-1.746732000	-0.240027000
C	-1.467538000	-0.866881000	-1.503266000
H	0.548691000	-0.377078000	-2.295589000
H	0.794953000	1.842043000	-1.409709000
H	-0.583694000	-1.926574000	1.700682000
H	-0.704283000	0.346335000	2.458567000
H	-2.693045000	-1.913218000	-0.021015000
H	-1.512822000	-1.501865000	-2.394878000
H	-1.777580000	2.463470000	-1.037748000
H	-2.246099000	1.898758000	1.539733000
H	-2.303454000	-0.163253000	-1.591522000
H	-1.198241000	-2.735324000	-0.442034000
H	-0.601404000	2.891485000	0.196065000
H	-2.745105000	0.750306000	0.319983000
Rh	0.865211000	-0.150990000	0.320255000
O	2.703394000	0.039815000	-0.268094000
H	2.897708000	0.329968000	-1.173894000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -498.46891$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -498.30781$

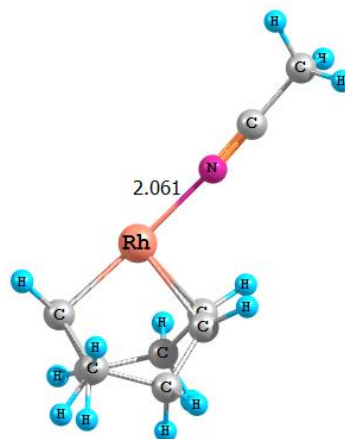
$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -498.26624$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -498.10514$



J

C	-0.289648000	-1.264723000	0.864820000
C	-1.782581000	-0.145905000	-1.249045000
C	-1.693479000	1.161176000	-0.762908000
C	-0.419392000	0.016966000	1.485690000
C	-2.166971000	1.650707000	0.594255000
C	-1.750949000	0.715641000	1.753770000
C	-1.419423000	-2.113243000	0.318896000
C	-2.441773000	-1.303315000	-0.510305000
H	-1.637005000	-0.285793000	-2.322000000
H	-1.508248000	1.949099000	-1.498366000
H	0.612056000	-1.828320000	1.106876000
H	0.403805000	0.323460000	2.130541000
H	-1.918741000	-2.641178000	1.145297000
H	-2.918464000	-1.964609000	-1.239949000
H	-3.256858000	1.793704000	0.584985000
H	-1.663988000	1.303082000	2.672457000
H	-3.245429000	-0.922421000	0.126382000
H	-0.972820000	-2.890697000	-0.310360000
H	-1.730496000	2.641429000	0.757990000
H	-2.522490000	-0.037144000	1.944825000
Rh	0.250660000	0.238836000	-0.511240000
N	2.257250000	0.057073000	-0.076435000
C	3.400979000	-0.007246000	0.094297000
C	4.839606000	-0.087315000	0.305079000
H	5.169322000	-1.127924000	0.220117000
H	5.359037000	0.515131000	-0.447196000
H	5.091652000	0.288600000	1.301940000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -555.21315$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -555.02061$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -555.00830$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -554.81576$ 

K

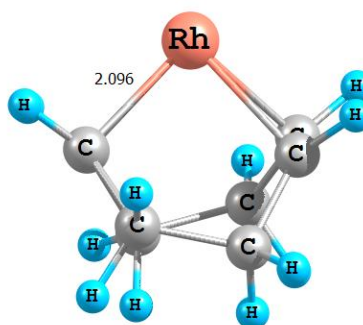
C	0.214749000	1.164138000	1.105605000
C	0.342153000	0.200804000	-1.505863000
C	0.216816000	-1.163603000	-1.105470000
C	0.342501000	-0.200060000	1.505988000
C	1.157648000	-1.913449000	-0.181756000
C	1.496409000	-1.111253000	1.096139000
C	1.153159000	1.916070000	0.181220000
C	1.494649000	1.113548000	-1.095591000
H	-0.202300000	0.496612000	-2.405746000
H	-0.403848000	-1.800213000	-1.743788000
H	-0.407228000	1.799333000	1.744041000
H	-0.201505000	-0.496468000	2.405931000
H	2.065801000	2.198369000	0.725539000
H	1.708986000	1.807037000	-1.913350000
H	2.071361000	-2.191670000	-0.726360000
H	1.710469000	-1.805057000	1.913696000
H	2.398648000	0.513560000	-0.953826000
H	0.661537000	2.853827000	-0.096459000
H	0.669413000	-2.853275000	0.094745000
H	2.399966000	-0.510157000	0.956077000
Rh	-1.132885000	-0.001091000	-0.000047000

$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -422.39358$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -422.24297$

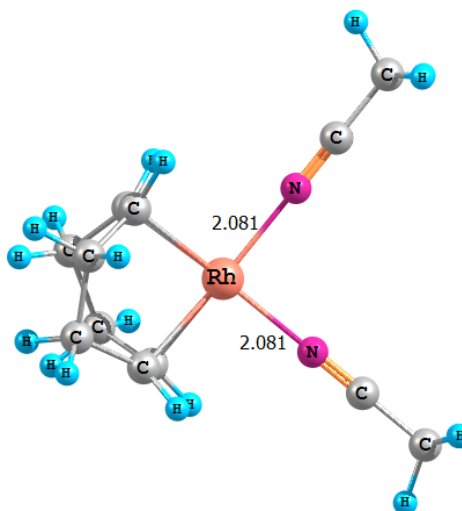
$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -422.27187$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -422.12126$



M

C	-1.343870000	-1.449521000	-0.749522000
C	-1.475193000	1.394576000	-0.643312000
C	-1.343918000	1.449463000	0.749502000
C	-1.475250000	-1.394632000	0.643279000
C	-2.235489000	0.766065000	1.767459000
C	-2.602795000	-0.685107000	1.384903000
C	-2.235367000	-0.766121000	-1.767544000
C	-2.602688000	0.685058000	-1.385023000
H	-0.943014000	2.152081000	-1.216997000
H	-0.740839000	2.260912000	1.156635000
H	-0.740752000	-2.260966000	-1.156605000
H	-0.943105000	-2.152125000	1.217010000
H	-3.145293000	-1.363170000	-1.929619000
H	-2.833196000	1.245921000	-2.296254000
H	-3.145421000	1.363121000	1.929477000
H	-2.833383000	-1.245971000	2.296113000
H	-3.512310000	0.707626000	-0.777675000
H	-1.700898000	-0.762277000	-2.723898000
H	-1.701085000	0.762209000	2.723849000
H	-3.512369000	-0.707662000	0.777481000
Rh	0.094767000	-0.000023000	0.000040000
N	1.565195000	1.471306000	-0.040655000
N	1.565263000	-1.471289000	0.040801000
C	2.379977000	2.292583000	-0.071093000
C	2.380144000	-2.292467000	0.071199000
C	3.406604000	3.326765000	-0.110113000
H	4.028769000	3.268456000	0.788696000
H	4.040143000	3.189337000	-0.992175000
H	2.940588000	4.316007000	-0.157147000
C	3.406861000	-3.326568000	0.109999000
H	4.009742000	-3.287537000	-0.802896000
H	4.059140000	-3.171403000	0.975289000
H	2.941476000	-4.314189000	0.187508000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -688.01945$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -687.78975$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -687.74503$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -687.51533$ 

NOTE: The following energies in solution are calculated with water as the solvent.

N

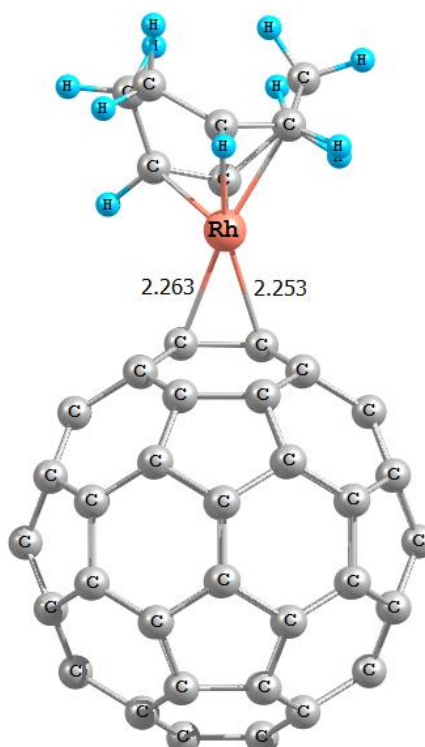
C	5.963555000	-1.035978000	-1.056910000
C	5.119910000	-0.191069000	1.525949000
C	4.855717000	1.143128000	1.094794000
C	5.953186000	0.318486000	-1.389464000
C	5.841453000	2.085315000	0.434432000
C	6.712867000	1.405993000	-0.646641000
C	6.680239000	-1.660816000	0.127307000
C	6.482445000	-0.877601000	1.446174000
H	4.446431000	-0.587521000	2.284641000
H	4.023485000	1.650015000	1.583353000
H	5.655089000	-1.738175000	-1.834851000
H	5.589586000	0.582314000	-2.383176000
H	7.751252000	-1.772982000	-0.095488000
H	6.576209000	-1.570828000	2.287472000
H	6.474310000	2.556971000	1.201594000
H	7.044161000	2.160968000	-1.366293000
H	7.272451000	-0.131455000	1.579189000
H	6.287317000	-2.675197000	0.251613000
H	5.264111000	2.896506000	-0.022535000
H	7.620969000	0.984872000	-0.205990000
Rh	4.058516000	-0.221838000	-0.311523000
C	-3.094087000	2.889696000	1.315183000
C	-2.394300000	2.377512000	2.482593000
C	-1.002431000	2.430446000	2.540777000
C	-0.253076000	2.998656000	1.434012000
C	-0.924787000	3.489319000	0.311834000
C	-2.375313000	3.437941000	0.252372000
C	-4.228478000	2.020750000	1.054855000
C	-4.229723000	0.970557000	2.060170000
C	-3.097804000	1.191269000	2.942952000
C	-2.381405000	0.104580000	3.445078000
C	-0.254033000	1.297216000	3.060647000
C	0.955308000	2.214471000	1.263892000
C	1.455093000	1.973398000	-0.013225000
C	0.758569000	2.477343000	-1.180377000
C	-0.410775000	3.232412000	-1.020334000
C	-1.543157000	3.000846000	-1.902928000
C	-2.758109000	3.135206000	-1.116546000
C	-3.844080000	2.296176000	-1.366555000
C	-4.595375000	1.728804000	-0.259381000
C	-4.599893000	-0.329310000	1.711892000
C	-4.980314000	-0.632747000	0.342979000
C	-4.978548000	0.375204000	-0.622585000
C	-4.462679000	0.104632000	-1.953272000
C	-3.762045000	1.291943000	-2.414522000
C	-2.597408000	1.165188000	-3.171151000
C	-1.464483000	2.036865000	-2.908980000
C	-0.250333000	1.256141000	-3.071992000
C	0.840740000	1.475331000	-2.230683000
C	0.958991000	1.158890000	2.276416000
C	1.208259000	-2.026541000	-1.042721000
C	1.570939000	-1.736608000	0.272195000
C	0.829668000	-2.295841000	1.380221000
C	-0.262493000	-3.130142000	1.124958000
C	-0.643183000	-3.435296000	-0.243661000
C	-0.615598000	-2.382087000	-2.478345000
C	0.085714000	-1.194522000	-2.940069000
C	1.205162000	-0.966830000	-2.049390000
C	1.586168000	0.338972000	-1.715016000
C	1.980780000	0.650052000	-0.342511000
C	2.013630000	-0.385322000	0.642992000
C	0.752969000	-1.288355000	2.425992000
C	-0.418457000	-1.159600000	3.177712000
C	-1.551729000	-2.029568000	2.914593000
C	-1.475540000	-2.996618000	1.910427000
C	-2.608762000	-3.220509000	1.027793000
C	-2.093447000	-3.491151000	-0.303800000
C	-2.761485000	-2.995712000	-1.424539000
C	-2.007579000	-2.429243000	-2.530894000
C	-0.634961000	-0.100968000	-3.429402000
C	-2.083620000	-0.155048000	-3.495574000
C	-2.755603000	-1.294612000	-3.048861000
C	-3.971831000	-1.163405000	-2.267454000
C	-3.974153000	-2.213477000	-1.261578000
C	-4.468376000	-1.953064000	0.016936000
C	-3.771134000	-2.465934000	1.184432000
C	-3.851656000	-1.461001000	2.232131000
C	-2.765920000	-1.248798000	3.082171000
C	1.462906000	-0.106260000	1.979193000
C	-0.930093000	0.158411000	3.503008000
C	0.080888000	-2.896916000	-1.309939000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2708.58046$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2708.07582$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2707.28775$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2706.78311$$



O

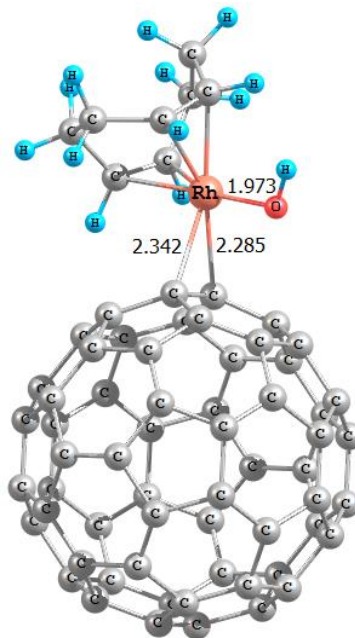
C	-5.670218000	-0.375965000	-1.445163000
C	-4.582670000	1.649147000	0.244397000
C	-4.940910000	1.000747000	1.429307000
C	-6.279183000	-0.863485000	-0.274170000
C	-6.344323000	0.575213000	1.830518000
C	-7.155855000	-0.043051000	0.668723000
C	-5.723813000	1.048838000	-1.956440000
C	-5.551229000	2.104221000	-0.842979000
H	-3.630223000	2.166394000	0.246896000
H	-4.242924000	1.080049000	2.263071000
H	-5.391782000	-1.110679000	-2.200208000
H	-6.429581000	-1.941508000	-0.215911000
H	-6.663487000	1.217139000	-2.506849000
H	-5.172043000	3.030729000	-1.288533000
H	-6.888202000	1.426374000	2.270156000
H	-7.932887000	-0.694111000	1.084335000
H	-6.519598000	2.360386000	-0.401300000
H	-4.916160000	1.164561000	-2.688015000
H	-6.249221000	-0.169175000	2.630460000
H	-7.684300000	0.735310000	0.109222000
Rh	-4.155104000	-0.554956000	0.114316000
C	2.811612000	2.943198000	1.603090000
C	2.027139000	3.502434000	0.514342000
C	0.636724000	3.390284000	0.528466000
C	-0.028978000	2.719252000	1.632796000
C	0.724756000	2.186624000	2.681206000
C	2.173247000	2.298971000	2.664701000
C	4.026476000	2.384006000	1.037694000
C	3.995118000	2.599504000	-0.400614000
C	2.759975000	3.291267000	-0.723879000
C	2.072417000	2.982182000	-1.899479000
C	-0.078721000	3.067136000	-0.693725000
C	-1.155866000	1.980447000	1.097562000
C	-1.494826000	0.736537000	1.621723000
C	-0.702611000	0.177039000	2.697122000
C	0.380430000	0.887549000	3.224322000
C	1.614980000	0.193418000	3.550542000
C	2.724481000	1.066333000	3.203588000
C	3.891852000	0.528131000	2.658625000
C	4.555355000	1.199964000	1.554271000
C	4.493530000	1.622239000	-1.264036000
C	5.043344000	0.389170000	-0.725481000
C	5.073624000	0.182468000	0.654573000
C	4.729228000	-1.118725000	1.203359000
C	3.999048000	-0.905488000	2.441562000
C	2.933821000	-1.743305000	2.776671000
C	1.716847000	-1.182287000	3.340542000
C	0.589132000	-1.923766000	2.800490000
C	-0.596754000	-1.254790000	2.479026000
C	-1.183305000	2.193418000	-0.349510000
C	-0.849778000	-2.330009000	-1.033044000
C	-1.385597000	-1.157993000	-1.554054000
C	-0.710273000	-0.487059000	-2.643786000
C	0.455869000	-1.024354000	-3.198032000
C	1.005015000	-2.253044000	-2.660753000
C	1.146152000	-3.451437000	-0.507623000
C	0.413315000	-3.239015000	0.729995000
C	-0.820724000	-2.550471000	0.410387000
C	-1.323308000	-1.582899000	1.271975000
C	-1.969690000	-0.360452000	0.753826000
C	-1.987133000	-0.144668000	-0.671119000
C	-0.817008000	0.945634000	-2.429440000
C	0.247087000	1.784949000	-2.770790000
C	1.462662000	1.225409000	-3.339259000
C	1.564715000	-0.150468000	-3.545814000
C	2.800711000	-0.844448000	-3.223604000
C	2.453779000	-2.145403000	-2.675978000
C	3.204606000	-2.683484000	-1.628997000
C	2.537174000	-3.353544000	-0.524045000
C	1.105894000	-2.938915000	1.906212000
C	2.555007000	-2.829206000	1.887869000
C	3.256556000	-3.033070000	0.698364000
C	4.364194000	-2.161200000	0.349460000
C	4.332777000	-1.945812000	-1.088914000
C	4.667054000	-0.696512000	-1.615491000
C	3.884635000	-0.134822000	-2.703721000
C	3.777930000	1.298724000	-2.486808000
C	2.591490000	1.965028000	-2.798654000
C	-1.559113000	1.160435000	-1.203292000
C	0.624271000	2.868470000	-1.883924000
C	0.363295000	-2.888701000	-1.594757000
O	-3.752911000	-2.438427000	-0.312826000
H	-4.528449000	-2.888308000	-0.684497000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2784.61863$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2784.10258$$

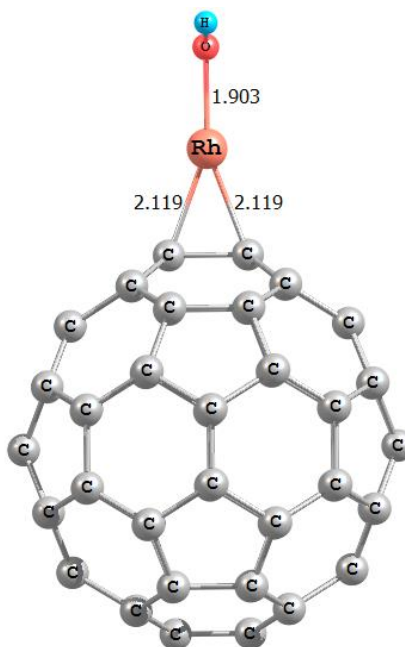
$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2783.28011$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2782.76406$$



P

Rh	-4.813404000	0.000036000	-0.009126000
C	-2.826233000	0.735764000	-0.044914000
C	-2.249431000	1.433699000	-1.216570000
C	-2.826238000	-0.735603000	-0.045531000
C	-2.275590000	1.431175000	1.144500000
C	-1.802227000	0.734329000	-2.331579000
C	-1.514906000	2.590632000	-0.753179000
C	-2.249477000	-1.432881000	-1.217385000
C	-2.275648000	-1.431729000	1.145691000
C	-1.532127000	2.589839000	0.699294000
C	-1.857235000	0.733544000	2.271458000
C	-1.802256000	-0.732892000	-2.332003000
C	-0.616600000	1.177446000	-3.037997000
C	-0.379109000	3.032027000	-1.438288000
C	-1.515005000	-2.590117000	-0.754663000
C	-1.532220000	-2.590160000	0.697810000
C	-1.857259000	-0.734755000	2.271036000
C	-0.413258000	3.030814000	1.412412000
C	-0.689071000	1.175888000	3.005996000
C	-0.616643000	-1.175652000	-3.038665000
C	0.115586000	0.001008000	-3.476410000
C	0.080307000	2.310004000	-2.606288000
C	0.786623000	3.483394000	-0.696090000
C	-0.379221000	-3.031156000	-1.440023000
C	-0.413371000	-3.031589000	1.410676000
C	-0.689113000	-1.177563000	3.005330000
C	0.018135000	2.308504000	2.590721000
C	0.769921000	3.483408000	0.698857000
C	0.032310000	-0.000981000	3.461076000
C	0.080222000	-2.308486000	-2.607608000
C	1.510681000	0.000979000	-3.466221000
C	1.533052000	2.308408000	-2.590625000
C	1.970521000	3.035320000	-1.409762000
C	0.786495000	-3.482996000	-0.698004000
C	0.018052000	-2.309963000	2.589403000
C	0.769792000	-3.483812000	0.698683000
C	1.470675000	2.307156000	2.610158000
C	1.936296000	3.034762000	1.440458000
C	1.427159000	-0.001012000	3.483904000
C	1.532969000	-2.306951000	-2.591943000
C	2.234502000	-1.175778000	-3.012314000
C	2.234544000	1.177450000	-3.011642000
C	3.090578000	2.602314000	-0.698084000
C	1.970412000	-3.034561000	-1.411502000
C	1.470589000	-2.308680000	2.608839000
C	1.936180000	-3.035631000	1.438719000
C	2.161689000	1.175866000	3.047381000
C	3.073107000	2.601987000	0.755812000
C	2.161646000	-1.177666000	3.046709000
C	3.400677000	-0.726780000	-2.272838000
C	3.400702000	0.727986000	-2.272422000
C	3.820535000	1.425645000	-1.138381000
C	3.090485000	-2.602002000	-0.699578000
C	3.073007000	-2.602505000	0.754319000
C	3.345090000	0.726626000	2.336307000
C	3.792148000	1.424845000	1.212962000
C	3.345062000	-0.728064000	2.335890000
C	3.820484000	-1.425105000	-1.139200000
C	4.254753000	0.697842000	0.042530000
C	3.792092000	-1.425654000	1.212142000
C	4.254727000	-0.697997000	0.042130000
O	-6.715765000	-0.000124000	-0.062097000
H	-7.168090000	-0.000264000	0.799736000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2472.50705$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2472.16779$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2471.33783$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2470.99857$ 

COD

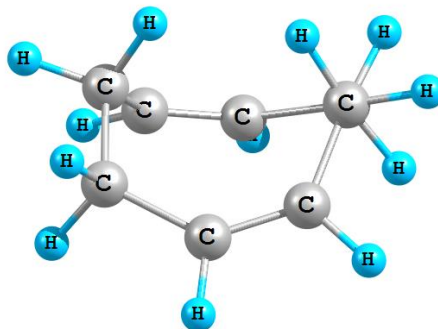
C	1.215278000	1.235989000	-0.495464000
C	0.007831000	-1.704672000	-0.218025000
C	-1.215377000	-1.235946000	-0.495314000
C	-0.007909000	1.704615000	-0.217940000
C	-1.923413000	0.011271000	-0.024557000
C	-1.083000000	1.107362000	0.665747000
C	1.923460000	-0.011055000	-0.024466000
C	1.083149000	-1.107490000	0.665428000
H	0.291009000	-2.635246000	-0.711120000
H	-1.822335000	-1.841702000	-1.170579000
H	1.821992000	1.841654000	-1.171016000
H	-0.291604000	2.634764000	-0.711550000
H	2.741401000	0.283415000	0.653185000
H	1.771517000	-1.909927000	0.959262000
H	-2.741803000	-0.283107000	0.652601000
H	-1.771208000	1.909783000	0.959992000
H	0.666337000	-0.724051000	1.600186000
H	2.425308000	-0.456013000	-0.896678000
H	-2.424705000	0.456468000	-0.896979000
H	-0.666024000	0.723515000	1.600249000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -312.02447$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -311.87480$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -311.85193$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -311.70226$$



Q

Rh	3.840604000	-0.834988000	-0.287687000
O	6.845689000	-0.869731000	1.747590000
H	7.391168000	-1.662081000	1.858687000
B	6.538443000	-0.696689000	0.367925000
O	7.635022000	-0.730240000	-0.576458000
H	8.403226000	-0.283653000	-0.195488000
O	5.615647000	-1.869487000	-0.172887000
H	5.992019000	-2.143657000	-1.028094000
C	5.520204000	0.584438000	0.187348000
C	5.070464000	0.931216000	-1.131076000
C	5.258459000	1.523842000	1.236618000
C	4.468375000	2.196423000	-1.385152000
H	5.448870000	0.371302000	-1.985326000
C	4.691317000	2.749639000	0.970784000
H	5.580726000	1.262260000	2.240037000
C	4.298025000	3.091305000	-0.351980000
H	4.177738000	2.460694000	-2.398067000
H	4.547238000	3.472515000	1.770074000
H	3.866845000	4.070296000	-0.544188000
C	-2.656050000	-0.665754000	3.361072000
C	-1.423072000	0.075972000	3.565438000
C	-1.364053000	1.433450000	3.249768000
C	-2.537170000	2.108129000	2.720220000
C	-3.721963000	1.396480000	2.523002000
C	-3.782105000	-0.019138000	2.849328000
C	-2.305177000	-1.996252000	2.890430000
C	-0.857312000	-2.075650000	2.807086000
C	-0.314517000	-0.797996000	3.219823000
C	0.806088000	-0.275667000	2.566828000
C	-0.193973000	1.977474000	2.578224000
C	-2.089862000	3.066459000	1.722973000
C	-2.846176000	3.274355000	0.568065000
C	-4.078067000	2.534317000	0.363243000
C	-4.508370000	1.614176000	1.321035000
C	-5.053920000	0.333240000	0.903123000
C	-4.604902000	-0.675647000	1.847787000
C	-4.267380000	-1.952734000	1.396066000
C	-3.095883000	-2.625379000	1.926951000
C	-0.254785000	-2.778740000	1.758241000
C	-1.079446000	-3.432163000	0.754865000
C	-2.469590000	-3.359258000	0.838527000
C	-3.259374000	-3.142647000	-0.363586000
C	-4.369354000	-2.273898000	-0.019092000
C	-4.805132000	-1.305007000	-0.925504000
C	-5.153013000	0.025158000	-0.454702000
C	-4.709374000	0.984502000	-1.452557000
C	-4.181439000	2.213472000	-1.052070000
C	-0.642038000	2.983902000	1.639178000
C	-0.968992000	1.965711000	-2.856645000
C	-0.173144000	2.587199000	-1.889418000
C	0.998052000	1.915094000	-1.365993000
C	1.341299000	0.651935000	-1.826629000
C	0.504233000	-0.004441000	-2.805625000
C	-1.855837000	-0.103562000	-3.528871000
C	-2.966147000	0.769116000	-3.185499000
C	-2.416992000	2.048991000	-2.768641000
C	-3.012834000	2.754833000	-1.721651000
C	-2.184693000	3.407767000	-0.719866000
C	-0.795029000	3.321867000	-0.800952000
C	1.104799000	2.236074000	0.061445000
C	1.550975000	1.279911000	0.967562000
C	1.996837000	-0.055821000	0.513961000
C	1.889098000	-0.367211000	-0.905740000
C	1.239846000	-1.646159000	-1.292880000
C	0.445401000	-1.420293000	-2.481722000
C	-0.738662000	-2.134978000	-2.683929000
C	-1.912576000	-1.461758000	-3.216822000
C	-4.088848000	0.247504000	-2.540141000
C	-4.148191000	-1.168181000	-2.214515000
C	-3.081593000	-2.005523000	-2.546573000
C	-2.627961000	-3.013661000	-1.602261000
C	-1.180775000	-3.091398000	-1.689506000
C	-0.419694000	-3.298063000	-0.534025000
C	0.808860000	-2.558052000	-0.334042000
C	0.912928000	-2.237240000	1.097449000
C	1.431097000	-1.011829000	1.494076000
C	-0.005666000	3.103056000	0.400362000
C	0.871543000	1.157837000	2.238572000
C	-0.623065000	0.640160000	-3.324758000

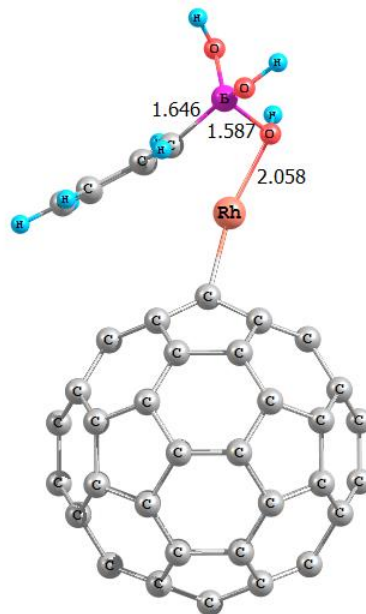
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$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2880.34058$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2879.49395$$

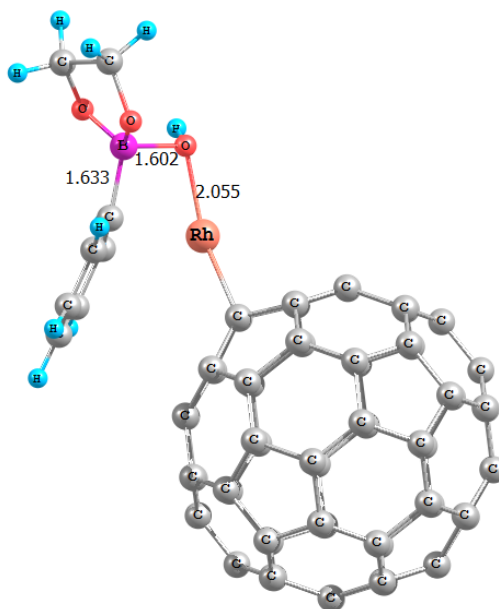
$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2879.03867$$

With Ph-B(OH)₂



Q

Rh	3.598767000	-0.639637000	-0.499846000
O	6.732766000	-0.840041000	1.442856000
B	6.313747000	-0.480695000	0.126379000
O	7.477965000	-0.359284000	-0.721782000
O	5.406030000	-1.617258000	-0.544045000
H	5.774457000	-1.785285000	-1.429243000
C	5.259402000	0.766365000	0.087426000
C	4.755116000	1.223983000	-1.177261000
C	5.017821000	1.594240000	1.230449000
C	4.113930000	2.492020000	-1.285516000
H	5.118250000	0.766200000	-2.096802000
C	4.402110000	2.818600000	1.105385000
H	5.394576000	1.251624000	2.189676000
C	3.951350000	3.274062000	-0.164003000
H	3.785703000	2.846547000	-2.258501000
H	4.267350000	3.456022000	1.975732000
H	3.486537000	4.253121000	-0.244936000
C	-2.797094000	-1.169149000	3.279040000
C	-1.581180000	-0.421885000	3.553815000
C	-1.570192000	0.967022000	3.424322000
C	-2.776579000	1.668620000	3.019364000
C	-3.944879000	0.951736000	2.754323000
C	-3.955132000	-0.496138000	2.886755000
C	-2.420861000	-2.411519000	2.623934000
C	-0.974352000	-2.431170000	2.496654000
C	-0.457550000	-1.204251000	3.066731000
C	0.629400000	-0.562669000	2.465339000
C	-0.435555000	1.634552000	2.805596000
C	-2.385156000	2.767418000	2.151741000
C	-3.178695000	3.104173000	1.053295000
C	-4.393677000	2.358984000	0.778384000
C	-4.769644000	1.303669000	1.611436000
C	-5.289666000	0.074124000	1.056636000
C	-4.785572000	-1.038042000	1.824793000
C	-4.424478000	-2.231250000	1.196192000
C	-3.219029000	-2.930671000	1.602742000
C	-0.380792000	-2.967016000	1.349016000
C	-1.212908000	-3.505954000	0.285376000
C	-2.601807000	-3.489460000	0.410496000
C	-3.430369000	-3.139080000	-0.732101000
C	-4.555345000	-2.360848000	-0.247191000
C	-5.042761000	-1.292771000	-1.002795000
C	-5.416857000	-0.050715000	-0.347784000
C	-5.029456000	1.048891000	-1.215909000
C	-4.526136000	2.228885000	-0.664807000
C	-0.938105000	2.744169000	2.023243000
C	-1.358561000	2.331334000	-2.559772000
C	-0.554870000	2.842684000	-1.536187000
C	0.649882000	2.144559000	-1.136928000
C	1.016198000	0.966360000	-1.772482000
C	0.171874000	0.421176000	-2.811652000
C	-2.203035000	0.344159000	-3.486548000
C	-3.328348000	1.125665000	-3.001791000
C	-2.805207000	2.354425000	-2.427693000
C	-3.392289000	2.893016000	-1.281459000
C	-2.556672000	3.431742000	-0.219576000
C	-1.167743000	3.402430000	-0.343915000
C	0.786437000	2.273197000	0.318427000
C	1.284453000	1.218422000	1.075647000
C	1.754747000	-0.028978000	0.434188000
C	1.617147000	-0.149647000	-1.011027000
C	0.994845000	-1.384228000	-1.553031000
C	0.162673000	-1.026376000	-2.681708000
C	-1.004737000	-1.745662000	-2.952351000
C	-2.211834000	-1.044970000	-3.360922000
C	-4.417451000	0.485804000	-2.407494000
C	-4.426094000	-0.962018000	-2.275925000
C	-3.345349000	-1.711980000	-2.743381000
C	-2.837190000	-2.823993000	-1.956416000
C	-1.391059000	-2.842130000	-2.087493000
C	-0.592766000	-3.177784000	-0.988443000
C	0.618542000	-2.431925000	-0.718228000
C	0.752124000	-2.303654000	0.740933000
C	1.245612000	-1.127055000	1.288331000
C	-0.339480000	3.050315000	0.797627000
C	0.644371000	0.883685000	2.330704000
C	-0.987393000	1.093316000	-3.211561000
C	8.062473000	-1.329150000	1.328751000
H	8.061843000	-2.420688000	1.181299000
H	8.620413000	-1.108157000	2.246280000
C	8.621669000	-0.605233000	0.089409000
H	9.354762000	-1.205684000	-0.463375000
H	9.099123000	0.347550000	0.366000000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2958.20348$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2957.71256$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2956.84167$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2956.35075$ With Ph-B(O-C₂H₄-O)

Q

Rh	3.046007000	-0.381969000	-0.683858000
O	6.287471000	-0.686605000	1.112830000
B	5.786627000	-0.207425000	-0.132763000
O	6.900005000	0.044505000	-1.013675000
O	4.877726000	-1.285589000	-0.894876000
H	5.220689000	-1.346317000	-1.804073000
C	4.684232000	0.994272000	0.023136000
C	4.117503000	1.588938000	-1.155416000
C	4.452054000	1.658681000	1.270314000
C	3.425288000	2.832445000	-1.079086000
H	4.464117000	1.267824000	-2.137246000
C	3.785114000	2.861311000	1.323925000
H	4.876795000	1.212843000	2.164972000
C	3.272301000	3.456424000	0.138612000
H	3.049301000	3.294293000	-1.987642000
H	3.656786000	3.375392000	2.273300000
H	2.766793000	4.416554000	0.199472000
C	-3.223903000	-1.701540000	3.104300000
C	-2.028819000	-0.955593000	3.460962000
C	-2.071174000	0.436518000	3.538999000
C	-3.312101000	1.142076000	3.267001000
C	-4.460756000	0.426360000	2.923369000
C	-4.415295000	-1.024473000	2.839499000
C	-2.820487000	-2.818326000	2.264644000
C	-1.377886000	-2.762527000	2.105955000
C	-0.890875000	-1.613098000	2.840716000
C	0.155752000	-0.847122000	2.318391000
C	-0.977782000	1.231858000	3.002352000
C	-2.983391000	2.370593000	2.563199000
C	-3.817256000	2.834223000	1.543974000
C	-5.011679000	2.090401000	1.187215000
C	-5.327371000	0.910103000	1.862535000
C	-5.817913000	-0.240946000	1.122496000
C	-5.253179000	-1.436043000	1.726074000
C	-4.865938000	-2.508552000	0.920364000
C	-3.625881000	-3.211562000	1.194038000
C	-0.795760000	-3.099170000	0.879130000
C	-1.635953000	-3.506569000	-0.235110000
C	-3.020720000	-3.564785000	-0.080400000
C	-3.891038000	-3.082121000	-1.141043000
C	-5.030502000	-2.429781000	-0.523015000
C	-5.576416000	-1.281997000	-1.101904000
C	-5.976492000	-0.165418000	-0.262339000
C	-5.650905000	1.064312000	-0.965679000
C	-5.177040000	2.169282000	-0.256395000
C	-1.540353000	2.423477000	2.403289000
C	-2.066118000	2.673553000	-2.180755000
C	-1.254879000	3.060467000	-1.108968000
C	-0.015804000	2.359697000	-0.842365000
C	0.375935000	1.303224000	-1.652787000
C	-0.475223000	0.884716000	-2.743816000
C	-2.862677000	0.814387000	-3.373459000
C	-4.002241000	1.471377000	-2.755601000
C	-3.508887000	2.622374000	-2.016822000
C	-4.084680000	2.962043000	-0.791108000
C	-3.240988000	3.369517000	0.321275000
C	-1.855712000	3.414898000	0.165510000
C	0.154993000	2.278744000	0.612617000
C	0.711052000	1.144445000	1.194868000
C	1.208064000	0.024213000	0.365800000
C	1.037384000	0.111870000	-1.078607000
C	0.444726000	-1.052499000	-1.784512000
C	-0.428913000	-0.565341000	-2.830229000
C	-1.576623000	-1.282640000	-3.179901000
C	-2.818252000	-0.577337000	-3.455433000
C	-5.051272000	0.708107000	-2.239996000
C	-5.004795000	-0.742546000	-2.324232000
C	-3.910469000	-1.371960000	-2.919896000
C	-3.342063000	-2.566449000	-2.316747000
C	-1.900281000	-2.508304000	-2.478652000
C	-1.061676000	-2.970712000	-1.458691000
C	0.128909000	-2.225732000	-1.106556000
C	0.295703000	-2.308327000	0.352772000
C	0.760258000	-1.206657000	1.058261000
C	-0.985607000	2.930742000	1.224854000
C	0.115823000	0.602749000	2.399393000
C	-1.667919000	1.562140000	-3.016265000
C	7.655863000	-1.078103000	0.916720000
C	7.691010000	-2.567351000	0.528927000
H	7.175604000	-2.745630000	-0.419105000
H	8.716410000	-2.946085000	0.446319000
H	7.172681000	-3.142681000	1.303010000
C	8.407563000	-0.879622000	2.235180000
H	8.286313000	0.137879000	2.614876000
H	8.013685000	-1.568904000	2.990086000
H	9.478530000	-1.084139000	2.116966000
C	8.112302000	-0.124349000	-0.257985000
C	9.186006000	-0.703969000	-1.182132000
H	9.416442000	0.015549000	-1.975578000
H	10.113137000	-0.909800000	-0.633694000
H	8.849298000	-1.629718000	-1.655550000
C	8.553883000	1.263536000	0.238298000
H	9.517218000	1.229108000	0.759810000
H	8.654193000	1.930205000	-0.624720000
H	7.808312000	1.694733000	0.913613000

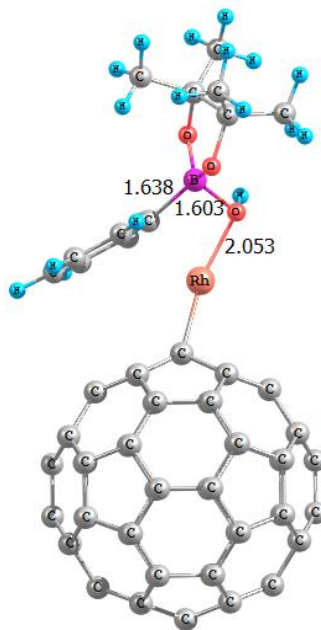
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3115.47051$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.87294$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.03025$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3113.43268$$

With Ph-B(O-C₂(Me)₂H₄-O)



Q-R

Rh	3.826601000	0.055534000	0.129188000
O	6.743622000	-2.283369000	0.759576000
H	6.662631000	-2.059882000	1.696023000
B	5.675153000	-1.792047000	0.001191000
O	5.585156000	-2.262301000	-1.316855000
H	6.404670000	-2.724429000	-1.544882000
O	4.333688000	-1.830514000	0.688247000
H	3.751651000	-2.448245000	0.207114000
C	5.948378000	0.172814000	-0.052841000
C	6.450420000	0.634544000	-1.290627000
C	6.410605000	0.811760000	1.123160000
C	7.368324000	1.682467000	-1.351858000
H	6.129044000	0.138385000	-2.202518000
C	7.320763000	1.870612000	1.063734000
H	6.064345000	0.472502000	2.098695000
C	7.799580000	2.304732000	-0.174624000
H	7.753386000	2.014435000	-2.313011000
H	7.663005000	2.348232000	1.978477000
H	8.513708000	3.122742000	-0.223528000
C	-0.917569000	1.023324000	-3.311255000
C	-2.369241000	1.034210000	-3.361789000
C	-3.085332000	1.998015000	-2.649514000
C	-2.378172000	2.991712000	-1.857517000
C	-0.984218000	2.977565000	-1.804206000
C	-0.236774000	1.975105000	-2.544861000
C	-0.480566000	-0.356947000	-3.294067000
C	-1.659799000	-1.207053000	-3.337216000
C	-2.829012000	-0.345268000	-3.378907000
C	-3.985056000	-0.704590000	-2.683505000
C	-4.288518000	1.624713000	-1.928256000
C	-3.149292000	3.236138000	-0.648849000
C	-2.494320000	3.461597000	0.565261000
C	-1.042845000	3.453401000	0.617685000
C	-0.300363000	3.212916000	-0.543181000
C	0.869931000	2.360330000	-0.498758000
C	0.908880000	1.586778000	-1.747652000
C	1.332814000	0.263697000	-1.736925000
C	0.617493000	-0.725908000	-2.511491000
C	-1.692360000	-2.393250000	-2.603748000
C	-0.547369000	-2.780867000	-1.795579000
C	0.582976000	-1.960885000	-1.747906000
C	1.281749000	-1.741555000	-0.499913000
C	1.848766000	-0.371872000	-0.502288000
C	1.807506000	0.395475000	0.745536000
C	1.255965000	1.769674000	0.699571000
C	0.477082000	2.000432000	1.897451000
C	-0.645036000	2.833415000	1.864313000
C	-4.328127000	2.390018000	-0.691648000
C	-3.060759000	0.423520000	3.280784000
C	-4.160377000	0.795634000	2.505416000
C	-4.862681000	-0.200718000	1.714960000
C	-4.436024000	-1.529742000	1.729733000
C	-3.291959000	-1.917230000	2.535055000
C	-1.164947000	-0.966830000	3.349394000
C	-0.712373000	0.408517000	3.363492000
C	-1.881482000	1.271925000	3.322507000
C	-1.848634000	2.458309000	2.589083000
C	-2.993393000	2.846797000	1.782870000
C	-4.125957000	2.032034000	1.741160000
C	-5.262988000	0.419442000	0.462691000
C	-5.225325000	-0.314582000	-0.723758000
C	-4.785159000	-1.699737000	-0.708468000
C	-4.397029000	-2.295226000	0.493307000
C	-3.227141000	-3.153784000	0.533776000
C	-2.541290000	-2.918137000	1.794262000
C	-1.146822000	-2.920025000	1.840251000
C	-0.441804000	-1.925099000	2.631646000
C	0.442606000	0.765051000	2.660772000
C	1.200668000	-0.232059000	1.937865000
C	0.763611000	-1.551234000	1.919914000
C	0.801559000	-2.321807000	0.669780000
C	-0.378800000	-3.163734000	0.630898000
C	-1.039438000	-3.394488000	-0.579587000
C	-2.491293000	-3.388488000	-0.629035000
C	-2.895595000	-2.768760000	-1.880735000
C	-4.019099000	-1.941150000	-1.919252000
C	-4.807909000	1.799699000	0.479432000
C	-4.729796000	0.300188000	-1.943846000
C	-2.616721000	-0.961050000	3.295986000

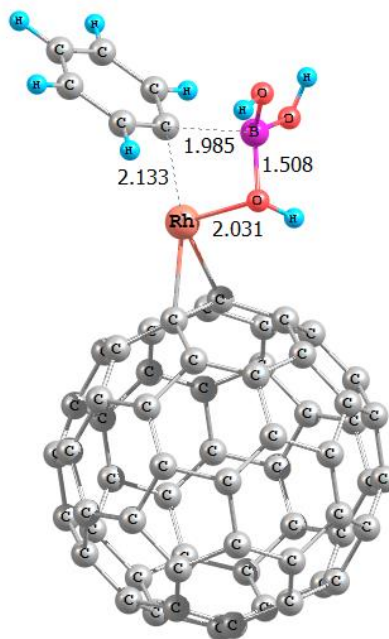
$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2880.78875$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2880.33658$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2879.48106$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2879.02890$

With Ph-B(OH)₂



Q-R

Rh	3.594519000	-0.407642000	-0.170244000
O	6.590084000	1.673880000	-1.140581000
B	5.499962000	1.353558000	-0.316318000
O	5.576966000	2.021725000	0.923523000
O	4.179126000	1.369736000	-0.977846000
H	3.623269000	2.073905000	-0.595709000
C	5.695459000	-0.620303000	0.018672000
C	6.182679000	-0.949300000	1.303889000
C	6.178718000	-1.361953000	-1.084821000
C	7.100816000	-1.984993000	1.480573000
H	5.850366000	-0.367947000	2.160252000
C	7.090105000	-2.405918000	-0.906441000
H	5.858846000	-1.101326000	-2.091007000
C	7.548557000	-2.718323000	0.375907000
H	7.473184000	-2.218935000	2.475044000
H	7.451493000	-2.965327000	-1.765712000
H	8.263015000	-3.525798000	0.514798000
C	-1.167000000	-0.776505000	3.381561000
C	-2.615021000	-0.677482000	3.444661000
C	-3.408345000	-1.642033000	2.820815000
C	-2.785266000	-2.746255000	2.108164000
C	-1.394672000	-2.837990000	2.043140000
C	-0.566916000	-1.835239000	2.692294000
C	-0.631956000	0.562186000	3.246486000
C	-1.746317000	1.496026000	3.227722000
C	-2.973811000	0.728299000	3.350029000
C	-4.110388000	1.112630000	2.636338000
C	-4.591567000	-1.242555000	2.080449000
C	-3.588829000	-3.032515000	0.930342000
C	-2.968043000	-3.403678000	-0.263974000
C	-1.520683000	-3.505400000	-0.330004000
C	-0.746629000	-3.225027000	0.800752000
C	0.481671000	-2.466950000	0.676817000
C	0.592916000	-1.598067000	1.856305000
C	1.111862000	-0.314563000	1.733371000
C	0.479115000	0.785035000	2.428104000
C	-1.704072000	2.617918000	2.399688000
C	-0.545164000	2.854382000	1.553646000
C	0.522284000	1.952939000	1.565530000
C	1.184603000	1.580802000	0.334065000
C	1.652296000	0.179289000	0.445291000
C	1.539764000	-0.683856000	-0.732531000
C	0.892969000	-2.005994000	-0.560991000
C	0.082555000	-2.277314000	-1.737427000
C	-1.096350000	-3.020611000	-1.626551000
C	-4.702463000	-2.101591000	0.911656000
C	-3.351807000	-0.565943000	-3.219202000
C	-4.464756000	-0.792338000	-2.407644000
C	-5.083136000	0.314262000	-1.697740000
C	-4.562115000	1.603093000	-1.826389000
C	-3.404036000	1.838926000	-2.669907000
C	-1.361834000	0.672294000	-3.418386000
C	-1.009819000	-0.728575000	-3.320634000
C	-2.237315000	-1.497946000	-3.199085000
C	-2.279527000	-2.619808000	-2.370804000
C	-3.438496000	-2.837254000	-1.526776000
C	-4.508774000	-1.961234000	-1.543937000
C	-5.509716000	-0.169981000	-0.395141000
C	-5.403690000	0.654438000	0.726342000
C	-4.864507000	1.997604000	0.592239000
C	-4.450731000	2.461952000	-0.657742000
C	-3.222893000	3.226989000	-0.778285000
C	-2.573183000	2.839841000	-2.020304000
C	-1.182921000	2.736715000	-2.077064000
C	-0.561800000	1.631458000	-2.788912000
C	0.125813000	-1.109493000	-2.599652000
C	0.963320000	-0.114224000	-1.968090000
C	0.623012000	1.230339000	-2.057910000
C	0.732805000	2.096552000	-0.876435000
C	-0.382902000	3.023081000	-0.898414000
C	-1.008632000	3.399481000	0.294208000
C	-2.456170000	3.502396000	0.355185000
C	-2.886789000	3.019039000	1.657026000
C	-4.066442000	2.281551000	1.772874000
C	-5.154544000	-1.576294000	-0.300511000
C	-4.935991000	0.107333000	1.989141000
C	-2.809485000	0.776595000	-3.353084000
C	6.822762000	2.727567000	0.944100000
H	6.620384000	3.804230000	0.845254000
H	7.334356000	2.553455000	1.896839000
C	7.602735000	2.169410000	-0.267614000
H	8.190115000	2.930884000	-0.790322000
H	8.275531000	1.352707000	0.031110000

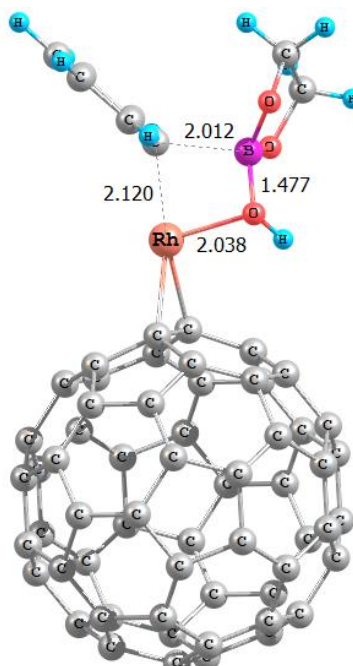
$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2958.19333$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2957.70488$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2956.82675$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2956.33830$

With Ph-B(O-C₂H₄-O)



Q-R

Rh	3.096438000	-1.405366000	0.048363000
O	5.666291000	1.010816000	-0.955609000
B	5.193615000	0.794709000	0.311956000
O	6.000546000	1.254784000	1.320409000
O	3.802490000	0.612150000	0.565087000
H	3.616653000	0.763254000	1.506523000
C	5.330224000	-1.778800000	0.159286000
C	4.750373000	-2.621595000	1.177270000
C	4.943611000	-2.092451000	-1.198201000
C	3.659381000	-3.472618000	0.916088000
H	5.078539000	-2.512707000	2.209913000
C	3.870572000	-2.950455000	-1.498163000
H	5.409970000	-1.542773000	-2.012783000
C	3.148048000	-3.558680000	-0.419275000
H	3.139271000	-3.992027000	1.716951000
H	3.511781000	-3.077640000	-2.516310000
H	2.267313000	-4.155201000	-0.625326000
C	-2.462715000	-2.934356000	1.722167000
C	-3.857841000	-2.531489000	1.706962000
C	-4.568027000	-2.515945000	0.504949000
C	-3.909738000	-2.902169000	-0.733213000
C	-2.567015000	-3.281433000	-0.719937000
C	-1.826252000	-3.297699000	0.530321000
C	-1.765890000	-2.100886000	2.677027000
C	-2.726796000	-1.179448000	3.262389000
C	-4.022498000	-1.446679000	2.661134000
C	-4.888489000	-0.390146000	2.373574000
C	-5.470239000	-1.418645000	0.207737000
C	-4.412658000	-2.047077000	-1.796545000
C	-3.552918000	-1.611998000	-2.807197000
C	-2.157365000	-2.013984000	-2.798405000
C	-1.670710000	-2.829868000	-1.771255000
C	-0.374948000	-2.558108000	-1.179123000
C	-0.472585000	-2.860618000	0.259330000
C	0.201364000	-2.066571000	1.179297000
C	-0.464450000	-1.669021000	2.399071000
C	-2.349317000	0.131011000	3.555225000
C	-0.994237000	0.578093000	3.274075000
C	-0.071428000	-0.304591000	2.703357000
C	0.840608000	0.142608000	1.673444000
C	1.129743000	-0.988901000	0.752578000
C	1.228015000	-0.692736000	-0.694138000
C	0.390743000	-1.495954000	-1.621354000
C	-0.123131000	-0.636892000	-2.664118000
C	-1.365036000	-0.892899000	-3.254589000
C	-5.374320000	-1.128672000	-1.215169000
C	-2.850549000	2.440208000	-2.678803000
C	-4.152582000	2.013274000	-2.410802000
C	-4.804046000	2.401803000	-1.171394000
C	-4.126834000	3.202175000	-0.248913000
C	-2.773231000	3.645328000	-0.526986000
C	-0.751400000	2.867843000	-1.709461000
C	-0.593351000	1.786752000	-2.656618000
C	-1.889115000	1.518731000	-3.260476000
C	-2.266660000	0.208448000	-3.554023000
C	-3.621331000	-0.237090000	-3.275189000
C	-4.545644000	0.646517000	-2.715207000
C	-5.599931000	1.276574000	-0.709847000
C	-5.692248000	0.998507000	0.654962000
C	-4.991793000	1.833839000	1.616398000
C	-4.223111000	2.912605000	1.174232000
C	-2.928551000	3.176327000	1.775098000
C	-2.029815000	3.624838000	0.722839000
C	-0.692715000	3.227179000	0.732011000
C	-0.037718000	2.838664000	-0.506223000
C	0.269797000	0.726990000	-2.358216000
C	1.028710000	0.713373000	-1.128549000
C	0.868020000	1.748097000	-0.217307000
C	0.770662000	1.455177000	1.221697000
C	-0.193536000	2.371270000	1.794992000
C	-1.057023000	1.946609000	2.810652000
C	-2.451011000	2.354042000	2.797656000
C	-3.251543000	1.231255000	3.258770000
C	-4.495739000	0.976185000	2.679095000
C	-5.439482000	0.191907000	-1.663986000
C	-5.627513000	-0.375943000	1.123154000
C	-2.145796000	3.273011000	-1.717534000
C	6.899674000	1.773985000	-0.816953000
C	7.918083000	1.226933000	-1.815857000
H	7.550371000	1.383416000	-2.835414000
H	8.878530000	1.746369000	-1.719791000
H	8.083617000	0.156762000	-1.673493000
C	6.546652000	3.226114000	-1.166822000
H	5.798287000	3.631385000	-0.478594000
H	7.428044000	3.876001000	-1.145657000
H	6.123092000	3.252747000	-2.175662000
C	7.288018000	1.565676000	0.710909000
C	8.208027000	0.363120000	0.957838000
H	7.777934000	-0.547752000	0.533953000
H	9.207488000	0.530055000	0.541810000
H	8.309226000	0.215489000	2.038296000
C	7.850537000	2.806520000	1.403514000
H	8.800275000	3.109528000	0.948049000
H	7.157287000	3.649631000	1.359174000
H	8.039978000	2.579581000	2.457646000

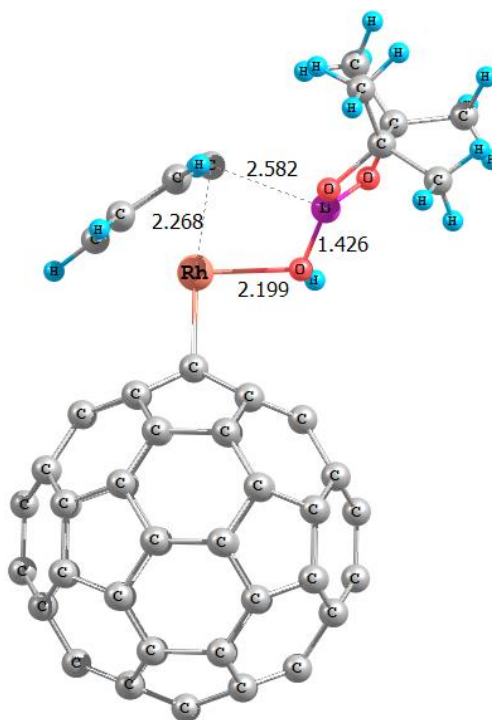
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3115.44889$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.85107$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.01156$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3113.41374$$

With Ph-B(O-C₂(Me)₂H₄-O)



Q-R

Rh	-3.044222000	0.855589000	-0.203431000
O	-6.261335000	-0.765330000	-1.193078000
B	-5.223571000	-0.648164000	-0.262391000
O	-5.533334000	-1.281134000	0.949087000
O	-3.846491000	-0.932678000	-0.741729000
H	-3.446979000	-1.607497000	-0.162220000
C	-5.072031000	1.397625000	-0.024385000
C	-5.416487000	1.896304000	1.252316000
C	-5.510303000	2.117267000	-1.159710000
C	-6.157915000	3.070621000	1.388913000
H	-5.119196000	1.341630000	2.138764000
C	-6.248640000	3.295554000	-1.022837000
H	-5.295866000	1.736432000	-2.154916000
C	-6.570821000	3.772197000	0.250402000
H	-6.422610000	3.435854000	2.378270000
H	-6.580432000	3.834789000	-1.906656000
H	-7.149845000	4.686035000	0.357354000
C	1.763537000	1.091569000	3.294991000
C	3.197797000	0.871758000	3.362940000
C	4.065952000	1.700708000	2.650301000
C	3.533928000	2.783929000	1.838335000
C	2.155854000	2.990989000	1.768112000
C	1.250746000	2.129451000	2.510356000
C	1.112219000	-0.201618000	3.287810000
C	2.140336000	-1.227695000	3.354819000
C	3.431631000	-0.562720000	3.401440000
C	4.523072000	-1.110768000	2.725012000
C	5.201389000	1.130818000	1.947667000
C	4.346230000	2.886368000	0.636406000
C	3.747357000	3.196574000	-0.586065000
C	2.313691000	3.418373000	-0.658053000
C	1.530727000	3.315136000	0.496343000
C	0.240158000	2.658480000	0.447000000
C	0.065362000	1.918721000	1.703926000
C	-0.562946000	0.679183000	1.701490000
C	-0.022311000	-0.401385000	2.496078000
C	1.991236000	-2.413106000	2.635186000
C	0.807056000	-2.625329000	1.818445000
C	-0.178182000	-1.636570000	1.747819000
C	-0.820232000	-1.324465000	0.488544000
C	-1.160510000	0.117603000	0.468491000
C	-0.983828000	0.850176000	-0.786228000
C	-0.223088000	2.120927000	-0.749233000
C	0.594558000	2.209508000	-1.940421000
C	1.834824000	2.853538000	-1.902435000
C	5.374548000	1.863547000	0.702953000
C	3.850590000	0.071744000	-3.261580000
C	4.987419000	0.274439000	-2.477604000
C	5.513915000	-0.810559000	-1.667462000
C	4.882245000	-2.056030000	-1.673565000
C	3.698508000	-2.266212000	-2.487867000
C	1.758090000	-1.000087000	-3.337502000
C	1.530537000	0.429330000	-3.372756000
C	2.821859000	1.096023000	-3.326949000
C	2.970600000	2.281758000	-2.607504000
C	4.154760000	2.494849000	-1.792776000
C	5.143120000	1.511031000	-1.728461000
C	5.994926000	-0.245738000	-0.417631000
C	5.829582000	-0.948983000	0.776739000
C	5.174303000	-2.246386000	0.771207000
C	4.708251000	-2.787601000	-0.428570000
C	3.417309000	-3.450070000	-0.473904000
C	2.790412000	-3.125406000	-1.745300000
C	1.413712000	-2.906376000	-1.808383000
C	0.883858000	-1.822532000	-2.619731000
C	0.439783000	0.974325000	-2.688850000
C	-0.474583000	0.119523000	-1.964300000
C	-0.253776000	-1.252284000	-1.926507000
C	-0.426339000	-1.989474000	-0.668628000
C	0.604420000	-3.008145000	-0.605579000
C	1.207845000	-3.324823000	0.615380000
C	2.641647000	-3.548935000	0.682477000
C	3.126621000	-2.985537000	1.932040000
C	4.367481000	-2.347134000	1.975507000
C	5.764955000	1.188758000	-0.455396000
C	5.426212000	-0.246900000	1.983863000
C	3.191595000	-1.224591000	-3.266600000
C	-6.921995000	-1.699994000	0.885262000
C	-7.190447000	-1.747788000	-0.675520000
C	-7.776581000	-0.655479000	1.616030000
H	-8.826626000	-0.963627000	1.664846000
H	-7.405556000	-0.546969000	2.640597000
H	-7.722002000	0.322217000	1.131686000
C	-7.038582000	-3.046614000	1.601160000
H	-6.804765000	-2.918105000	2.663310000
H	-8.057483000	-3.444092000	1.525842000
H	-6.345579000	-3.785149000	1.191485000
C	-8.603084000	-1.345065000	-1.099445000
H	-9.350061000	-2.029181000	-0.679900000
H	-8.842032000	-0.327287000	-0.783011000
H	-8.682366000	-1.386193000	-2.190781000
C	-6.824217000	-3.099349000	-1.310128000
H	-6.850321000	-2.995218000	-2.399296000
H	-5.814362000	-3.415328000	-1.028897000
H	-7.525499000	-3.890163000	-1.021825000

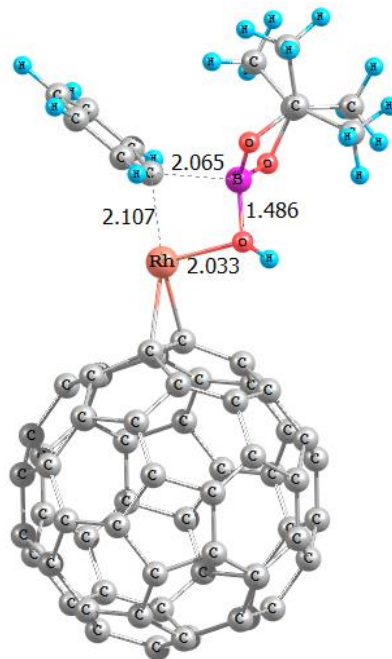
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3115.45844$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.86119$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) =$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3113.41253$$

With Ph-B(O-C₂(Me)₂H₄-O), second structure



R

Rh	-3.783302000	0.850727000	-0.272811000
O	-7.234533000	0.454457000	1.047756000
H	-6.533045000	-0.220213000	0.977382000
B	-7.017800000	1.571582000	0.324210000
O	-7.916332000	2.596099000	0.255718000
H	-8.712978000	2.402092000	0.770609000
O	-5.832467000	1.761077000	-0.413789000
H	-5.854784000	2.612777000	-0.878307000
C	-4.560760000	-0.951450000	-0.141007000
C	-5.064504000	-1.559921000	-1.305197000
C	-4.744690000	-1.599567000	1.094779000
C	-5.738661000	-2.782433000	-1.231970000
H	-4.928070000	-1.082207000	-2.272367000
C	-5.427178000	-2.823555000	1.159216000
H	-4.343005000	-1.163430000	2.005343000
C	-5.924468000	-3.417708000	-0.000850000
H	-6.118614000	-3.239018000	-2.142950000
H	-5.560886000	-3.309461000	2.122878000
H	-6.449608000	-4.367322000	0.051984000
C	-6.610186000	2.370988000	-1.277413000
C	0.649494000	2.858388000	-1.801226000
C	1.323764000	2.143384000	-2.796809000
C	0.764473000	0.902803000	-3.290423000
C	-0.443856000	0.431187000	-2.767648000
C	-1.150637000	1.183502000	-1.755894000
C	-0.641456000	2.669070000	0.163398000
C	0.599130000	3.336581000	0.503242000
C	1.396442000	3.453532000	-0.705979000
C	2.783389000	3.313073000	-0.646745000
C	2.766487000	1.990748000	-2.731179000
C	1.858422000	-0.022764000	-3.536580000
C	1.699243000	-1.380226000	-3.256623000
C	0.439744000	-1.872669000	-2.722053000
C	-0.610842000	-0.982255000	-2.476707000
C	-1.426521000	-1.106756000	-1.289228000
C	-1.879471000	0.242860000	-0.866110000
C	-1.909925000	0.540557000	0.579982000
C	-1.212228000	1.765922000	1.052214000
C	1.224940000	3.081596000	1.728088000
C	0.634754000	2.134558000	2.650707000
C	-0.554353000	1.483875000	2.308140000
C	-0.720567000	0.070019000	2.596294000
C	-1.486552000	-0.523917000	1.523130000
C	-1.162484000	-1.798567000	1.077094000
C	-1.132571000	-2.097208000	-0.361279000
C	-0.035881000	-3.013875000	-0.597784000
C	0.733462000	-2.913921000	-1.761217000
C	3.098305000	0.650977000	-3.189471000
C	4.034927000	-2.661877000	-0.123719000
C	4.608724000	-1.750807000	-1.012728000
C	5.172433000	-0.506669000	-0.515339000
C	5.142809000	-0.223500000	0.851098000
C	4.548017000	-1.172419000	1.777862000
C	2.744587000	-2.854464000	1.833266000
C	1.994681000	-3.447642000	0.737771000
C	2.795168000	-3.332724000	-0.470698000
C	2.176495000	-3.070614000	-1.694446000
C	2.774483000	-2.122532000	-2.620680000
C	3.965469000	-1.475551000	-2.285669000
C	4.876084000	0.538110000	-1.481518000
C	4.558030000	1.824866000	-1.042503000
C	4.527121000	2.120018000	0.381984000
C	4.814963000	1.116458000	1.309143000
C	4.020168000	0.996130000	2.519551000
C	3.854865000	-0.419288000	2.809026000
C	2.645061000	-0.890176000	3.322971000
C	2.078130000	-2.133022000	2.825366000
C	0.610297000	-3.288213000	0.674612000
C	-0.085416000	-2.536875000	1.705523000
C	0.635357000	-1.974791000	2.763836000
C	0.310494000	-0.640303000	3.219481000
C	1.550909000	0.034672000	3.566942000
C	1.709803000	1.392561000	3.289347000
C	2.968726000	1.883893000	2.755455000
C	2.668102000	2.928295000	1.788933000
C	3.432242000	3.041208000	0.625806000
C	4.130870000	-0.060501000	-2.575767000
C	3.482566000	2.564135000	-1.678608000
C	4.003780000	-2.366355000	1.300708000

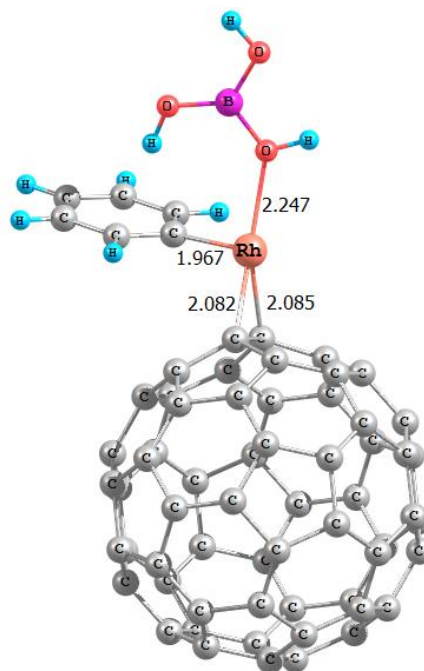
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2880.85226$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2880.39926$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2879.54568$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2879.09268$$

With Ph-B(OH)₂



R

Rh	-3.675845000	0.073678000	-0.556277000
O	-5.683476000	-2.767513000	-0.564616000
B	-6.308804000	-1.644228000	-0.108175000
O	-7.370344000	-1.854919000	0.724135000
O	-5.867243000	-0.390091000	-0.485311000
H	-6.342264000	0.356045000	-0.077100000
C	-4.211231000	1.900820000	-0.068606000
C	-4.757401000	2.150888000	1.204204000
C	-4.227798000	2.929554000	-1.026783000
C	-5.312753000	3.401070000	1.506378000
H	-4.726923000	1.380263000	1.971847000
C	-4.785396000	4.174366000	-0.717151000
H	-3.803505000	2.763426000	-2.013218000
C	-5.329132000	4.414834000	0.547406000
H	-5.723719000	3.579382000	2.497568000
H	-4.789804000	4.959775000	-1.469524000
H	-5.756861000	5.385430000	0.783703000
C	-0.920336000	-2.292283000	-0.154703000
C	0.165019000	-3.191059000	0.180217000
C	0.753615000	-3.145028000	1.448760000
C	0.281737000	-2.183716000	2.422678000
C	-0.756672000	-1.310000000	2.085609000
C	-1.379141000	-1.375020000	0.782860000
C	-0.756951000	-1.894535000	-1.561838000
C	0.428476000	-2.553303000	-2.071048000
C	0.998713000	-3.352961000	-0.999333000
C	2.383366000	-3.462631000	-0.867706000
C	2.195412000	-3.252175000	1.585173000
C	1.429008000	-1.693328000	3.169594000
C	1.488905000	-0.353856000	3.554361000
C	0.404151000	0.552946000	3.213015000
C	-0.695995000	0.084993000	2.487171000
C	-1.288060000	0.884779000	1.437529000
C	-1.831756000	-0.0115293000	0.388294000
C	-1.667745000	0.386434000	-1.025855000
C	-1.056822000	-0.596875000	-1.957895000
C	1.272064000	-1.893226000	-2.971266000
C	0.962691000	-0.539448000	-3.379393000
C	-0.174966000	0.094698000	-2.870491000
C	-0.114059000	1.488727000	-2.466835000
C	-0.964005000	1.661945000	-1.309526000
C	-0.559853000	2.512009000	-0.288215000
C	-0.724336000	2.112861000	1.116711000
C	0.425865000	2.599655000	1.851658000
C	0.977871000	1.840784000	2.888799000
C	2.614116000	-2.354596000	2.649833000
C	4.442700000	1.747548000	1.612564000
C	4.746772000	0.443528000	2.008382000
C	5.222370000	-0.520518000	1.029997000
C	5.379289000	-0.142497000	-0.304366000
C	5.067180000	1.212609000	-0.716991000
C	3.521839000	3.044668000	-0.120173000
C	2.684226000	3.204632000	1.058056000
C	3.257492000	2.406584000	2.130399000
C	2.420659000	1.738526000	3.026388000
C	2.737331000	0.380852000	3.438844000
C	3.876624000	-0.253496000	2.939922000
C	4.644874000	-1.813752000	1.356690000
C	4.242903000	-2.676401000	0.334820000
C	4.406401000	-2.282388000	-1.056246000
C	4.965142000	-1.041460000	-1.369036000
C	4.397680000	-0.238889000	-2.439105000
C	4.460502000	1.156678000	-2.035587000
C	3.418535000	2.025726000	-2.364703000
C	2.938658000	2.989223000	-1.387436000
C	1.298885000	3.294429000	0.920890000
C	0.689548000	3.237311000	-0.397414000
C	1.496781000	3.093815000	-1.530558000
C	1.085432000	2.197847000	-2.589086000
C	2.270955000	1.535190000	-3.109320000
C	2.211168000	0.196394000	-3.496674000
C	3.295430000	-0.708884000	-3.155273000
C	2.713516000	-2.001055000	-2.829153000
C	3.259131000	-2.770731000	-1.799639000
C	3.813691000	-1.649338000	2.536970000
C	2.994764000	-3.408078000	0.450904000
C	4.605921000	2.141938000	0.221426000
C	-7.560285000	-3.282364000	0.793721000
H	-7.645958000	-3.579859000	1.842043000
H	-8.492241000	-3.534900000	0.277057000
C	-6.310872000	-3.884506000	0.093070000
H	-6.565046000	-4.641685000	-0.653198000
H	-5.599167000	-4.314701000	0.805157000

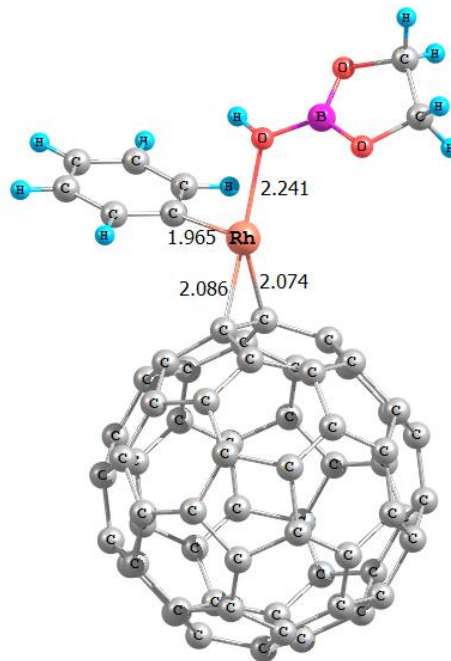
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2958.25162$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2957.76665$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2956.88292$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2956.39795$$

With Ph-B(O-C₂H₄-O)



R

Rh	-3.123821000	-0.796126000	0.256036000
O	-5.630285000	1.597955000	0.156557000
B	-6.160564000	0.343820000	0.142313000
O	-7.510966000	0.271626000	-0.023260000
O	-5.343536000	-0.763775000	0.294726000
H	-5.768024000	-1.629297000	0.171636000
C	-3.284597000	-2.745998000	0.053530000
C	-3.545191000	-3.305222000	-1.210293000
C	-3.299659000	-3.584540000	1.182060000
C	-3.815588000	-4.672745000	-1.338659000
H	-3.523748000	-2.678182000	-2.098416000
C	-3.571333000	-4.950574000	1.045370000
H	-3.089342000	-3.176575000	2.167423000
C	-3.828673000	-5.499042000	-0.213111000
H	-4.009292000	-5.090070000	-2.324349000
H	-3.575354000	-5.586100000	1.928124000
H	-4.034320000	-6.561216000	-0.315889000
C	-0.760810000	1.930754000	-0.367721000
C	0.191686000	2.942000000	-0.778046000
C	0.888430000	2.808244000	-1.984100000
C	0.664136000	1.643774000	-2.814551000
C	-0.245064000	0.664600000	-2.402097000
C	-0.981177000	0.816585000	-1.167673000
C	-0.658178000	1.783252000	1.092453000
C	0.356525000	2.705845000	1.558833000
C	0.882281000	3.421174000	0.407778000
C	2.237550000	3.747127000	0.345069000
C	2.301122000	3.139755000	-2.047072000
C	1.936547000	1.250569000	-3.398378000
C	2.244415000	-0.1100979000	-3.555407000
C	1.293859000	-1.119318000	-3.137630000
C	0.073750000	-0.743187000	-2.566046000
C	-0.470941000	-1.454613000	-1.437258000
C	-1.243605000	-0.525145000	-0.585413000
C	-1.141307000	-0.674164000	0.882074000
C	-0.781461000	0.528815000	1.677467000
C	1.212368000	2.344562000	2.605909000
C	1.089344000	1.035180000	3.210082000
C	0.111387000	0.144875000	2.742295000
C	0.437023000	-1.262253000	2.575887000
C	-0.269731000	-1.752251000	1.413416000
C	0.353536000	-2.663885000	0.571094000
C	0.250836000	-2.516178000	-0.887710000
C	1.524130000	-2.902126000	-1.461266000
C	2.036132000	-2.225120000	-2.572742000
C	2.949955000	2.176989000	-2.922835000
C	5.314759000	-1.344069000	-1.119391000
C	5.439891000	-0.082244000	-1.704134000
C	5.667275000	1.085946000	-0.869232000
C	5.764628000	0.945928000	0.516087000
C	5.639303000	-0.368011000	1.125137000
C	4.466224000	-2.504391000	0.742381000
C	3.771838000	-2.982398000	-0.442801000
C	4.301121000	-2.268290000	-1.594015000
C	3.450103000	-1.897528000	-2.636853000
C	3.579911000	-0.583541000	-3.246164000
C	4.554079000	0.305966000	-2.788149000
C	4.920227000	2.195892000	-1.437519000
C	4.297160000	3.120527000	-0.596742000
C	4.399043000	2.974638000	0.847528000
C	5.119803000	1.909890000	1.392327000
C	4.597602000	1.192584000	2.542966000
C	4.918459000	-0.215878000	2.377235000
C	4.005365000	-1.192251000	2.780436000
C	3.773656000	-2.360560000	1.946116000
C	2.412234000	-3.288234000	-0.377815000
C	1.688741000	-3.138245000	0.873629000
C	2.359949000	-2.688808000	2.015455000
C	1.719141000	-1.727406000	2.885960000
C	2.732728000	-0.799472000	3.361938000
C	2.424980000	0.551795000	3.521491000
C	3.375509000	1.568479000	3.103942000
C	2.624567000	2.676614000	2.535542000
C	3.127645000	3.364216000	1.429383000
C	4.232520000	1.714354000	-2.623268000
C	2.962748000	3.600268000	-0.906879000
C	5.416828000	-1.490056000	0.324584000
C	-7.946015000	1.629875000	-0.367917000
C	-8.051427000	1.676144000	-1.896588000
H	-8.435380000	2.640874000	-2.243133000
H	-7.080863000	1.499784000	-2.371566000
H	-8.739604000	0.893145000	-2.229451000
C	-9.311883000	1.869870000	0.268597000
H	-9.293896000	1.695282000	1.346586000
H	-9.648140000	2.896515000	0.085245000
H	-10.047131000	1.189760000	-0.172858000
C	-6.768031000	2.518317000	0.210695000
C	-6.424147000	3.754495000	-0.615056000
H	-7.273888000	4.445641000	-0.649979000
H	-5.580582000	4.278450000	-0.155034000
H	-6.142231000	3.493769000	-1.637404000
C	-6.955777000	2.894170000	1.685033000
H	-6.026278000	3.332365000	2.060893000
H	-7.758516000	3.627403000	1.813088000
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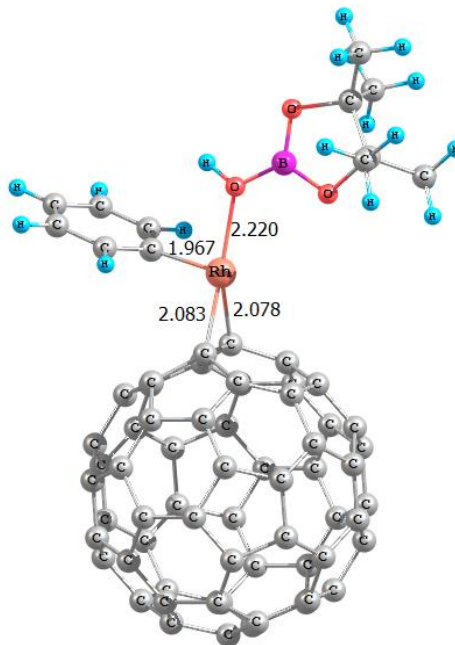
$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3115.52224$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.93034$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -3114.07303$$

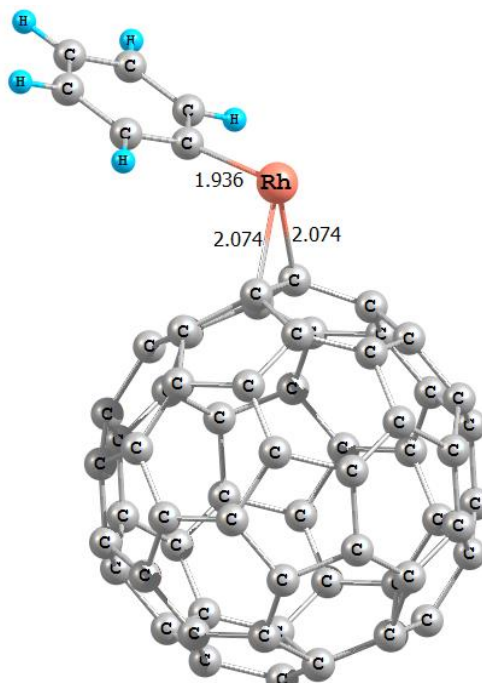
$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) =$$

With Ph-B(O-C₂(Me)₂H₄-O)



S

Rh	-4.098977000	-1.479571000	0.000158000
C	-5.214644000	0.102770000	-0.000037000
C	-5.725191000	0.589107000	1.216742000
C	-5.725662000	0.588456000	-1.216870000
C	-6.777585000	1.510018000	1.209411000
H	-5.304056000	0.256971000	2.162357000
C	-6.778056000	1.509373000	-1.209621000
H	-5.304898000	0.255822000	-2.162476000
C	-7.304657000	1.969672000	-0.000128000
H	-7.175505000	1.877222000	2.152324000
H	-7.176336000	1.876067000	-2.152580000
H	-8.114195000	2.694486000	-0.000162000
C	-0.720985000	-2.804433000	0.735822000
C	0.596696000	-3.214773000	1.177137000
C	1.173341000	-2.633121000	2.311010000
C	0.452616000	-1.607606000	3.035439000
C	-0.812689000	-1.208440000	2.594856000
C	-1.417883000	-1.828182000	1.437482000
C	-0.721019000	-2.804500000	-0.735509000
C	0.596641000	-3.214874000	-1.176852000
C	1.410694000	-3.467560000	0.000135000
C	2.764551000	-3.131258000	0.000088000
C	2.581320000	-2.276613000	2.308711000
C	1.411487000	-0.612050000	3.486686000
C	1.066062000	0.739350000	3.485840000
C	-0.252947000	1.154556000	3.036020000
C	-1.173356000	0.198930000	2.594130000
C	-2.006136000	0.452225000	1.439710000
C	-2.274019000	-0.831070000	0.742775000
C	-2.274044000	-0.831134000	-0.742553000
C	-1.417946000	-1.828304000	-1.437217000
C	1.173234000	-2.633210000	-2.310801000
C	0.452475000	-1.607863000	-3.035281000
C	-0.812811000	-1.208662000	-2.594676000
C	-1.173476000	0.198709000	-2.594049000
C	-2.006204000	0.452104000	-1.439613000
C	-1.856133000	1.639269000	-0.735028000
C	-1.856101000	1.639333000	0.735021000
C	-0.895097000	2.629975000	1.176351000
C	-0.111164000	2.398887000	2.311022000
C	2.729539000	-1.026603000	3.036591000
C	3.181563000	2.937721000	0.727490000
C	3.881243000	1.951207000	1.425284000
C	4.606485000	0.922604000	0.697695000
C	4.606451000	0.922544000	-0.697948000
C	3.881175000	1.951089000	-1.425590000
C	1.863886000	3.348630000	-1.177147000
C	1.047005000	3.598339000	-0.000154000
C	1.863944000	3.348728000	1.176824000
C	1.295811000	2.761030000	2.308713000
C	2.024594000	1.734755000	3.035951000
C	3.290627000	1.337313000	2.601866000
C	4.462433000	-0.327572000	1.425050000
C	4.321531000	-1.528833000	0.727592000
C	4.321499000	-1.528896000	-0.727625000
C	4.462362000	-0.327692000	-1.425190000
C	3.650324000	-0.071680000	-2.602381000
C	3.290502000	1.337093000	-2.602088000
C	2.024450000	1.734500000	-3.036151000
C	1.295703000	2.760832000	-2.308959000
C	-0.301492000	3.242320000	-0.000107000
C	-0.895151000	2.629876000	-1.176486000
C	-0.111272000	2.398690000	-2.311172000
C	-0.253092000	1.154300000	-3.036065000
C	1.065897000	0.739055000	-3.485906000
C	1.411323000	-0.612346000	-3.486661000
C	2.729394000	-1.026859000	-3.036588000
C	2.581212000	-2.276811000	-2.308600000
C	3.361771000	-2.520965000	-1.176922000
C	3.650446000	-0.071461000	2.602257000
C	3.361826000	-2.520864000	1.177018000
C	3.181528000	2.937658000	-0.727842000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2628.35041$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2627.94061$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2627.05970$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -2626.64990$ 

T

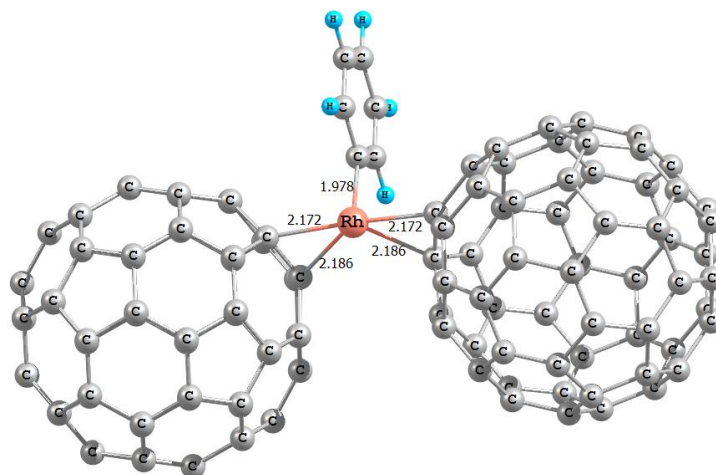
Rh	-0.000019000	1.347420000	-0.845958000
C	2.163630000	1.238763000	-0.998754000
C	2.682127000	0.544732000	-2.199681000
C	1.725104000	0.431856000	0.135052000
C	3.110235000	2.345573000	-0.744624000
C	2.670629000	-0.842698000	-2.297374000
C	3.803506000	1.292589000	-2.726122000
C	1.818262000	-1.041149000	0.022708000
C	2.241736000	0.759496000	1.478539000
C	4.067689000	2.402263000	-1.827114000
C	3.510147000	2.673322000	0.545248000
C	2.232611000	-1.651954000	-1.155883000
C	3.772623000	-1.535933000	-2.934283000
C	4.863959000	0.630555000	-3.352479000
C	2.236950000	-1.582641000	1.297560000
C	2.501708000	-0.471330000	2.194545000
C	3.070418000	1.857617000	1.678833000
C	5.384259000	2.810180000	-1.590053000
C	4.876003000	3.085195000	0.800562000
C	3.063084000	-2.839454000	-1.107454000
C	4.015747000	-2.768116000	-2.202296000
C	4.848724000	-0.814299000	-3.459390000
C	6.232044000	1.051347000	-3.099871000
C	3.031415000	-2.730963000	1.352622000
C	3.550956000	-0.552038000	3.114349000
C	4.166697000	1.780559000	2.625009000
C	5.797611000	3.160465000	-0.247277000
C	6.486339000	2.117971000	-2.236968000
C	5.282892000	2.536998000	2.084156000
C	3.454222000	-3.372464000	0.123883000
C	5.319724000	-3.231324000	-2.025171000
C	6.207172000	-1.293558000	-3.269816000
C	7.063713000	-0.139601000	-3.048639000
C	4.1271165000	-2.811357000	2.304713000
C	4.402447000	0.599712000	3.333806000
C	4.381837000	-1.743956000	3.166050000
C	7.156732000	2.683760000	-0.055950000
C	7.584079000	2.039839000	-1.287223000
C	6.589356000	2.080553000	2.269996000
C	4.812794000	-3.850883000	0.310365000
C	5.727514000	-3.781462000	-0.742065000
C	6.438693000	-2.477856000	-2.567821000
C	8.115779000	-0.216472000	-2.134590000
C	5.229732000	-3.503498000	1.658825000
C	5.762574000	0.125172000	3.523788000
C	5.750306000	-1.324677000	3.419717000
C	7.546010000	2.157783000	1.177149000
C	8.381877000	0.895638000	-1.236279000
C	6.833919000	0.852171000	3.001568000
C	7.095373000	-3.364719000	-0.490180000
C	7.534203000	-2.557849000	-1.618152000
C	8.356340000	-1.449788000	-1.405246000
C	6.544178000	-3.101170000	1.901077000
C	6.809698000	-1.989069000	2.799425000
C	8.376131000	0.967586000	1.229854000
C	7.786843000	0.348766000	0.047554000
C	7.936842000	0.161130000	2.358109000
C	7.495242000	-3.029436000	0.804929000
C	8.770620000	-1.100927000	-0.056495000
C	7.925362000	-1.231475000	2.258319000
C	8.350005000	-1.875047000	1.026026000
C	-1.725104000	0.431990000	0.135132000
C	-1.818208000	-1.041055000	0.023138000
C	-2.163594000	1.238598000	-0.998929000
C	-2.241868000	0.759950000	1.478485000
C	-2.232465000	-1.652174000	-1.155322000
C	-2.236983000	-1.582230000	1.298093000
C	-2.681979000	0.544234000	-2.199704000
C	-3.110246000	2.345438000	-0.745156000
C	-2.501848000	-0.470696000	2.194781000
C	-3.070589000	1.858108000	1.678443000
C	-2.670428000	-0.843219000	-2.297047000
C	-3.062882000	-2.839704000	-1.106655000
C	-3.031407000	-2.730569000	1.353401000
C	-3.803377000	1.291924000	-2.726437000
C	-4.067634000	2.401820000	-1.827730000
C	-3.510282000	2.673476000	0.544608000
C	-3.551161000	-0.551197000	3.114521000
C	-4.166939000	1.781262000	2.624564000
C	-3.772354000	-1.536658000	-2.933860000
C	-4.015480000	-2.768674000	-2.201588000
C	-3.454106000	-3.372393000	0.124799000
C	-4.127234000	-2.810734000	2.305426000
C	-4.863730000	0.629683000	-3.352691000
C	-5.384236000	2.809736000	-1.590865000
C	-4.876162000	3.085382000	0.799718000
C	-4.402702000	0.600581000	3.333640000
C	-4.382003000	-1.743130000	3.166470000
C	-5.283129000	2.537517000	2.083431000
C	-4.848444000	-0.815194000	-3.459228000
C	-5.319451000	-3.231879000	-2.024435000
C	-4.812679000	-3.850807000	0.311306000
C	-5.229722000	-3.503088000	1.659643000
C	-6.231849000	1.050482000	-3.100280000
C	-5.797693000	3.160349000	-0.248208000
C	-6.486236000	2.117310000	-2.237671000
C	-5.762821000	0.126031000	3.523633000
C	-5.750502000	-1.323839000	3.419937000
C	-6.589587000	2.085575000	2.269295000
C	-6.206881000	-1.294462000	-3.269640000
C	-6.338415000	-2.478597000	-2.567857000
C	-5.727321000	-3.781688000	-0.741210000
C	-6.544202000	-3.100752000	1.901699000
C	-7.063477000	-0.140479000	-3.048801000
C	-7.156812000	2.683652000	-0.056852000
C	-7.584051000	2.039403000	-1.287991000
C	-6.834155000	0.852863000	3.001157000
C	-6.809837000	-1.988433000	2.799751000
C	-7.546177000	2.157999000	1.176359000
C	-7.533995000	-2.558369000	-1.617747000
C	-7.095204000	-3.364919000	-0.489536000
C	-7.495174000	-3.029316000	0.805459000
C	-8.115603000	-0.217147000	-2.134816000
C	-8.381805000	0.895185000	-1.236806000
C	-7.937013000	0.161619000	2.357797000
C	-7.925465000	-1.231008000	2.258349000
C	-8.376251000	0.967770000	1.229305000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4914.51647$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4913.75189$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4912.08742$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4911.32284$$



C	-8.356190000	-1.450284000	-1.405181000
C	-8.350004000	-1.874914000	1.026202000
C	-8.786868000	0.348635000	0.047133000
C	-8.770577000	-1.101086000	-0.056548000
C	-0.000079000	3.167467000	-0.071301000
C	-0.000411000	4.201785000	-1.018296000
C	0.000191000	3.470635000	1.291547000
C	-0.000439000	5.535246000	-0.595808000
H	-0.000639000	3.982468000	-2.085150000
C	0.000139000	4.809221000	1.704817000
H	0.000443000	2.679110000	2.033505000
C	-0.000172000	5.841972000	0.767100000
H	-0.000680000	6.330499000	-1.337274000
H	0.000339000	5.037003000	2.768182000
H	-0.000221000	6.878192000	1.093754000

T-U

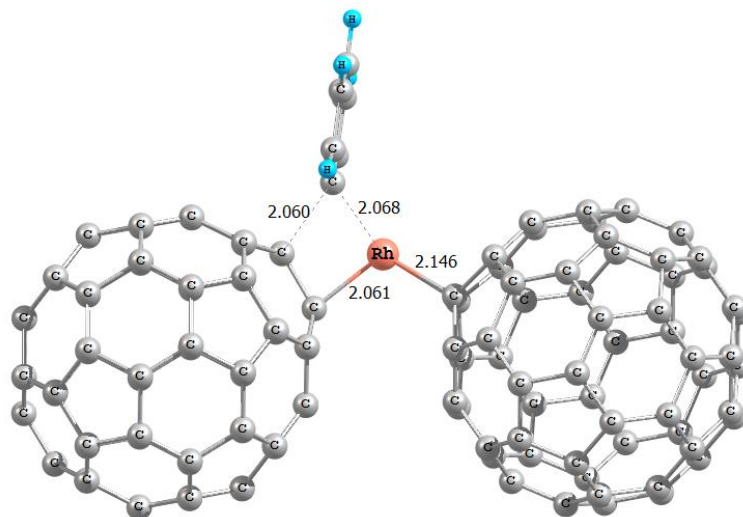
Rh	0.083837000	2.063135000	-0.049263000
C	1.824632000	1.013317000	-0.772234000
C	1.885012000	-0.290728000	-1.465147000
C	1.810723000	1.023224000	0.687084000
C	2.803785000	1.876264000	-1.471557000
C	1.848728000	-1.485292000	-0.754381000
C	2.753552000	-0.171911000	-2.616672000
C	1.858862000	-0.267981000	1.403419000
C	2.774961000	1.900690000	1.391204000
C	3.317394000	1.166773000	-2.622917000
C	3.629698000	2.750133000	-0.773674000
C	1.835365000	-1.473359000	0.711981000
C	2.656640000	-2.611222000	-1.179951000
C	3.527910000	-1.256523000	-3.039495000
C	2.703365000	-0.128591000	2.569669000
C	3.266331000	1.210636000	2.564249000
C	3.615307000	2.761441000	0.693903000
C	4.632432000	1.371556000	-3.051570000
C	4.997218000	2.958129000	-1.204964000
C	2.633829000	-2.591907000	1.172764000
C	3.141521000	-3.295488000	0.007142000
C	3.477401000	-2.504621000	-2.306550000
C	4.897606000	-1.044437000	-3.478410000
C	3.468619000	-1.205597000	3.026514000
C	4.572424000	1.422887000	3.015225000
C	4.974113000	2.977825000	1.148954000
C	5.490976000	2.286270000	-2.327342000
C	5.438209000	0.241643000	-3.484957000
C	5.828488000	3.098545000	-0.020754000
C	3.432232000	-2.465752000	2.313455000
C	4.424610000	-3.842927000	0.024541000
C	4.816320000	-3.068707000	-2.286212000
C	5.695218000	-2.166626000	-3.012512000
C	4.829380000	-0.985658000	3.488739000
C	5.445247000	2.325131000	2.292131000
C	5.369627000	0.300580000	3.483561000
C	6.831021000	1.725592000	-2.307500000
C	6.798647000	0.460524000	-3.023602000
C	7.117289000	2.564675000	-0.003465000
C	4.771167000	-3.029698000	2.329208000
C	5.257655000	-3.704745000	1.208430000
C	5.280718000	-3.724645000	-1.144884000
C	7.002211000	-1.957003000	-2.568851000
C	5.635758000	-2.115324000	3.057469000
C	6.785334000	1.764626000	2.308610000
C	6.738811000	0.511907000	3.045359000
C	7.628277000	1.861514000	-1.169360000
C	7.564939000	-0.616193000	-2.574324000
C	7.604675000	1.881219000	1.184075000
C	6.626027000	-3.494814000	0.770603000
C	6.640260000	-3.507130000	-0.683909000
C	7.484669000	-2.641187000	-1.381157000
C	6.951274000	-1.912975000	2.636085000
C	7.513848000	-0.572122000	2.629750000
C	8.425523000	0.741621000	-0.702359000
C	8.394975000	-0.472914000	-1.390412000
C	8.411083000	0.753859000	0.752123000
C	7.456626000	-2.617036000	1.469572000
C	8.345702000	-1.724229000	-0.652804000
C	8.366843000	-0.448820000	1.459915000
C	8.332057000	-1.712502000	0.742912000
C	-1.533256000	0.785924000	-0.086858000
C	-1.756124000	-0.040152000	-1.310468000
C	-2.294450000	2.073790000	0.030852000
C	-1.648048000	-0.191345000	1.033598000
C	-2.541144000	0.393976000	-2.366683000
C	-1.765808000	-1.438320000	-0.948005000
C	-3.248280000	2.392784000	-1.082575000
C	-3.128814000	2.248035000	1.267019000
C	-1.697186000	-1.531262000	0.498917000
C	-2.318875000	0.100814000	2.209490000
C	-3.310199000	1.641224000	-2.242183000
C	-3.350036000	-0.547372000	-3.111918000
C	-2.527555000	-2.361006000	-1.671960000
C	-4.455172000	2.959055000	-0.533153000
C	-4.383225000	2.867838000	0.913644000
C	-3.086255000	1.350499000	2.320070000
C	-2.389800000	-2.543387000	1.170593000
C	-3.056011000	-0.932914000	2.904010000
C	-4.575895000	1.452690000	-2.920688000
C	-4.603909000	0.102649000	-3.455539000
C	-3.339622000	-1.905861000	-2.779337000
C	-3.258864000	-3.405142000	-0.972213000
C	-5.681489000	2.796147000	-1.185274000
C	-5.541823000	2.614446000	1.654958000
C	-4.281516000	1.067714000	3.088373000
C	-3.086247000	-2.238389000	2.401308000
C	-3.190834000	-3.495073000	0.418080000
C	-4.266272000	-0.339918000	3.447581000
C	-5.743459000	2.024668000	-2.406942000
C	-5.794246000	-0.624682000	-3.455161000
C	-4.579454000	-2.661348000	-2.768992000
C	-4.529678000	-3.590622000	-1.651696000
C	-6.883455000	2.521609000	-0.414154000
C	-5.489868000	1.693132000	2.768162000
C	-6.814737000	2.432319000	0.975533000
C	-4.325891000	-2.994133000	2.415005000
C	-4.390705000	-3.773711000	1.188967000
C	-5.455235000	-1.068940000	3.469532000
C	-6.981820000	1.266066000	-2.399250000
C	-7.006453000	-0.032882000	-2.911506000
C	-5.782905000	-2.034930000	-3.100458000
C	-5.683663000	-3.856364000	-0.912171000
C	-7.687572000	1.573151000	-1.165728000
C	-6.727785000	0.933616000	2.783957000
C	-7.548480000	1.391158000	1.674709000
C	-5.487445000	-2.422756000	2.939347000
C	-5.612869000	-3.949342000	0.537259000
C	-6.710777000	-0.419856000	3.125778000
C	-7.739252000	-1.074416000	-2.215758000
C	-6.982283000	-2.312085000	-2.332183000
C	-6.934793000	-3.204582000	-1.259348000
C	-8.390978000	0.570496000	-0.495578000
C	-8.319771000	0.477432000	0.953704000
C	-6.757293000	-2.606355000	2.261748000
C	-6.820029000	-3.354522000	1.084509000
C	-7.514514000	-1.369059000	2.378484000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4914.47803$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4913.71252$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4912.05336$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4911.28785$$



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C	-7.637900000	-2.894839000	-0.025533000
C	-8.302410000	-0.930089000	1.312459000
C	-8.363998000	-1.707789000	0.085992000
C	-1.104006000	3.755162000	0.011526000
C	-1.081256000	4.467451000	-1.202816000
C	-1.041534000	4.444201000	1.236647000
C	-0.895908000	5.851981000	-1.183125000
H	-1.201911000	3.948105000	-2.148579000
C	-0.858952000	5.829659000	1.236288000
H	-1.127312000	3.905783000	2.175379000
C	-0.783982000	6.534244000	0.031738000
H	-0.855381000	6.397897000	-2.122065000
H	-0.789561000	6.358277000	2.183400000
H	-0.658942000	7.613202000	0.039726000

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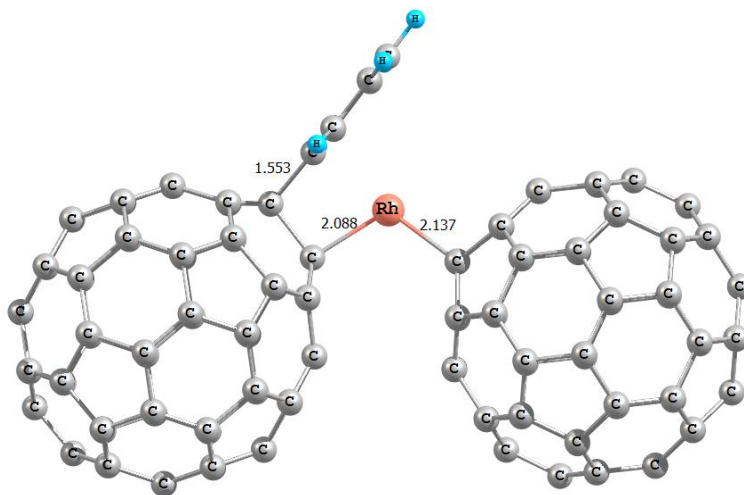
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C	1.779620000	-0.131821000	-1.434992000
C	1.781898000	1.172087000	0.734900000
C	2.815736000	1.977689000	-1.432556000
C	1.689743000	-1.327864000	-0.734050000
C	2.644031000	-0.052305000	-2.592667000
C	1.779436000	-0.132115000	1.434560000
C	2.815524000	1.977397000	1.432520000
C	3.280605000	1.252871000	-2.593935000
C	3.695607000	2.797159000	-0.734468000
C	1.689655000	-1.328008000	0.733354000
C	2.428448000	-2.492629000	-1.176807000
C	3.353367000	-1.173949000	-3.034147000
C	2.643661000	-0.052837000	2.592388000
C	3.280224000	1.252343000	2.594025000
C	3.695503000	2.797008000	0.734929000
C	4.600736000	1.389673000	-3.034676000
C	5.067832000	2.935319000	-1.176890000
C	2.428283000	-2.492866000	1.175980000
C	2.885392000	-3.213030000	-0.000452000
C	3.242062000	-2.423264000	-2.311553000
C	4.728914000	-1.032965000	-3.484294000
C	3.352916000	-1.174575000	3.033748000
C	4.600289000	1.389052000	3.034986000
C	5.067659000	2.935080000	1.177585000
C	5.514472000	2.249152000	-2.310990000
C	5.339187000	0.221155000	-3.485383000
C	5.916357000	3.019216000	0.000418000
C	3.241724000	-2.423734000	2.310865000
C	4.135214000	-3.832402000	-0.000421000
C	4.547601000	-3.060594000	-2.308803000
C	5.467891000	-2.201438000	-3.035938000
C	4.728400000	-1.033685000	3.484121000
C	5.514134000	2.248684000	2.311616000
C	5.338673000	0.220436000	3.485563000
C	6.821558000	1.615993000	-2.308554000
C	6.713861000	0.361161000	-3.035412000
C	7.174497000	2.416565000	0.000452000
C	4.547260000	-3.061063000	2.308177000
C	4.985759000	-3.751691000	1.176666000
C	4.985754000	-3.751452000	-1.177366000
C	6.788451000	-2.067854000	-2.602827000
C	5.467443000	-2.202062000	3.035632000
C	6.821220000	1.615521000	2.309241000
C	6.713409000	0.360532000	3.035815000
C	7.635262000	1.697441000	-1.176617000
C	7.423892000	-0.759892000	-2.602240000
C	7.635093000	1.697204000	1.177444000
C	6.359145000	-3.613442000	0.727274000
C	6.359253000	-3.613293000	-0.727742000
C	7.243352000	-2.788036000	-1.425724000
C	6.788067000	-2.068391000	2.602744000
C	7.423510000	-0.760430000	2.602521000
C	8.374377000	0.531858000	-0.727057000
C	8.270804000	-0.672965000	-1.424947000
C	8.374275000	0.531710000	0.727730000
C	7.243141000	-2.788332000	1.425559000
C	8.160027000	-1.926379000	-0.697881000
C	8.270601000	-0.673260000	1.425373000
C	8.159929000	-1.926526000	0.698032000
C	-1.600613000	1.293978000	0.000072000
C	-1.722796000	0.363300000	-1.170383000
C	-2.563151000	2.552220000	0.000044000
C	-1.722858000	0.363290000	1.170492000
C	-2.497585000	0.623988000	-2.288202000
C	-1.576078000	-1.001670000	-0.724520000
C	-3.549486000	2.584164000	-1.178327000
C	-3.549509000	2.584191000	1.178395000
C	-1.576115000	-1.001672000	0.724631000
C	-2.497663000	0.623987000	2.288296000
C	-3.443146000	1.761979000	-2.279872000
C	-3.130487000	-0.458988000	-3.006685000
C	-2.157185000	-2.062216000	-1.425269000
C	-4.851516000	2.993776000	-0.726072000
C	-4.851537000	2.993783000	0.726091000
C	-3.443220000	1.761979000	2.279927000
C	-2.157239000	-2.062219000	1.425363000
C	-3.130589000	-0.458992000	3.006751000
C	-4.628173000	1.356297000	-3.005157000
C	-4.439727000	-0.011641000	-3.451780000
C	-2.954994000	-1.786945000	-2.597036000
C	-2.776472000	-3.157856000	-0.697258000
C	-6.008235000	2.628568000	-1.425193000
C	-6.008281000	2.628573000	1.425166000
C	-4.628272000	1.356294000	3.005173000
C	-2.955084000	-1.786947000	2.597103000
C	-2.776495000	-3.157862000	0.697332000
C	-4.439843000	-0.011643000	3.451801000
C	-5.893171000	1.788912000	-2.593191000
C	-5.518090000	-0.896662000	-3.469274000
C	-4.079434000	-2.703626000	-2.599693000
C	-3.968858000	-3.554987000	-1.425208000
C	-7.203993000	2.233834000	-0.697131000
C	-5.893256000	1.788907000	2.593163000
C	-7.204013000	2.233834000	0.697061000
C	-4.079521000	-2.703635000	2.599727000
C	-3.968907000	-3.554992000	1.425242000
C	-5.518205000	-0.896665000	3.469259000
C	-7.014477000	0.867023000	-2.599790000
C	-6.829768000	-0.449499000	-3.026163000
C	-5.336357000	-2.270593000	-3.029042000
C	-5.116753000	-3.935470000	-0.727249000
C	-7.826775000	1.141583000	-1.425171000
C	-7.014564000	0.867021000	2.599728000
C	-7.826821000	1.141582000	1.425080000
C	-5.336457000	-2.270599000	3.029031000
C	-5.116778000	-3.935473000	0.727244000
C	-6.829866000	-0.449953000	3.026103000
C	-7.452442000	-1.542478000	-2.304381000
C	-6.528047000	-2.667502000	-2.304374000
C	-6.422190000	-3.483590000	-1.175784000
C	-8.422110000	0.088964000	-0.727171000
C	-8.422135000	0.088964000	0.727059000
C	-6.528123000	-2.667507000	2.304324000
C	-6.422290000	-3.483590000	1.175734000
C	-7.452517000	-1.542481000	2.304299000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4914.51438$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4913.74627$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4912.09510$$

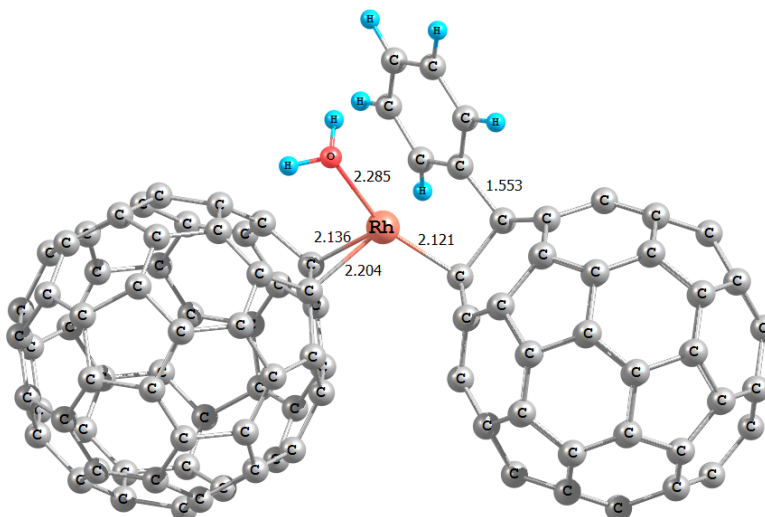
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C	-7.229219000	-3.203906000	-0.000038000
C	-8.232061000	-1.279377000	1.175429000
C	-8.116225000	-2.125763000	-0.000053000
C	-1.560636000	3.738022000	0.000012000
C	-1.086748000	4.291913000	-1.220449000
C	-1.086655000	4.291826000	1.220475000
C	-0.227025000	5.396985000	-1.210625000
H	-1.459847000	3.905513000	-2.162944000
C	-0.226952000	5.396924000	1.210670000
H	-1.459702000	3.905366000	2.162967000
C	0.196611000	5.953880000	0.000030000
H	0.103105000	5.823510000	-2.153370000
H	0.103227000	5.823395000	2.153424000
H	0.856340000	6.816517000	0.000030000

V

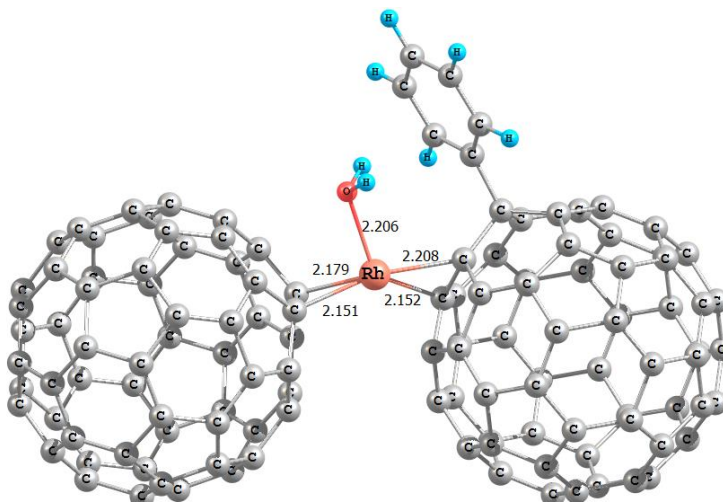
Rh	0.141395000	2.420280000	-0.478912000
C	1.773590000	1.046044000	-1.030858000
C	1.692646000	-0.401728000	-1.334292000
C	1.838452000	1.451489000	0.384471000
C	2.827211000	1.550429000	-1.944635000
C	1.578201000	-1.353118000	-0.329148000
C	2.503867000	-0.700843000	-2.494519000
C	1.817859000	0.385267000	1.418949000
C	2.955544000	2.343532000	0.799744000
C	3.204334000	0.510751000	-2.875655000
C	3.778900000	2.483941000	-1.538047000
C	1.645738000	-0.949448000	1.078691000
C	2.235111000	-2.636744000	-0.452864000
C	3.135712000	-1.942075000	-2.629253000
C	2.738608000	0.725974000	2.481958000
C	3.439902000	1.939066000	2.100420000
C	3.848804000	2.877482000	-0.120759000
C	4.509284000	0.441431000	-3.374376000
C	5.137670000	2.406855000	-2.038490000
C	2.341672000	-1.990629000	1.805917000
C	2.707486000	-3.033352000	0.863022000
C	2.996446000	-2.935163000	-1.586372000
C	4.494945000	-2.013203000	-3.141018000
C	3.411827000	-0.270586000	3.196673000
C	4.784213000	2.112075000	2.448008000
C	5.244028000	3.050607000	0.222186000
C	5.497990000	1.410848000	-2.950157000
C	5.167075000	-0.847685000	-3.509018000
C	6.040844000	2.759782000	-0.956734000
C	3.207148000	-1.661258000	2.852694000
C	3.923099000	-3.703989000	0.997856000
C	4.267132000	-3.624661000	-1.445321000
C	5.195016000	-3.056199000	-2.409249000
C	4.811923000	-0.094481000	3.548910000
C	5.706903000	2.681398000	1.488932000
C	5.483891000	1.072007000	3.185155000
C	6.770170000	0.724840000	-2.810712000
C	6.566307000	-0.672569000	-3.157244000
C	7.267631000	2.106992000	-0.827147000
C	4.477198000	-2.352926000	2.989032000
C	4.828739000	-3.353040000	2.080605000
C	4.721741000	-4.002045000	-0.180067000
C	6.538678000	-2.887670000	-2.069592000
C	5.470953000	-1.383720000	3.420650000
C	6.979492000	1.995532000	1.623395000
C	6.842447000	0.999355000	2.673652000
C	7.638772000	1.065863000	-1.771786000
C	7.238508000	-1.671486000	-2.451447000
C	7.743933000	1.712931000	0.489252000
C	6.185466000	-3.428172000	1.569743000
C	6.118942000	-3.828110000	0.172063000
C	7.010806000	-3.282617000	-0.753492000
C	6.775278000	-1.454639000	2.928099000
C	7.474915000	-0.238620000	2.546445000
C	8.337674000	0.026275000	-1.038088000
C	8.142310000	-1.315519000	-1.370717000
C	8.403880000	0.426779000	0.358984000
C	7.140085000	-2.497538000	1.984432000
C	8.001888000	-2.311140000	-0.321007000
C	8.270881000	-0.530645000	1.366549000
C	8.065150000	-1.926803000	1.019513000
C	-1.557577000	1.236184000	-0.019542000
C	-1.794460000	0.471961000	-1.288813000
C	-2.516417000	2.476433000	0.229036000
C	-1.602359000	0.151941000	1.016533000
C	-2.648062000	0.880584000	-2.303362000
C	-1.623671000	-0.942921000	-1.049870000
C	-3.596672000	2.654460000	-0.848704000
C	-3.410387000	2.338485000	1.477437000
C	-1.509897000	-1.140084000	0.379215000
C	-2.282436000	0.250722000	2.219268000
C	-3.584599000	1.996997000	-2.060173000
C	-3.344595000	-0.097900000	-3.110802000
C	-2.263289000	-1.898441000	-1.842668000
C	-4.856141000	2.992817000	-0.243507000
C	-4.741061000	2.799082000	1.190743000
C	-3.219287000	1.375532000	2.444448000
C	-2.037627000	-2.291031000	0.972347000
C	-2.866930000	-0.923643000	2.828592000
C	-4.826537000	1.691488000	-2.737264000
C	-4.683476000	0.399733000	-3.382233000
C	-3.148726000	-1.468930000	-2.900852000
C	-2.829935000	-3.086763000	-1.225072000
C	-6.067578000	2.728254000	-0.891870000
C	-5.841568000	2.339532000	1.923497000
C	-4.347058000	0.868091000	3.196820000
C	-2.735164000	-2.183608000	2.230341000
C	-2.719035000	-3.278993000	0.151917000
C	-4.133822000	-0.547269000	3.433676000
C	-6.051770000	2.058742000	-2.170064000
C	-5.766648000	-0.478717000	-3.433984000
C	-4.276060000	-2.380991000	-2.938279000
C	-4.078723000	-3.384972000	-1.903283000
C	-7.205111000	2.234230000	-0.131680000
C	-5.638976000	1.348455000	2.952601000
C	-7.094046000	2.043047000	1.245056000
C	-3.862519000	-3.096588000	2.197014000
C	-3.852071000	-3.778118000	0.911185000
C	-5.213764000	-1.431083000	3.416912000
C	-7.176746000	1.142612000	-2.213228000
C	-7.035910000	-0.102374000	-2.829887000
C	-5.560677000	-1.898810000	-3.202497000
C	-5.170082000	-3.862498000	-1.175095000
C	-7.891062000	1.250064000	-0.951030000
C	-6.761890000	0.428984000	2.920771000
C	-7.663779000	0.858643000	1.863566000
C	-5.078047000	-2.731146000	2.780033000
C	-5.054342000	-4.062178000	0.261110000
C	-6.553886000	-0.933435000	3.146664000
C	-7.607099000	-1.285795000	-2.217111000
C	-6.693597000	-2.396238000	-2.445780000
C	-6.504097000	-3.358972000	-1.451932000
C	-8.437257000	0.109442000	-0.358544000
C	-8.320838000	-0.090209000	1.077197000
C	-6.326663000	-3.029167000	2.104981000
C	-6.316751000	-3.681562000	0.869810000
C	-7.239740000	-1.918547000	2.332863000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.94330$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.15131$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4988.52850$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4987.73651$ 

C	-8.292955000	-1.183635000	-1.004490000
C	-7.213022000	-3.246842000	-0.187990000
C	-8.105602000	-1.506522000	1.317030000
C	-8.090482000	-2.183170000	0.031074000
C	-1.559725000	3.695188000	0.329178000
C	-1.742021000	4.882379000	-0.432684000
C	-0.595367000	3.706133000	1.379466000
C	-0.997977000	6.020415000	-0.167044000
H	-2.487417000	4.893191000	-1.221329000
C	0.139714000	4.885795000	1.649766000
H	-0.574440000	2.901269000	2.106620000
C	-0.051316000	6.024980000	0.882290000
H	-1.156792000	6.918151000	-0.757829000
H	0.837003000	4.895503000	2.482657000
H	0.501434000	6.933323000	1.107937000
O	1.226175000	4.145432000	-1.512775000
H	2.166939000	3.973664000	-1.705192000
H	1.187194000	4.918452000	-0.921857000

X

Rh	-0.067947000	1.516067000	-0.583205000
C	1.913965000	0.780081000	-1.111718000
C	2.103804000	-0.570912000	-1.683398000
C	1.776091000	0.903727000	0.338452000
C	2.902084000	1.638955000	-1.799306000
C	2.068429000	-1.709722000	-0.885935000
C	3.055763000	-0.492362000	-2.770568000
C	1.842175000	-0.328319000	1.156551000
C	2.635599000	1.885804000	1.041847000
C	3.548320000	0.871626000	-2.842148000
C	3.624937000	2.608606000	-1.113030000
C	1.936523000	-1.583876000	0.568580000
C	2.965682000	-2.815397000	-1.153928000
C	3.915541000	-1.560992000	-3.043770000
C	2.579338000	-0.050874000	2.369464000
C	3.070485000	1.314372000	2.298690000
C	3.490106000	2.730601000	0.342074000
C	4.881925000	1.117458000	-3.184712000
C	5.011010000	2.858510000	-1.451777000
C	2.750609000	-2.614912000	1.180341000
C	3.387005000	-3.376409000	0.119280000
C	3.869333000	-2.750005000	-2.218637000
C	5.303608000	-1.305027000	-3.391386000
C	3.356830000	-1.043627000	2.973350000
C	4.322494000	1.634601000	2.832906000
C	4.794525000	3.059172000	0.882852000
C	5.630329000	2.133461000	-2.474633000
C	5.776871000	0.005692000	-3.460591000
C	5.734780000	3.137938000	-0.222363000
C	3.444017000	-2.355622000	2.365956000
C	4.690043000	-3.847107000	0.280587000
C	5.228947000	-3.233060000	-2.048277000
C	6.116578000	-2.339940000	-2.774751000
C	4.661980000	-0.710988000	3.520676000
C	5.204123000	2.526500000	2.108952000
C	5.134753000	0.599768000	3.452268000
C	6.991274000	1.653964000	-2.305194000
C	7.082609000	0.337830000	-2.915551000
C	7.043414000	2.682609000	-0.061895000
C	4.803822000	-2.839147000	2.531616000
C	5.414719000	-3.569634000	1.510537000
C	5.631964000	-3.771789000	-0.824749000
C	7.370478000	-2.021882000	-2.249763000
C	5.557555000	-1.822345000	3.246898000
C	6.565462000	2.047124000	2.275469000
C	6.522901000	0.854945000	3.106412000
C	7.684350000	1.922783000	-1.123357000
C	7.863006000	-0.655620000	-2.320864000
C	7.466745000	2.122885000	1.211899000
C	6.801658000	-3.315970000	1.164701000
C	6.935919000	-3.440437000	-0.278650000
C	7.789029000	-2.583599000	-0.976746000
C	6.890968000	-1.577957000	2.913334000
C	7.383400000	-0.211958000	2.841416000
C	8.496819000	0.890290000	-0.505616000
C	8.585500000	-0.373785000	-1.092014000
C	8.362687000	1.014051000	0.937510000
C	7.526000000	-2.340098000	1.851932000
C	8.540483000	-1.565510000	-0.260763000
C	8.322461000	-1.030831000	1.735516000
C	8.412354000	-1.446648000	1.124306000
C	-2.248213000	1.803777000	-0.381409000
C	-2.547103000	1.223192000	-1.700168000
C	-3.203864000	2.868397000	0.228383000
C	-1.775890000	0.697174000	0.438498000
C	-3.642029000	1.573008000	-2.479693000
C	-2.021851000	-0.121790000	-1.748721000
C	-4.535846000	2.909667000	-0.571582000
C	-3.756255000	2.372549000	1.599891000
C	-1.478246000	-0.437979000	-0.431747000
C	-2.130275000	0.501711000	1.784627000
C	-4.686300000	2.406449000	-1.851083000
C	-4.294690000	0.556452000	-3.263816000
C	-2.614185000	-1.094807000	-2.549319000
C	-5.659534000	2.875971000	0.324758000
C	-5.182949000	2.549206000	1.657600000
C	-3.185106000	1.359913000	2.346304000
C	-1.638413000	-1.757785000	0.084721000
C	-2.292341000	-0.817261000	2.278344000
C	-5.967393000	1.907184000	-2.300320000
C	-5.731202000	0.764566000	-3.165776000
C	-3.786819000	-0.754824000	-3.321277000
C	-2.77785000	-2.440527000	-2.012341000
C	-6.915586000	2.419298000	-0.099088000
C	-5.976617000	1.769196000	2.511300000
C	-3.983270000	0.534127000	3.224373000
C	-2.050427000	-1.939986000	1.442403000
C	-2.306241000	-2.760487000	-0.736140000
C	-3.444977000	-0.813319000	3.180907000
C	-7.072411000	1.921843000	-1.443832000
C	-6.601163000	-0.325206000	-3.135520000
C	-4.691422000	-1.883762000	-3.263185000
C	-4.067748000	-2.928926000	-2.463648000
C	-7.728211000	1.597491000	0.784372000
C	-5.362682000	0.738303000	3.315550000
C	-7.270336000	1.279654000	2.060751000
C	-2.967641000	-3.071105000	1.491926000
C	-3.121507000	-3.582895000	0.141958000
C	-4.303560000	-1.904078000	3.222094000
C	-7.977039000	0.787157000	-1.407267000
C	-7.474318000	-0.316136000	-2.233556000
C	-6.073392000	-1.679412000	-3.183866000
C	-4.847767000	-3.721790000	-1.619183000
C	-8.383569000	0.584580000	-0.027685000
C	-6.260474000	-0.399756000	3.359835000
C	-7.443272000	-0.065841000	2.583284000
C	-4.061963000	-3.058030000	2.357261000
C	-4.364355000	-4.054316000	-0.288860000
C	-5.739756000	-1.696618000	3.309952000
C	-7.913286000	-1.658498000	-1.717689000
C	-6.877277000	-2.500806000	-2.302908000
C	-6.280823000	-3.506024000	-1.537894000
C	-8.544098000	-0.710468000	0.470055000
C	-8.063722000	-1.042308000	1.802174000
C	-5.348499000	-3.550419000	1.913440000
C	-5.499457000	-4.040790000	0.613768000
C	-6.384556000	-2.710096000	2.499492000

 $E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.93143$ $G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.14185$ $E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4988.51354$ $G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4987.72396$ 

C	-8.304605000	-1.853893000	-0.391345000
C	-6.685530000	-3.701871000	-0.155724000
C	-7.524955000	-2.391049000	1.760046000
C	-7.676688000	-2.895425000	0.405095000
C	-2.512815000	4.240290000	0.322145000
C	-2.643785000	5.186720000	-0.702440000
C	-1.664381000	4.534144000	1.402447000
C	-1.937168000	6.393154000	-0.657251000
H	-3.306446000	4.983033000	-1.538262000
C	-0.955372000	5.739224000	1.447350000
H	-1.561626000	3.819798000	2.214181000
C	-1.088106000	6.674011000	0.414532000
H	-2.058415000	7.115328000	-1.460215000
H	-0.309433000	5.950225000	2.295420000
H	-0.541727000	7.611962000	0.451846000
O	0.594155000	3.610353000	-0.791138000
H	0.178086000	3.985175000	-1.585733000
H	0.179529000	4.088804000	-0.045384000

X-Y

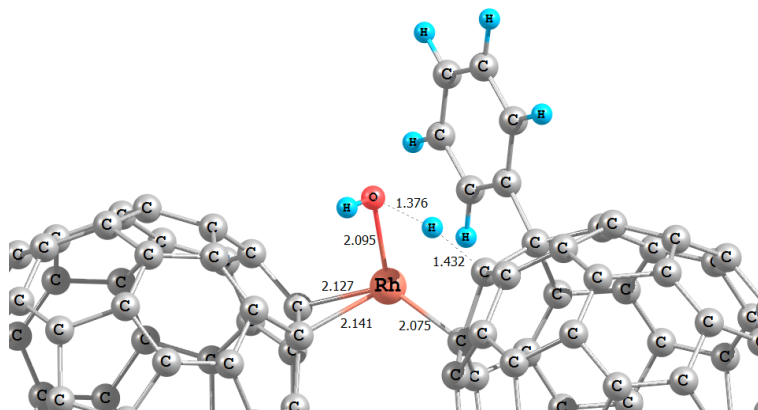
Rh	0.017428000	1.662517000	-0.207535000
C	1.709631000	0.425097000	-0.640305000
C	1.747057000	-1.018682000	-0.313687000
C	2.030575000	1.383696000	0.419740000
C	2.403570000	0.554014000	-1.942576000
C	1.998450000	-1.458035000	0.980180000
C	2.308085000	-1.737536000	-1.435925000
C	2.577768000	0.860768000	1.760826000
C	3.036188000	2.431767000	0.132028000
C	2.713870000	-0.768310000	-2.439718000
C	3.277382000	1.606677000	-2.190016000
C	2.317455000	-0.497894000	2.044302000
C	2.796721000	-2.646793000	1.201992000
C	3.070564000	-2.891137000	-1.231751000
C	3.448556000	1.661760000	2.311836000
C	3.853361000	2.631567000	1.308118000
C	3.598233000	2.570815000	-1.130636000
C	3.865149000	-0.989528000	-3.200159000
C	4.479822000	1.384081000	-2.968650000
C	3.312579000	-1.105698000	2.904427000
C	3.608919000	-2.431645000	2.387650000
C	3.320863000	-3.355267000	0.116816000
C	4.272760000	-3.116918000	-2.018196000
C	4.405318000	1.085405000	3.153048000
C	5.199726000	2.989229000	1.183955000
C	4.995662000	2.926620000	-1.267738000
C	4.768091000	0.110804000	-3.469289000
C	4.661925000	-2.185980000	-2.981365000
C	5.541512000	2.197158000	-2.400681000
C	4.336162000	-0.329041000	3.456248000
C	4.910703000	-2.929216000	2.442420000
C	4.677959000	-3.870493000	0.171514000
C	5.267404000	-3.723415000	-1.149228000
C	5.805582000	1.452032000	3.017607000
C	5.783711000	3.140130000	-0.132561000
C	6.194462000	2.383580000	2.054258000
C	6.126965000	-0.399830000	-3.418695000
C	6.061861000	-1.820587000	-3.116700000
C	6.847615000	1.709387000	-2.356013000
C	5.693339000	-0.844602000	3.507690000
C	5.975495000	-2.118794000	3.011825000
C	5.457640000	-3.660088000	1.310230000
C	6.612752000	-3.372296000	-1.277818000
C	6.602981000	0.257081000	3.237473000
C	7.141424000	2.625963000	-0.083390000
C	7.397157000	2.159221000	1.269593000
C	7.145744000	0.382877000	-2.872297000
C	7.017834000	-2.401244000	-2.281328000
C	7.663936000	1.925834000	-1.172411000
C	7.176651000	-2.344539000	2.228376000
C	6.856619000	-3.297747000	1.176772000
C	7.425168000	-3.155306000	-0.091352000
C	7.156791000	0.039974000	2.482619000
C	8.162475000	1.010636000	1.478929000
C	8.1441421000	-0.221412000	-2.005802000
C	8.078405000	-1.585525000	-1.714859000
C	8.461166000	0.732450000	-0.954503000
C	8.049910000	-1.286687000	1.968258000
C	8.329990000	-2.052078000	-0.361666000
C	8.705190000	0.282928000	0.344643000
C	8.636125000	-1.136926000	0.646690000
C	-2.167431000	1.781814000	-0.871811000
C	-2.902105000	1.321619000	-2.120990000
C	-2.956266000	2.738958000	0.125199000
C	-1.663890000	0.453013000	-0.326361000
C	-4.146695000	1.802813000	-2.481069000
C	-2.574424000	-0.051807000	-2.426571000
C	-4.423860000	2.951947000	-0.296645000
C	-3.185525000	2.080250000	1.502949000
C	-1.830553000	-0.594143000	-1.322411000
C	-1.675680000	0.138627000	1.055327000
C	-4.927831000	2.637396000	-1.539601000
C	-5.084357000	0.948061000	-3.181863000
C	-3.455863000	-0.880346000	-3.135437000
C	-5.286106000	2.878132000	0.851468000
C	-4.519679000	2.341258000	1.960793000
C	-2.526925000	0.955732000	1.951872000
C	-1.962360000	-1.921892000	-0.942775000
C	-1.891986000	-1.259536000	1.436368000
C	-6.322509000	2.281283000	-1.691659000
C	-6.422555000	1.244529000	-2.701077000
C	-4.746630000	-0.366717000	-3.523422000
C	-3.616506000	-2.266034000	-2.734207000
C	-6.643068000	2.563929000	0.723151000
C	-5.139172000	1.515968000	2.907155000
C	-3.156911000	0.073153000	2.907091000
C	-2.002187000	-2.268528000	0.472106000
C	-2.881079000	-2.779468000	-1.661864000
C	-2.777353000	-1.289767000	2.586547000
C	-7.175805000	2.257853000	-0.582478000
C	-7.365408000	0.223951000	-2.568090000
C	-5.720621000	-1.432989000	-3.368073000
C	-5.020047000	-2.611005000	-2.880324000
C	-7.281789000	1.688411000	1.693964000
C	-4.439789000	0.352366000	3.391710000
C	-6.544795000	1.175772000	2.761576000
C	-2.971733000	-3.332014000	0.625640000
C	-3.514107000	-3.651461000	-0.688804000
C	-3.704056000	-2.324953000	2.748660000
C	-8.145927000	1.189186000	-0.433888000
C	-8.239350000	0.191023000	-1.406025000
C	-7.003981000	-1.144818000	-2.900490000
C	-5.629674000	-3.449447000	-1.945166000
C	-8.211311000	0.835654000	0.976767000
C	-5.404247000	-0.720872000	3.549899000
C	-6.709620000	-0.211060000	3.160618000
C	-3.806143000	-3.367868000	1.747538000
C	-4.861732000	-3.981570000	-0.828876000
C	-5.045058000	-2.031931000	3.233216000
C	-8.405511000	-1.195351000	-1.011990000
C	-7.640494000	-2.020592000	-1.934259000
C	-6.966934000	-3.150941000	-1.464669000
C	-8.368552000	-0.499152000	1.355744000
C	-7.602522000	-1.033019000	2.469850000
C	-5.208104000	-3.711870000	1.598795000
C	-5.727159000	-4.012930000	0.338091000
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$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.88209$

$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.09725$

$E_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4988.45492$

$G_s(\text{M06}/6\text{-}311\text{G}(\text{d},\text{p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4987.67007$



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C	-7.027209000	-3.498950000	-0.055181000
C	-7.227918000	-2.398085000	2.143778000
C	-7.763975000	-2.708541000	0.829665000
C	-2.202686000	4.077919000	0.271075000
C	-2.438970000	5.135881000	-0.614080000
C	-1.216311000	4.229841000	1.257254000
C	-1.700055000	6.316140000	-0.522740000
H	-3.203450000	5.039447000	-1.379505000
C	-0.475891000	5.412182000	1.346879000
H	-1.040621000	3.435918000	1.978061000
C	-0.714576000	6.458289000	0.456193000
H	-1.897631000	7.126693000	-1.218995000
H	0.279778000	5.513359000	2.121223000
H	-0.142128000	7.378865000	0.526754000
O	0.127306000	3.070330000	-1.755710000
H	0.479349000	2.603125000	-2.533805000
H	-1.109076000	2.536221000	-1.472465000

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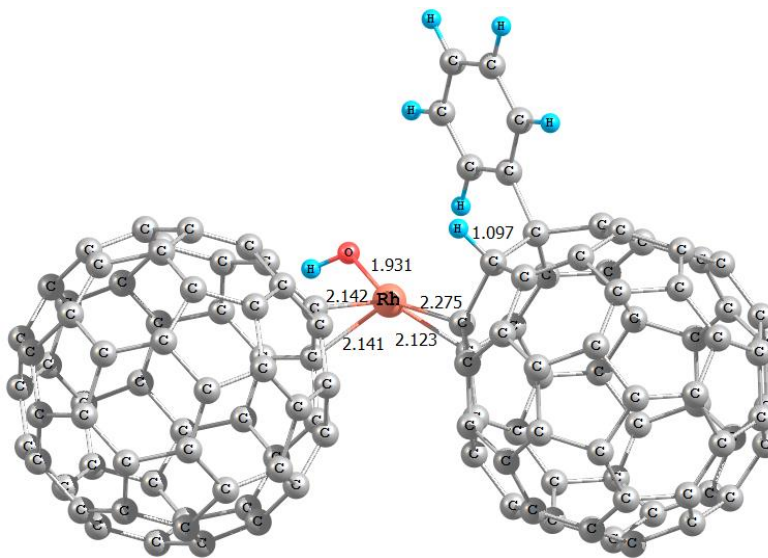
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C	1.799451000	0.765569000	1.275748000
C	2.841922000	2.423457000	-0.342804000
C	1.714384000	-0.862138000	-1.126260000
C	2.667774000	1.081684000	-2.260812000
C	1.795998000	-0.716247000	1.347127000
C	2.842285000	1.186934000	2.249806000
C	3.308909000	2.258849000	-1.700516000
C	3.733132000	2.844601000	0.634375000
C	1.708832000	-1.491568000	0.199227000
C	2.439761000	-1.729668000	-2.027601000
C	3.371145000	0.253898000	-3.142645000
C	2.658838000	-1.144451000	2.425897000
C	3.303265000	0.031331000	2.984717000
C	3.731949000	2.215398000	1.961462000
C	4.631076000	2.561594000	-2.043857000
C	5.105393000	3.152389000	0.294279000
C	2.435734000	-2.739585000	0.097735000
C	2.889830000	-2.888050000	-1.274647000
C	3.253971000	-1.183749000	-3.023754000
C	4.747456000	0.566035000	-3.491313000
C	3.363420000	-2.349948000	2.340951000
C	4.624742000	-0.043150000	3.436922000
C	5.104532000	2.144545000	2.420304000
C	5.549660000	3.020670000	-1.024212000
C	5.364076000	1.695347000	-2.953554000
C	5.953913000	2.721480000	1.392774000
C	3.247681000	-3.167003000	1.151461000
C	4.134509000	-3.455427000	-1.542747000
C	4.545457000	-1.768900000	-3.298447000
C	5.479723000	-0.686009000	-3.588115000
C	4.738999000	-2.424424000	2.805714000
C	5.544826000	1.037454000	3.149904000
C	5.356703000	-1.295385000	3.343187000
C	6.853872000	2.441270000	-1.295511000
C	6.739652000	1.620938000	-2.489899000
C	7.208905000	2.171985000	1.133277000
C	4.548572000	-3.751175000	0.874391000
C	4.983624000	-3.891225000	-0.445113000
C	4.986629000	-2.880786000	-2.572275000
C	6.800373000	-0.758930000	-3.141134000
C	5.472241000	-3.291814000	1.898245000
C	6.849187000	0.460026000	2.876555000
C	6.733312000	-0.983917000	2.995840000
C	7.667082000	2.025330000	-0.239295000
C	7.443396000	0.418514000	-2.580736000
C	7.664097000	1.014696000	1.887516000
C	6.357964000	-3.581697000	-0.794341000
C	6.359429000	-2.956679000	-2.108523000
C	7.248655000	-1.916772000	-2.386542000
C	6.793666000	-2.992082000	1.561878000
C	7.437069000	-1.814550000	2.121901000
C	8.399179000	0.775833000	-0.334176000
C	8.289613000	-0.012585000	-1.481311000
C	8.396992000	0.151088000	0.980381000
C	7.245470000	-3.140062000	0.188981000
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C	8.285497000	-1.235808000	1.094330000
C	8.168396000	-2.055341000	-0.100402000
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C	-3.203591000	2.895279000	-0.404390000
C	-1.447277000	0.850030000	-0.274523000
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C	-2.174308000	-0.222264000	-2.274721000
C	-4.632796000	2.795772000	-0.978012000
C	-3.493552000	2.467312000	1.046331000
C	-1.453530000	-0.407213000	-1.036579000
C	-1.674759000	0.731624000	1.138917000
C	-4.953812000	2.182517000	-2.168241000
C	-4.697679000	0.215175000	-3.446721000
C	-2.851529000	-1.293783000	-2.881257000
C	-5.599845000	2.804647000	0.085154000
C	-4.895929000	2.605579000	1.337136000
C	-2.743208000	1.566938000	1.773992000
C	-1.475180000	-1.660748000	-0.425979000
C	-1.788046000	-0.596476000	1.766430000
C	-6.262584000	1.596162000	-2.363009000
C	-6.109089000	0.387126000	-3.150655000
C	-4.144036000	-1.069336000	-3.480445000
C	-2.864433000	-2.592650000	-2.242225000
C	-6.880728000	2.268100000	-0.089496000
C	-5.500161000	1.881087000	2.370313000
C	-3.357935000	0.786606000	2.828163000
C	-1.646032000	-1.756718000	1.017829000
C	-2.195492000	-2.763654000	-1.029237000
C	-2.775255000	-0.541523000	2.817470000
C	-7.222521000	1.648212000	-1.346744000
C	-6.911973000	-0.724486000	-2.894383000
C	-4.975853000	-2.226289000	-3.203295000
C	-4.181987000	-3.172263000	-2.434270000
C	-7.498281000	1.498840000	0.979170000
C	-4.710591000	0.948284000	3.137921000
C	-6.824173000	1.312876000	2.186330000
C	-2.468848000	-2.913410000	1.301314000
C	-2.810172000	-3.539492000	0.035880000
C	-3.562499000	-1.657989000	3.115714000
C	-8.048859000	0.488206000	-1.068732000
C	-7.897372000	-0.675013000	-1.826242000
C	-6.332155000	-2.058528000	-2.914535000
C	-4.772770000	-3.909207000	-1.408265000
C	-8.222768000	0.396873000	0.373225000
C	-5.536279000	-0.209535000	3.431244000
C	-6.844823000	0.015014000	2.839361000
C	-3.410298000	-2.868802000	2.334542000
C	-4.074960000	-4.099288000	-0.148543000
C	-4.974669000	-1.487652000	3.416538000
C	-7.916425000	-1.973018000	-1.178386000
C	-6.949674000	-2.827055000	-1.851549000
C	-6.186772000	-3.734795000	-1.111384000
C	-8.238714000	-0.852964000	0.996470000
C	-7.537948000	-1.047864000	2.255180000
C	-4.726640000	-3.446940000	2.142158000
C	-5.053572000	-4.049048000	0.925308000
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$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.93619$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.14333$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4988.50519$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4987.71233$$



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C	-6.951328000	-2.376652000	2.241293000
C	-7.289122000	-3.003681000	0.974368000
C	-2.669645000	4.340138000	-0.493736000
C	-2.888504000	5.096637000	-1.654709000
C	-1.888550000	4.890483000	0.529918000
C	-2.333027000	6.368660000	-1.789218000
H	-3.498484000	4.691668000	-2.457062000
C	-1.323668000	6.161869000	0.390214000
H	-1.707977000	4.340709000	1.448317000
C	-1.545954000	6.903978000	-0.767091000
H	-2.517000000	6.940577000	-2.694891000
H	-0.708421000	6.558249000	1.192316000
H	-1.111370000	7.895923000	-0.874478000
O	0.822207000	3.494031000	1.923271000
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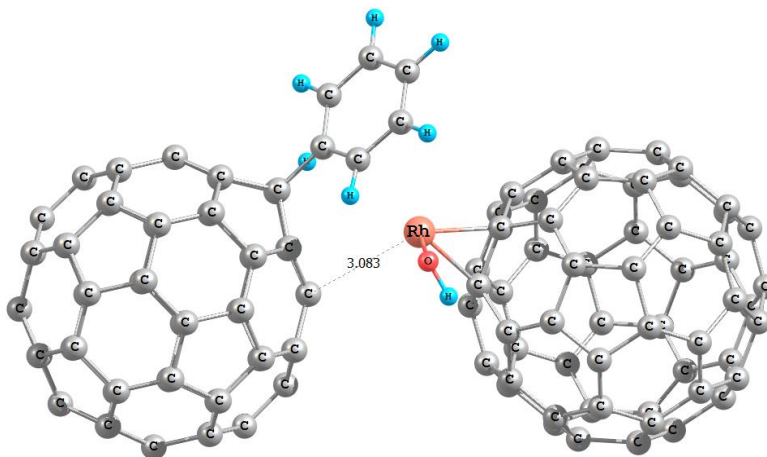
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C	-2.927895000	1.824412000	1.138929000
C	-1.994583000	0.464380000	-0.795597000
C	-3.607767000	2.423097000	-1.035822000
C	-2.752496000	0.746820000	1.999280000
C	-4.117956000	2.639217000	1.245506000
C	-1.944385000	-0.683407000	0.143334000
C	-2.612757000	-0.084618000	-2.031384000
C	-4.537152000	3.007176000	-0.096293000
C	-4.076804000	1.911900000	-2.237342000
C	-2.244110000	-0.538520000	1.491466000
C	-3.745335000	0.458845000	3.014447000
C	-5.074774000	2.377076000	2.230371000
C	-2.335066000	-1.887770000	-0.552221000
C	-2.752332000	-1.518020000	-1.893294000
C	-3.568334000	0.628568000	-2.747261000
C	-5.898553000	3.099840000	-0.402029000
C	-5.487077000	1.987932000	-2.557069000
C	-2.935116000	-1.595929000	2.198075000
C	-3.860732000	-0.984726000	3.137924000
C	-4.884959000	1.261982000	3.133548000
C	-6.490674000	2.464484000	1.908888000
C	-2.987894000	-2.921672000	0.126696000
C	-3.809425000	-2.197404000	-2.506366000
C	-4.676698000	-0.065607000	-3.372649000
C	-6.384677000	2.578489000	-1.661083000
C	-6.893243000	2.817416000	0.620892000
C	-5.859700000	0.770504000	-3.257088000
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C	-6.180829000	0.653062000	3.375172000
C	-7.174943000	1.396471000	2.617946000
C	-4.092339000	-3.621543000	-0.509090000
C	-4.794022000	-1.454892000	-3.263141000
C	-4.494454000	-3.266399000	-1.796686000
C	-7.682262000	1.970153000	-1.425172000
C	-7.997978000	2.118385000	-0.013528000
C	-7.109550000	0.190794000	-3.037656000
C	-4.593483000	-3.376795000	1.774549000
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C	-6.289391000	-0.734130000	3.493050000
C	-8.235555000	0.723243000	2.009050000
C	-5.087020000	-3.903707000	0.512129000
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C	-8.038591000	0.800445000	-2.099102000
C	-8.655703000	1.091650000	0.666564000
C	-7.228459000	-1.253385000	-2.915350000
C	-6.893701000	-2.703807000	2.359264000
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C	-6.865303000	-3.449972000	-1.138275000
C	-8.724209000	-0.265758000	-1.392349000
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C	-8.223824000	-1.535355000	-1.897090000
C	-7.367645000	-3.207651000	1.146248000
C	-8.837711000	-1.243748000	0.870594000
C	-8.046076000	-2.611500000	-1.025207000
C	-8.357335000	-2.461684000	0.386654000
C	2.689396000	1.493170000	1.860972000
C	3.968377000	1.374190000	2.693305000
C	2.807198000	2.372719000	0.524836000
C	2.348575000	0.014650000	1.655832000
C	5.107773000	2.111943000	2.461623000
C	4.083717000	0.043847000	3.227294000
C	4.238244000	2.905852000	0.273565000
C	2.622601000	1.535811000	-0.757421000
C	3.084120000	-0.792650000	2.589354000
C	1.954588000	-0.526741000	0.453830000
C	5.246324000	2.895610000	1.211837000
C	6.407411000	1.563014000	2.781816000
C	5.329176000	-0.493774000	3.572417000
C	4.574332000	2.776104000	-1.119515000
C	3.578220000	1.933237000	-1.754189000
C	2.089977000	0.261982000	-0.793946000
C	3.363156000	-2.137372000	2.318600000
C	2.260989000	-1.904131000	0.139875000
C	6.630475000	2.806745000	0.796438000
C	7.346081000	1.983911000	1.759659000
C	6.521530000	0.284831000	3.341915000
C	5.626149000	-1.885632000	3.271421000
C	5.906640000	2.716634000	-1.543698000
C	3.942701000	1.072064000	-2.794098000
C	2.483771000	-0.657431000	-1.844867000
C	2.942633000	-2.706762000	1.061649000
C	4.664825000	-2.689120000	2.658460000
C	2.586453000	-1.987787000	-1.272892000
C	6.963001000	2.733422000	-0.560664000
C	8.360639000	1.130310000	1.335793000
C	7.567321000	-0.615845000	2.891742000
C	7.013976000	-1.960492000	2.849103000
C	6.290285000	1.804056000	-2.609194000
C	3.383058000	-0.258114000	-2.839170000
C	5.329505000	1.000975000	-3.222770000
C	3.982086000	-3.612508000	0.607579000
C	5.048788000	-3.603305000	1.596881000
C	3.576627000	-2.867568000	-1.712266000
C	8.007990000	1.829560000	-1.006170000
C	8.092860000	1.042804000	-0.077469000
C	8.468585000	-0.202377000	1.908407000
C	7.384344000	-2.835699000	1.825837000
C	7.592625000	1.254598000	-2.275747000
C	4.421907000	-1.166166000	-3.290044000
C	5.627364000	-0.387633000	-3.528469000
C	4.293660000	-3.691388000	-0.751554000
C	6.381806000	-3.673644000	1.187177000
C	4.518291000	-2.444921000	-2.736439000
C	8.994310000	-0.342916000	-0.379839000
C	8.855887000	-1.112944000	0.848080000
C	8.323385000	-2.403443000	0.805661000
C	7.880070000	-0.080907000	-2.565395000
C	6.877298000	-0.918711000	-3.204225000
C	5.678065000	-3.767550000	-1.176035000
C	6.702374000	-3.757739000	-0.226823000
C	5.816882000	-2.997517000	-2.403693000

$$E_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.91440$$

$$G_g(\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4990.12345$$

$$E_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4988.48275$$

$$G_s(\text{M06}/6\text{-}311\text{G}(\text{d,p})//\text{B3LYP}/6\text{-}31\text{G}(\text{d})) = -4987.69180$$



C	8.595406000	-0.895319000	-1.599226000
C	7.902870000	-2.973842000	-0.462946000
C	6.974390000	-2.250013000	-2.631988000
C	8.036696000	-2.236227000	-1.640490000
C	1.788995000	3.536234000	0.567404000
C	1.554314000	4.259639000	1.743042000
C	1.068965000	3.900181000	-0.593754000
C	0.595546000	5.278178000	1.780324000
H	2.125166000	4.043798000	2.641907000
C	0.086960000	4.904116000	-0.543388000
H	1.331027000	3.485901000	-1.562221000
C	-0.156870000	5.590523000	0.648450000
H	0.435463000	5.822418000	2.707158000
H	-0.456898000	5.148942000	-1.450093000
H	-0.914104000	6.367687000	0.689338000
O	-0.503894000	2.290754000	-2.632190000
H	-0.989390000	1.581497000	-3.087698000
H	1.899401000	1.952096000	2.466329000