Electronic Supplementary Material (ESI) for Dalton Transactions


# Electronic Supplementary Information

# Proposal for Halogen Atom Transfer Mechanism for Ullmann O-Arylation of Phenols with Aryl Halides

Songlin Zhang*, Zhenzhong Zhu, and Yuqiang Ding*

*The Key Laboratory of Food Colloids and Biotechnology, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, Wuxi 214122, Jiangsu Province, China*

Contents

## 1. Additional Computational Results

a. Reductive elimination of oxidative addition complex **PDb**

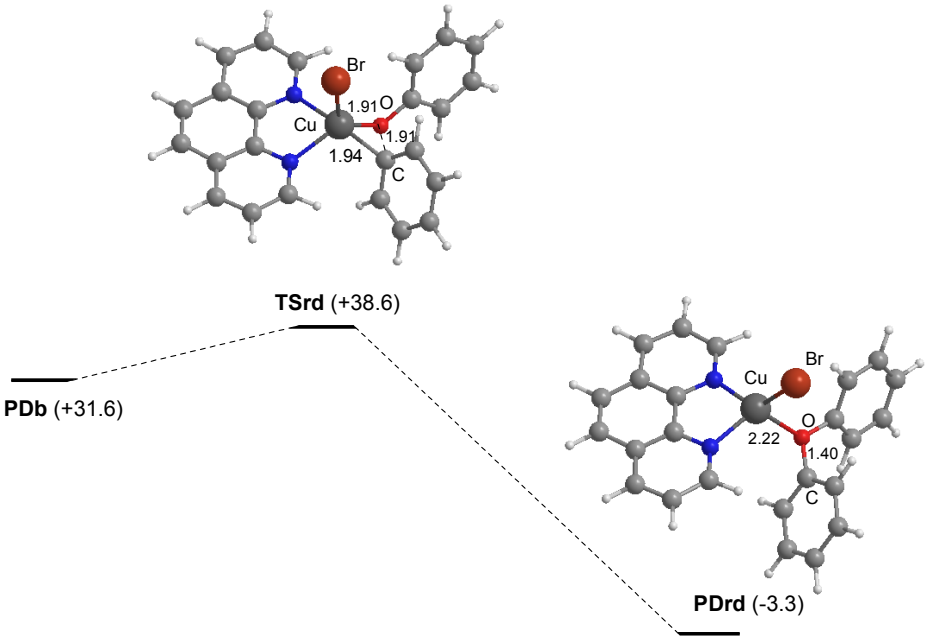


*Figure S1*. Reaction coordinates of reductive elimination of complex **PDb**.

b. Oxidative addition of complex **A** with phenyl bromide

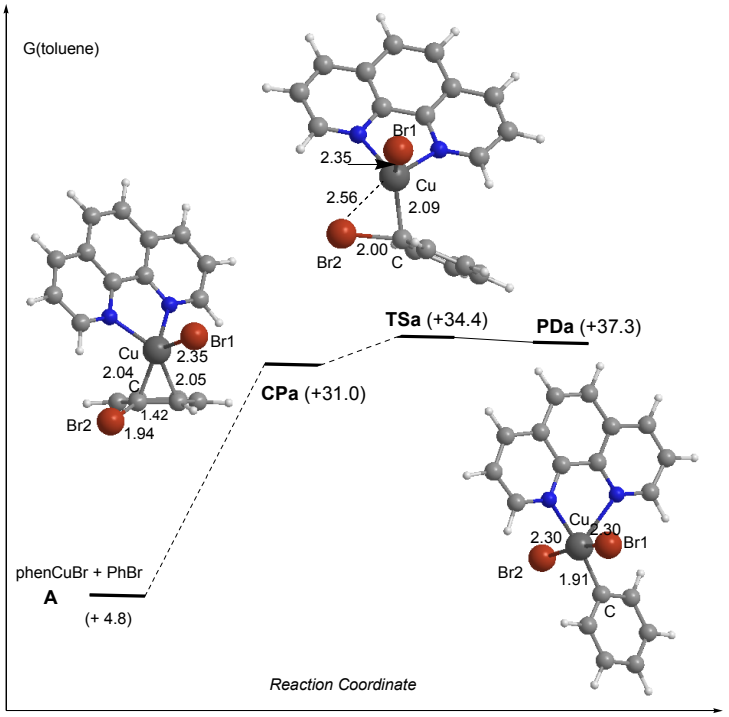

*Figure S2*. Reaction coordinates of oxidative addition of complex A with phenyl bromide.

c. Oxidative addition of complex **E** with phenyl bromide

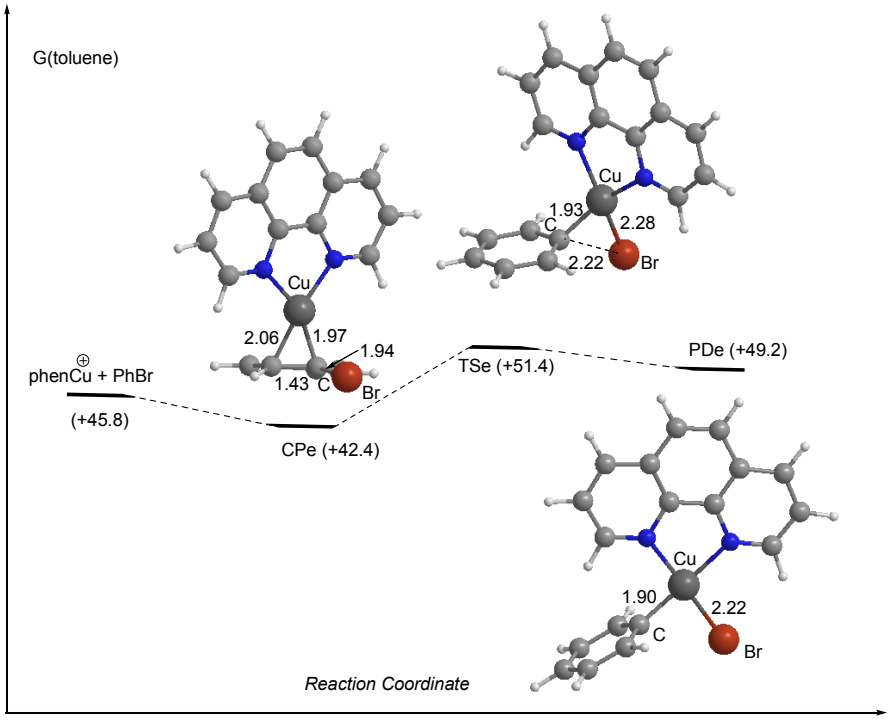


*Figure S3*. Reaction coordinates of oxidative addition of complex **E** with phenyl bromide.

# 2. Optimized Cartesian Coordinates from B3LYP/6-31G(d) Calculations

**PhBr**
SCF Done: E(RB+HF-LYP) = -2803.35368043 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 35 | 0 | -1.810705 | -0.000003 | -0.000017 |
| 2 | 6 | 0 | 0.103827 | 0.000210 | -0.000030 |
| 3 | 6 | 0 | 0.784807 | -1.215747 | -0.000043 |
| 4 | 6 | 0 | 2.180984 | -1.207838 | 0.000095 |
| 5 | 6 | 0 | 2.881291 | -0.000164 | -0.000032 |
| 6 | 6 | 0 | 2.181256 | 1.207696 | -0.000120 |
| 7 | 6 | 0 | 0.785071 | 1.215899 | 0.000149 |
| 8 | 1 | 0 | 0.232807 | -2.149474 | 0.000074 |
| 9 | 1 | 0 | 2.718628 | -2.152104 | 0.000153 |
| 10 | 1 | 0 | 3.967516 | -0.000473 | -0.000054 |
| 11 | 1 | 0 | 2.718886 | 2.151954 | -0.000386 |
| 12 | 1 | 0 | 0.233442 | 2.149881 | 0.000687 |

**PhOH**
SCF Done: E(RB+HF-LYP) = -307.464867405 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.263830 | 1.199685 | -0.000001 |
| 2 | 6 | 0 | 0.940934 | -0.024501 | -0.000002 |
| 3 | 6 | 0 | 0.221015 | -1.224128 | 0.000000 |
| 4 | 6 | 0 | -1.171630 | -1.190400 | 0.000001 |
| 5 | 6 | 0 | -1.857308 | 0.027668 | 0.000000 |
| 6 | 6 | 0 | -1.131626 | 1.219386 | 0.000000 |
| 7 | 8 | 0 | 2.307040 | -0.111940 | -0.000003 |
| 8 | 1 | 0 | 0.765962 | -2.162936 | 0.000004 |
| 9 | 1 | 0 | -1.725537 | -2.125600 | 0.000003 |
| 10 | 1 | 0 | -2.943114 | 0.046915 | 0.000002 |
| 11 | 1 | 0 | -1.650029 | 2.174659 | 0.000000 |
| 12 | 1 | 0 | 0.826722 | 2.131893 | 0.000001 |
| 13 | 1 | 0 | 2.678383 | 0.784330 | 0.000032 |

**$Ph_2O$**
SCF Done: E(RB+HF-LYP) = -538.512821128 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.266139 | -1.070218 | 0.663286 |
| 2 | 6 | 0 | -1.201582 | -0.499251 | -0.037345 |
| 3 | 6 | 0 | -1.390041 | 0.657502 | -0.799801 |
| 4 | 6 | 0 | -2.654753 | 1.245209 | -0.844699 |
| 5 | 6 | 0 | -3.726633 | 0.684369 | -0.147143 |
| 6 | 6 | 0 | -3.526699 | -0.476984 | 0.602304 |
| 7 | 8 | 0 | -0.000011 | -1.180971 | 0.000088 |
| 8 | 6 | 0 | 1.201575 | -0.499304 | 0.037446 |
| 9 | 6 | 0 | 2.266044 | -1.070176 | -0.663403 |
| 10 | 6 | 0 | 3.526607 | -0.476941 | -0.602537 |
| 11 | 6 | 0 | 3.726638 | 0.684326 | 0.147021 |
| 12 | 6 | 0 | 2.654852 | 1.245080 | 0.844789 |
| 13 | 6 | 0 | 1.390141 | 0.657370 | 0.800000 |
| 14 | 1 | 0 | -0.558942 | 1.085621 | -1.350478 |
| 15 | 1 | 0 | -2.801432 | 2.144084 | -1.437762 |
| 16 | 1 | 0 | -4.708556 | 1.146781 | -0.189143 |
| 17 | 1 | 0 | -4.353621 | -0.923556 | 1.147992 |
| 18 | 1 | 0 | -2.089674 | -1.971852 | 1.241313 |
| 19 | 1 | 0 | 0.559107 | 1.085397 | 1.350851 |
| 20 | 1 | 0 | 2.801616 | 2.143885 | 1.437940 |
| 21 | 1 | 0 | 4.708559 | 1.146748 | 0.188942 |
| 22 | 1 | 0 | 4.353456 | -0.923450 | -1.148387 |
| 23 | 1 | 0 | 2.089516 | -1.971771 | -1.241475 |

**phen**
SCF Done: E(RB+HF-LYP) = -571.610386722 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.179083 | -0.362687 | 0.000000 |
| 2 | 6 | 0 | -1.553016 | -1.570952 | 0.000000 |
| 3 | 6 | 0 | -0.121148 | -1.658607 | 0.000000 |
| 4 | 6 | 0 | 0.671302 | -0.473718 | 0.000000 |
| 5 | 6 | 0 | 0.000000 | 0.821521 | 0.000000 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -1.424856 | 0.857505 | 0.000000 |
| 7 | 6 | 0 | 0.554479 | -2.899024 | 0.000000 |
| 8 | 6 | 0 | 1.933280 | -2.920409 | 0.000000 |
| 9 | 6 | 0 | 2.619106 | -1.688314 | 0.000000 |
| 10 | 7 | 0 | 2.023819 | -0.506919 | 0.000000 |
| 11 | 6 | 0 | -2.048786 | 2.124712 | 0.000000 |
| 12 | 6 | 0 | -1.271243 | 3.263448 | 0.000000 |
| 13 | 6 | 0 | 0.130933 | 3.113199 | 0.000000 |
| 14 | 7 | 0 | 0.752815 | 1.945632 | 0.000000 |
| 15 | 1 | 0 | 3.708855 | -1.675690 | 0.000000 |
| 16 | 1 | 0 | 2.486124 | -3.855100 | 0.000000 |
| 17 | 1 | 0 | -0.022223 | -3.821234 | 0.000000 |
| 18 | 1 | 0 | 0.769666 | 3.996243 | 0.000000 |
| 19 | 1 | 0 | -1.716067 | 4.254110 | 0.000000 |
| 20 | 1 | 0 | -3.134810 | 2.185116 | 0.000000 |
| 21 | 1 | 0 | -2.128976 | -2.493351 | 0.000000 |
| 22 | 1 | 0 | -3.264803 | -0.301133 | 0.000000 |

**A**

SCF Done: E(RB+HF-LYP) = -4783.71761682 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.161127 | 1.328738 | 0.000402 |
| 2 | 6 | 0 | 1.381033 | 0.719609 | 0.000010 |
| 3 | 6 | 0 | 2.605383 | 1.426212 | -0.000192 |
| 4 | 6 | 0 | 2.535981 | 2.837121 | -0.000082 |
| 5 | 6 | 0 | 1.297144 | 3.451514 | 0.000242 |
| 6 | 6 | 0 | 0.134132 | 2.661268 | 0.000487 |
| 7 | 6 | 0 | 3.834468 | 0.682990 | -0.000375 |
| 8 | 6 | 0 | 3.834844 | -0.681134 | -0.000261 |
| 9 | 6 | 0 | 2.606183 | -1.425064 | -0.000053 |
| 10 | 6 | 0 | 1.381443 | -0.719177 | -0.000047 |
| 11 | 6 | 0 | 2.537665 | -2.836025 | 0.000183 |
| 12 | 6 | 0 | 1.299195 | -3.451139 | 0.000369 |
| 13 | 6 | 0 | 0.135705 | -2.661609 | 0.000188 |
| 14 | 7 | 0 | 0.161838 | -1.329035 | -0.000084 |
| 15 | 29 | 0 | -1.298747 | -0.000991 | -0.000081 |
| 16 | 35 | 0 | -3.521650 | 0.000001 | -0.000104 |
| 17 | 1 | 0 | -0.850855 | -3.115286 | 0.000160 |
| 18 | 1 | 0 | 1.209409 | -4.532628 | 0.000587 |
| 19 | 1 | 0 | 3.453279 | -3.421462 | 0.000189 |
| 20 | 1 | 0 | -0.852733 | 3.114296 | 0.000795 |
| 21 | 1 | 0 | 1.206760 | 4.532953 | 0.000381 |
| 22 | 1 | 0 | 3.451232 | 3.423131 | -0.000249 |
| 23 | 1 | 0 | 4.772590 | -1.230393 | -0.000359 |
| 24 | 1 | 0 | 4.771912 | 1.232762 | -0.000574 |

**CPa**

SCF Done: E(RB+HF-LYP) = -7587.09403852 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.261857 | 1.307611 | -0.002863 |
| 2 | 6 | 0 | -2.260497 | 0.422414 | -0.244990 |
| 3 | 6 | 0 | -3.624492 | 0.801008 | -0.319900 |
| 4 | 6 | 0 | -3.928525 | 2.165875 | -0.127867 |
| 5 | 6 | 0 | -2.905435 | 3.057685 | 0.128805 |
| 6 | 6 | 0 | -1.583161 | 2.581868 | 0.183169 |
| 7 | 6 | 0 | -1.894933 | -0.963670 | -0.403843 |
| 8 | 6 | 0 | -2.904534 | -1.932424 | -0.626886 |
| 9 | 6 | 0 | -4.274550 | -1.512597 | -0.714109 |
| 10 | 6 | 0 | -4.619887 | -0.202599 | -0.568803 |
| 11 | 6 | 0 | -2.499521 | -3.279404 | -0.740253 |
| 12 | 6 | 0 | -1.159317 | -3.593428 | -0.627829 |
| 13 | 6 | 0 | -0.229332 | -2.562861 | -0.410436 |
| 14 | 7 | 0 | -0.576989 | -1.282519 | -0.310057 |
| 15 | 29 | 0 | 0.578235 | 0.271395 | 0.361392 |
| 16 | 35 | 0 | 0.610860 | -0.042770 | 2.694544 |
| 17 | 1 | 0 | -0.756730 | 3.256507 | 0.385283 |
| 18 | 1 | 0 | -3.104828 | 4.112113 | 0.290467 |
| 19 | 1 | 0 | -4.962275 | 2.498499 | -0.176175 |
| 20 | 1 | 0 | 0.832094 | -2.770977 | -0.326795 |
| 21 | 1 | 0 | -0.812258 | -4.618709 | -0.703572 |
| 22 | 1 | 0 | -3.244627 | -4.052751 | -0.908159 |
| 23 | 1 | 0 | -5.661028 | 0.103472 | -0.627869 |
| 24 | 1 | 0 | -5.036057 | -2.267660 | -0.890281 |
| 25 | 6 | 0 | 2.186475 | 0.372264 | -0.896628 |
| 26 | 6 | 0 | 2.258157 | 1.416915 | 0.068381 |
| 27 | 6 | 0 | 1.986458 | 2.741877 | -0.368769 |
| 28 | 6 | 0 | 1.617307 | 3.003449 | -1.675151 |
| 29 | 6 | 0 | 1.550481 | 1.953657 | -2.617571 |
| 30 | 6 | 0 | 1.862354 | 0.658337 | -2.247155 |

| | | | | | |
|---|---|---|---|---|---|
| 31 | 1 | 0 | 2.788537 | 1.266042 | 1.000883 |
| 32 | 1 | 0 | 2.095956 | 3.552699 | 0.346827 |
| 33 | 1 | 0 | 1.413475 | 4.023184 | -1.990415 |
| 34 | 1 | 0 | 1.280899 | 2.164823 | -3.648651 |
| 35 | 1 | 0 | 1.865096 | -0.145697 | -2.975639 |
| 36 | 35 | 0 | 3.158927 | -1.269739 | -0.546167 |

**TSa**

SCF Done: E(RB+HF-LYP) = -7587.08356114 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -0.696722 | 1.356552 | 0.069240 |
| 2 | 6 | 0 | -1.993777 | 1.003965 | -0.129240 |
| 3 | 6 | 0 | -3.064591 | 1.928464 | -0.052485 |
| 4 | 6 | 0 | -2.742953 | 3.268455 | 0.251761 |
| 5 | 6 | 0 | -1.422197 | 3.614878 | 0.465847 |
| 6 | 6 | 0 | -0.429329 | 2.625315 | 0.367533 |
| 7 | 6 | 0 | -2.269180 | -0.384393 | -0.405874 |
| 8 | 6 | 0 | -3.607126 | -0.813709 | -0.588664 |
| 9 | 6 | 0 | -4.667213 | 0.152218 | -0.523404 |
| 10 | 6 | 0 | -4.406897 | 1.465403 | -0.267526 |
| 11 | 6 | 0 | -3.817932 | -2.190964 | -0.814533 |
| 12 | 6 | 0 | -2.733621 | -3.048022 | -0.838633 |
| 13 | 6 | 0 | -1.443353 | -2.522599 | -0.651226 |
| 14 | 7 | 0 | -1.211308 | -1.231099 | -0.449155 |
| 15 | 29 | 0 | 0.543635 | -0.282896 | 0.262177 |
| 16 | 35 | 0 | 0.752253 | -0.887803 | 2.521948 |
| 17 | 1 | 0 | 0.616011 | 2.863434 | 0.535127 |
| 18 | 1 | 0 | -1.140893 | 4.633948 | 0.710907 |
| 19 | 1 | 0 | -3.534961 | 4.009551 | 0.322094 |
| 20 | 1 | 0 | -0.567423 | -3.165677 | -0.659606 |
| 21 | 1 | 0 | -2.862603 | -4.113558 | -0.999086 |
| 22 | 1 | 0 | -4.828832 | -2.564139 | -0.957311 |
| 23 | 1 | 0 | -5.217912 | 2.186628 | -0.209763 |
| 24 | 1 | 0 | -5.688549 | -0.188316 | -0.672179 |
| 25 | 6 | 0 | 2.271059 | 0.232451 | -0.791394 |
| 26 | 6 | 0 | 3.088647 | 0.684527 | 0.259309 |
| 27 | 6 | 0 | 3.538718 | 2.005174 | 0.243869 |
| 28 | 6 | 0 | 3.250436 | 2.844120 | -0.836816 |
| 29 | 6 | 0 | 2.495267 | 2.360501 | -1.910864 |
| 30 | 6 | 0 | 2.033659 | 1.046078 | -1.912409 |
| 31 | 1 | 0 | 3.315414 | 0.025533 | 1.088325 |
| 32 | 1 | 0 | 4.136916 | 2.367681 | 1.075227 |
| 33 | 1 | 0 | 3.624854 | 3.863913 | -0.849984 |
| 34 | 1 | 0 | 2.284514 | 2.999833 | -2.764066 |
| 35 | 1 | 0 | 1.473095 | 0.656324 | -2.755033 |
| 36 | 35 | 0 | 2.147846 | -1.737354 | -1.093374 |

**PDa**

SCF Done: E(RB+HF-LYP) = -7587.09860692 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.855885 | 1.422677 | -0.432346 |
| 2 | 6 | 0 | 2.524424 | 0.131529 | -0.039465 |
| 3 | 6 | 0 | 3.508901 | -0.785470 | 0.316685 |
| 4 | 6 | 0 | 4.848781 | -0.389847 | 0.295393 |
| 5 | 6 | 0 | 5.197594 | 0.909737 | -0.077130 |
| 6 | 6 | 0 | 4.200387 | 1.812190 | -0.443616 |
| 7 | 29 | 0 | 0.687753 | -0.371205 | 0.025629 |
| 8 | 35 | 0 | 0.870927 | -0.870524 | -2.210061 |
| 9 | 7 | 0 | -0.847145 | 1.493680 | -0.078262 |
| 10 | 6 | 0 | -2.106350 | 1.000683 | -0.077370 |
| 11 | 6 | 0 | -3.257852 | 1.828185 | -0.132237 |
| 12 | 6 | 0 | -3.048840 | 3.224060 | -0.178399 |
| 13 | 6 | 0 | -1.760465 | 3.717417 | -0.156195 |
| 14 | 6 | 0 | -0.686591 | 2.807434 | -0.103178 |
| 15 | 6 | 0 | -4.562634 | 1.230731 | -0.130808 |
| 16 | 6 | 0 | -4.715027 | -0.120846 | -0.062027 |
| 17 | 6 | 0 | -3.576006 | -0.990596 | 0.014875 |
| 18 | 6 | 0 | -2.271819 | -0.432712 | 0.005609 |
| 19 | 6 | 0 | -3.686479 | -2.394144 | 0.108621 |
| 20 | 6 | 0 | -2.543476 | -3.164291 | 0.191788 |
| 21 | 6 | 0 | -1.293547 | -2.526482 | 0.176777 |
| 22 | 7 | 0 | -1.164221 | -1.208062 | 0.084872 |
| 23 | 35 | 0 | 0.803860 | -0.304823 | 2.325913 |
| 24 | 1 | 0 | 0.338130 | 3.167181 | -0.071200 |
| 25 | 1 | 0 | -1.563722 | 4.784372 | -0.178617 |
| 26 | 1 | 0 | -3.904374 | 3.893194 | -0.222963 |
| 27 | 1 | 0 | -0.370853 | -3.094324 | 0.239728 |
| 28 | 1 | 0 | -2.593351 | -4.245151 | 0.267465 |
| 29 | 1 | 0 | -4.671245 | -2.853945 | 0.116862 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 1 | 0 | -5.431136 | 1.882048 | -0.181358 |
| 31 | 1 | 0 | -5.706084 | -0.566331 | -0.058259 |
| 32 | 1 | 0 | 3.245123 | -1.795261 | 0.613789 |
| 33 | 1 | 0 | 5.618479 | -1.103825 | 0.578321 |
| 34 | 1 | 0 | 6.240923 | 1.213456 | -0.088444 |
| 35 | 1 | 0 | 4.460093 | 2.821771 | -0.753279 |
| 36 | 1 | 0 | 2.093895 | 2.118077 | -0.768236 |

**B**

SCF Done: E(RB+HF-LYP) = -2518.83274992 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 29 | 0 | 0.609920 | 0.052312 | -0.520798 |
| 2 | 7 | 0 | -0.778161 | 1.269580 | -0.323771 |
| 3 | 6 | 0 | -2.010948 | 0.724245 | -0.066755 |
| 4 | 6 | 0 | -2.093731 | -0.711266 | 0.019355 |
| 5 | 7 | 0 | -0.953301 | -1.406133 | -0.211777 |
| 6 | 6 | 0 | -0.989964 | -2.728126 | -0.115329 |
| 7 | 6 | 0 | -2.162853 | -3.440601 | 0.201865 |
| 8 | 6 | 0 | -3.334435 | -2.739955 | 0.422024 |
| 9 | 6 | 0 | -3.327980 | -1.330208 | 0.335558 |
| 10 | 6 | 0 | -4.486439 | -0.509205 | 0.543708 |
| 11 | 6 | 0 | -4.410664 | 0.848462 | 0.444149 |
| 12 | 6 | 0 | -3.170264 | 1.507789 | 0.141447 |
| 13 | 6 | 0 | -3.040256 | 2.910205 | 0.048033 |
| 14 | 6 | 0 | -0.695720 | 2.605729 | -0.403469 |
| 15 | 1 | 0 | 0.290556 | 3.009148 | -0.602603 |
| 16 | 1 | 0 | -1.658519 | 4.525987 | -0.307130 |
| 17 | 1 | 0 | -3.909088 | 3.544948 | 0.198655 |
| 18 | 1 | 0 | -5.293808 | 1.461937 | 0.600940 |
| 19 | 1 | 0 | -5.430844 | -0.991958 | 0.781034 |
| 20 | 1 | 0 | -4.258968 | -3.259226 | 0.661424 |
| 21 | 1 | 0 | -2.136555 | -4.523970 | 0.261421 |
| 22 | 1 | 0 | -0.048333 | -3.239333 | -0.299128 |
| 23 | 8 | 0 | 2.131220 | -0.914891 | -0.566903 |
| 24 | 6 | 0 | 3.297555 | -0.438666 | -0.142590 |
| 25 | 6 | 0 | 4.487776 | -1.164723 | -0.367324 |
| 26 | 6 | 0 | 5.714053 | -0.683777 | 0.085606 |
| 27 | 6 | 0 | 5.802256 | 0.527089 | 0.780075 |
| 28 | 6 | 0 | 4.630694 | 1.253241 | 1.016095 |
| 29 | 6 | 0 | 3.402140 | 0.780415 | 0.566108 |
| 30 | 1 | 0 | 4.421338 | -2.105267 | -0.907946 |
| 31 | 1 | 0 | 6.615664 | -1.262627 | -0.106482 |
| 32 | 1 | 0 | 6.762263 | 0.895609 | 1.131376 |
| 33 | 1 | 0 | 4.675244 | 2.195499 | 1.559494 |
| 34 | 1 | 0 | 2.476648 | 1.326714 | 0.744431 |
| 35 | 6 | 0 | -1.798355 | 3.452766 | -0.229940 |

**CPb**

SCF Done: E(RB+HF-LYP) = -5322.20611232 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.925353 | 2.814933 | -0.782936 |
| 2 | 6 | 0 | -1.292103 | 2.365081 | 0.508231 |
| 3 | 6 | 0 | -2.068304 | 3.246853 | 1.299486 |
| 4 | 6 | 0 | -2.451895 | 4.496385 | 0.821896 |
| 5 | 6 | 0 | -2.081088 | 4.924239 | -0.457758 |
| 6 | 6 | 0 | -1.313756 | 4.068121 | -1.251669 |
| 7 | 8 | 0 | -0.949672 | 1.176708 | 0.983291 |
| 8 | 29 | 0 | 0.190802 | -0.029743 | 0.088395 |
| 9 | 7 | 0 | 1.667556 | -0.033155 | -1.201230 |
| 10 | 6 | 0 | 2.877179 | -0.233934 | -0.593277 |
| 11 | 6 | 0 | 4.109255 | -0.202135 | -1.291056 |
| 12 | 6 | 0 | 4.063962 | -0.016629 | -2.687921 |
| 13 | 6 | 0 | 2.834161 | 0.141073 | -3.305247 |
| 14 | 6 | 0 | 1.667454 | 0.135148 | -2.529372 |
| 15 | 6 | 0 | 2.865336 | -0.438687 | 0.828616 |
| 16 | 6 | 0 | 4.086606 | -0.544262 | 1.538583 |
| 17 | 6 | 0 | 5.321099 | -0.491331 | 0.806896 |
| 18 | 6 | 0 | 5.330988 | -0.342834 | -0.548161 |
| 19 | 6 | 0 | 4.009996 | -0.705239 | 2.937524 |
| 20 | 6 | 0 | 2.766607 | -0.755242 | 3.544618 |
| 21 | 6 | 0 | 1.610815 | -0.670865 | 2.751847 |
| 22 | 7 | 0 | 1.645425 | -0.528935 | 1.427267 |
| 23 | 6 | 0 | -3.135354 | -1.688667 | -0.240081 |
| 24 | 6 | 0 | -4.028766 | -2.650065 | -0.702361 |
| 25 | 6 | 0 | -5.346843 | -2.602132 | -0.243517 |
| 26 | 6 | 0 | -5.743032 | -1.608837 | 0.654330 |
| 27 | 6 | 0 | -4.820417 | -0.659141 | 1.096956 |
| 28 | 6 | 0 | -3.494875 | -0.685677 | 0.653350 |
| 29 | 35 | 0 | -1.308747 | -1.761187 | -0.883071 |

| | | | | | |
|---|---|---|---|---|---|
| 30 | 1 | 0 | 0.622036 | -0.723441 | 3.197887 |
| 31 | 1 | 0 | 2.671258 | -0.876976 | 4.618854 |
| 32 | 1 | 0 | 4.922416 | -0.787065 | 3.522306 |
| 33 | 1 | 0 | 0.696028 | 0.297162 | -2.987170 |
| 34 | 1 | 0 | 2.759197 | 0.290679 | -4.377509 |
| 35 | 1 | 0 | 4.986736 | 0.008760 | -3.261080 |
| 36 | 1 | 0 | 6.253791 | -0.579703 | 1.357885 |
| 37 | 1 | 0 | 6.271509 | -0.312454 | -1.091876 |
| 38 | 1 | 0 | -2.762682 | 0.049222 | 0.982584 |
| 39 | 1 | 0 | -5.126899 | 0.118426 | 1.791100 |
| 40 | 1 | 0 | -6.770449 | -1.574697 | 1.006031 |
| 41 | 1 | 0 | -6.060130 | -3.343952 | -0.592410 |
| 42 | 1 | 0 | -3.708758 | -3.416479 | -1.400448 |
| 43 | 1 | 0 | -2.352884 | 2.919951 | 2.296897 |
| 44 | 1 | 0 | -3.048173 | 5.148669 | 1.457871 |
| 45 | 1 | 0 | -2.382621 | 5.901213 | -0.825783 |
| 46 | 1 | 0 | -1.012787 | 4.379827 | -2.250682 |
| 47 | 1 | 0 | -0.328209 | 2.148995 | -1.402848 |

**TSb**

SCF Done: E(RB+HF-LYP) = -5322.19465127 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.475175 | 2.655674 | 1.586136 |
| 2 | 6 | 0 | -1.328000 | 1.708047 | 1.000741 |
| 3 | 6 | 0 | -2.305710 | 2.098476 | 0.072491 |
| 4 | 6 | 0 | -2.318045 | 3.417520 | -0.373327 |
| 5 | 6 | 0 | -1.422390 | 4.359252 | 0.147699 |
| 6 | 6 | 0 | -0.502824 | 3.972690 | 1.125566 |
| 7 | 29 | 0 | -0.158955 | 0.128173 | 0.055788 |
| 8 | 35 | 0 | -1.662570 | 0.056248 | 2.066125 |
| 9 | 7 | 0 | 1.553641 | 1.049722 | -0.580342 |
| 10 | 6 | 0 | 2.628507 | 0.217937 | -0.526563 |
| 11 | 6 | 0 | 3.868119 | 0.514576 | -1.144802 |
| 12 | 6 | 0 | 3.958187 | 1.721491 | -1.869890 |
| 13 | 6 | 0 | 2.854200 | 2.551869 | -1.937414 |
| 14 | 6 | 0 | 1.672912 | 2.180889 | -1.274390 |
| 15 | 6 | 0 | 4.955865 | -0.413047 | -1.007774 |
| 16 | 6 | 0 | 4.814413 | -1.566659 | -0.295621 |
| 17 | 6 | 0 | 3.567550 | -1.901361 | 0.332835 |
| 18 | 6 | 0 | 2.472614 | -1.010057 | 0.208977 |
| 19 | 6 | 0 | 3.357845 | -3.085287 | 1.070692 |
| 20 | 6 | 0 | 2.114529 | -3.324193 | 1.628101 |
| 21 | 6 | 0 | 1.087560 | -2.385322 | 1.436481 |
| 22 | 7 | 0 | 1.248843 | -1.261546 | 0.743329 |
| 23 | 8 | 0 | -1.224014 | -0.310425 | -1.468645 |
| 24 | 1 | 0 | 0.797139 | 2.821348 | -1.295125 |
| 25 | 1 | 0 | 2.887428 | 3.486044 | -2.488729 |
| 26 | 1 | 0 | 4.888822 | 1.984738 | -2.365727 |
| 27 | 1 | 0 | 0.096267 | -2.550406 | 1.850634 |
| 28 | 1 | 0 | 1.918613 | -4.224740 | 2.201076 |
| 29 | 1 | 0 | 4.170855 | -3.796559 | 1.190614 |
| 30 | 1 | 0 | 5.901483 | -0.175001 | -1.487736 |
| 31 | 1 | 0 | 5.645724 | -2.259917 | -0.198466 |
| 32 | 1 | 0 | -2.996890 | 1.367057 | -0.328508 |
| 33 | 1 | 0 | -3.047477 | 3.713526 | -1.122207 |
| 34 | 1 | 0 | -1.455495 | 5.390066 | -0.193673 |
| 35 | 1 | 0 | 0.179407 | 4.700823 | 1.556592 |
| 36 | 1 | 0 | 0.212359 | 2.357792 | 2.370043 |
| 37 | 6 | 0 | -2.247147 | -1.141116 | -1.499828 |
| 38 | 6 | 0 | -3.417509 | -0.811552 | -2.231183 |
| 39 | 6 | 0 | -4.507511 | -1.677514 | -2.284107 |
| 40 | 6 | 0 | -4.485304 | -2.904454 | -1.614162 |
| 41 | 6 | 0 | -3.338079 | -3.251710 | -0.892871 |
| 42 | 6 | 0 | -2.241645 | -2.396359 | -0.837664 |
| 43 | 1 | 0 | -3.430552 | 0.135425 | -2.766134 |
| 44 | 1 | 0 | -5.387936 | -1.390839 | -2.857164 |
| 45 | 1 | 0 | -5.339019 | -3.575587 | -1.655238 |
| 46 | 1 | 0 | -3.296891 | -4.206436 | -0.370304 |
| 47 | 1 | 0 | -1.347258 | -2.675621 | -0.284632 |

**PDb**

SCF Done: E(RB+HF-LYP) = -5322.21641926 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.784187 | 2.579290 | 0.035076 |
| 2 | 6 | 0 | 1.309504 | 1.899977 | -1.111629 |
| 3 | 6 | 0 | 1.588821 | 2.472378 | -2.374649 |
| 4 | 6 | 0 | 2.275997 | 3.676457 | -2.476980 |
| 5 | 6 | 0 | 2.735485 | 4.342144 | -1.334503 |
| 6 | 6 | 0 | 2.490138 | 3.777035 | -0.082512 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 8 | 0 | 0.587108 | 0.784357 | -1.069947 |
| 8 | 29 | 0 | 0.463151 | -0.288361 | 0.448561 |
| 9 | 7 | 0 | -1.289295 | 0.678774 | 0.946794 |
| 10 | 6 | 0 | -2.423807 | 0.381901 | 0.265616 |
| 11 | 6 | 0 | -3.625607 | 1.110889 | 0.461780 |
| 12 | 6 | 0 | -3.610714 | 2.159584 | 1.406311 |
| 13 | 6 | 0 | -2.451502 | 2.431655 | 2.102448 |
| 14 | 6 | 0 | -1.308883 | 1.656583 | 1.844662 |
| 15 | 6 | 0 | -2.400288 | -0.709552 | -0.682991 |
| 16 | 6 | 0 | -3.573679 | -1.007068 | -1.425003 |
| 17 | 6 | 0 | -4.768751 | -0.244674 | -1.205303 |
| 18 | 6 | 0 | -4.794971 | 0.767793 | -0.295557 |
| 19 | 6 | 0 | -3.498793 | -2.061885 | -2.361101 |
| 20 | 6 | 0 | -2.310908 | -2.744426 | -2.518710 |
| 21 | 6 | 0 | -1.207694 | -2.377078 | -1.723237 |
| 22 | 7 | 0 | -1.248285 | -1.403094 | -0.827401 |
| 23 | 6 | 0 | 2.072363 | -1.199872 | 0.013575 |
| 24 | 6 | 0 | 1.986167 | -2.570868 | -0.220063 |
| 25 | 6 | 0 | 3.120642 | -3.264830 | -0.654802 |
| 26 | 6 | 0 | 4.333273 | -2.596262 | -0.823371 |
| 27 | 6 | 0 | 4.410046 | -1.230538 | -0.550339 |
| 28 | 6 | 0 | 3.278276 | -0.526100 | -0.123783 |
| 29 | 35 | 0 | 0.662892 | -1.144132 | 2.564794 |
| 30 | 1 | 0 | -0.257196 | -2.892474 | -1.827551 |
| 31 | 1 | 0 | -2.214209 | -3.553586 | -3.235368 |
| 32 | 1 | 0 | -4.376000 | -2.319140 | -2.949400 |
| 33 | 1 | 0 | -0.385781 | 1.828744 | 2.387093 |
| 34 | 1 | 0 | -2.406007 | 3.225764 | 2.839923 |
| 35 | 1 | 0 | -4.514386 | 2.739257 | 1.575864 |
| 36 | 1 | 0 | -5.656006 | -0.493588 | -1.781403 |
| 37 | 1 | 0 | -5.703375 | 1.340751 | -0.130425 |
| 38 | 1 | 0 | 3.354096 | 0.537661 | 0.077943 |
| 39 | 1 | 0 | 5.351404 | -0.699590 | -0.668928 |
| 40 | 1 | 0 | 5.215674 | -3.138840 | -1.152158 |
| 41 | 1 | 0 | 3.053775 | -4.334943 | -0.837072 |
| 42 | 1 | 0 | 1.064873 | -3.112549 | -0.033898 |
| 43 | 1 | 0 | 1.237443 | 1.948865 | -3.259059 |
| 44 | 1 | 0 | 2.465886 | 4.097754 | -3.461936 |
| 45 | 1 | 0 | 3.281282 | 5.277327 | -1.421478 |
| 46 | 1 | 0 | 2.849361 | 4.271560 | 0.817456 |
| 47 | 1 | 0 | 1.616959 | 2.144321 | 1.018570 |

**TSrd**

SCF Done: E(RB+HF-LYP) = -5322.20111610 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.489381 | 1.786321 | 0.585452 |
| 2 | 6 | 0 | -1.559199 | 1.445577 | -0.394414 |
| 3 | 6 | 0 | -1.277605 | 2.299028 | -1.462693 |
| 4 | 6 | 0 | -1.837603 | 3.578831 | -1.471314 |
| 5 | 6 | 0 | -2.718349 | 3.969449 | -0.459336 |
| 6 | 6 | 0 | -3.043172 | 3.068395 | 0.558083 |
| 7 | 29 | 0 | -0.174902 | 0.154242 | 0.039592 |
| 8 | 35 | 0 | -0.090628 | -0.107716 | 2.431982 |
| 9 | 8 | 0 | -1.618894 | -0.321351 | -1.115656 |
| 10 | 6 | 0 | -2.742229 | -1.009700 | -0.772823 |
| 11 | 6 | 0 | -2.913731 | -1.639531 | 0.470581 |
| 12 | 6 | 0 | -4.066136 | -2.390904 | 0.708246 |
| 13 | 6 | 0 | -5.048234 | -2.527065 | -0.274634 |
| 14 | 6 | 0 | -4.878386 | -1.888732 | -1.507054 |
| 15 | 6 | 0 | -3.741431 | -1.123701 | -1.754217 |
| 16 | 7 | 0 | 1.145358 | -1.438215 | -0.394662 |
| 17 | 6 | 0 | 2.437210 | -1.040785 | -0.452536 |
| 18 | 6 | 0 | 3.516712 | -1.950349 | -0.558172 |
| 19 | 6 | 0 | 3.194783 | -3.324413 | -0.613707 |
| 20 | 6 | 0 | 1.870860 | -3.716734 | -0.555404 |
| 21 | 6 | 0 | 0.869945 | -2.734600 | -0.438635 |
| 22 | 6 | 0 | 4.858066 | -1.439549 | -0.587941 |
| 23 | 6 | 0 | 5.102387 | -0.100942 | -0.500893 |
| 24 | 6 | 0 | 4.028227 | 0.845536 | -0.384683 |
| 25 | 6 | 0 | 2.692853 | 0.375242 | -0.377537 |
| 26 | 6 | 0 | 4.222631 | 2.239085 | -0.266911 |
| 27 | 6 | 0 | 3.124494 | 3.068652 | -0.147527 |
| 28 | 6 | 0 | 1.835212 | 2.506531 | -0.160318 |
| 29 | 7 | 0 | 1.619406 | 1.202054 | -0.283079 |
| 30 | 1 | 0 | 0.949048 | 3.128695 | -0.076150 |
| 31 | 1 | 0 | 3.238785 | 4.142889 | -0.046135 |
| 32 | 1 | 0 | 5.231652 | 2.643206 | -0.265075 |
| 33 | 1 | 0 | -0.181006 | -3.001346 | -0.371997 |
| 34 | 1 | 0 | 1.593018 | -4.765007 | -0.590150 |
| 35 | 1 | 0 | 3.991038 | -4.059855 | -0.695425 |
| 36 | 1 | 0 | 6.122309 | 0.274078 | -0.511653 |
| 37 | 1 | 0 | 5.680515 | -2.145147 | -0.669847 |
| 38 | 1 | 0 | -2.737657 | 1.090816 | 1.377573 |

| | | | | | |
|---|---|---|---|---|---|
| 39 | 1 | 0 | -3.736122 | 3.357877 | 1.343911 |
| 40 | 1 | 0 | -3.165033 | 4.959534 | -0.475641 |
| 41 | 1 | 0 | -1.604387 | 4.256439 | -2.289201 |
| 42 | 1 | 0 | -0.638569 | 1.966246 | -2.274534 |
| 43 | 1 | 0 | -3.595272 | -0.618203 | -2.704053 |
| 44 | 1 | 0 | -5.639455 | -1.980892 | -2.278141 |
| 45 | 1 | 0 | -5.940066 | -3.117010 | -0.081574 |
| 46 | 1 | 0 | -4.192423 | -2.872569 | 1.674779 |
| 47 | 1 | 0 | -2.161967 | -1.512611 | 1.245519 |

**PDrd**

SCF Done: E(RB+HF-LYP) = -5322.24154531 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.576321 | 1.048918 | 0.221967 |
| 2 | 6 | 0 | 2.689933 | 0.378377 | -0.190677 |
| 3 | 6 | 0 | 3.939301 | 1.008845 | -0.405186 |
| 4 | 6 | 0 | 4.016067 | 2.396114 | -0.158739 |
| 5 | 6 | 0 | 2.885439 | 3.068165 | 0.272705 |
| 6 | 6 | 0 | 1.686099 | 2.359441 | 0.446756 |
| 7 | 6 | 0 | 2.553863 | -1.037154 | -0.404012 |
| 8 | 6 | 0 | 3.663418 | -1.792616 | -0.854888 |
| 9 | 6 | 0 | 4.914381 | -1.122987 | -1.078440 |
| 10 | 6 | 0 | 5.048037 | 0.215781 | -0.857183 |
| 11 | 6 | 0 | 3.471274 | -3.176551 | -1.050303 |
| 12 | 6 | 0 | 2.228811 | -3.727888 | -0.789299 |
| 13 | 6 | 0 | 1.192310 | -2.901918 | -0.327577 |
| 14 | 7 | 0 | 1.335848 | -1.589865 | -0.127237 |
| 15 | 29 | 0 | 0.123660 | -0.236186 | 0.679055 |
| 16 | 8 | 0 | -1.648433 | 0.028729 | -0.627673 |
| 17 | 6 | 0 | -2.771997 | -0.797831 | -0.772561 |
| 18 | 6 | 0 | -3.032865 | -1.727228 | 0.231745 |
| 19 | 6 | 0 | -4.097901 | -2.614592 | 0.063591 |
| 20 | 6 | 0 | -4.892074 | -2.564778 | -1.083711 |
| 21 | 6 | 0 | -4.621099 | -1.615372 | -2.071898 |
| 22 | 6 | 0 | -3.555263 | -0.727010 | -1.924620 |
| 23 | 6 | 0 | -1.824532 | 1.406346 | -0.781253 |
| 24 | 6 | 0 | -2.545311 | 2.125979 | 0.172421 |
| 25 | 6 | 0 | -2.672065 | 3.506647 | 0.019115 |
| 26 | 6 | 0 | -2.087379 | 4.156338 | -1.072366 |
| 27 | 6 | 0 | -1.365694 | 3.420610 | -2.014372 |
| 28 | 6 | 0 | -1.233996 | 2.036882 | -1.874580 |
| 29 | 35 | 0 | -0.808186 | -0.190616 | 2.781404 |
| 30 | 1 | 0 | 0.781352 | 2.858841 | 0.780397 |
| 31 | 1 | 0 | 2.908681 | 4.134828 | 0.472026 |
| 32 | 1 | 0 | 4.956738 | 2.919810 | -0.307509 |
| 33 | 1 | 0 | 0.213166 | -3.312116 | -0.098567 |
| 34 | 1 | 0 | 2.044995 | -4.788632 | -0.927115 |
| 35 | 1 | 0 | 4.296378 | -3.792999 | -1.397166 |
| 36 | 1 | 0 | 6.003450 | 0.707683 | -1.020520 |
| 37 | 1 | 0 | 5.761534 | -1.711472 | -1.421086 |
| 38 | 1 | 0 | -2.961154 | 1.604937 | 1.027995 |
| 39 | 1 | 0 | -3.225110 | 4.076657 | 0.760510 |
| 40 | 1 | 0 | -2.191532 | 5.231901 | -1.185277 |
| 41 | 1 | 0 | -0.907759 | 3.919769 | -2.864096 |
| 42 | 1 | 0 | -0.674861 | 1.444648 | -2.592323 |
| 43 | 1 | 0 | -3.331435 | 0.009740 | -2.689598 |
| 44 | 1 | 0 | -5.236440 | -1.566918 | -2.966421 |
| 45 | 1 | 0 | -5.721905 | -3.255453 | -1.205048 |
| 46 | 1 | 0 | -4.312769 | -3.338099 | 0.845436 |
| 47 | 1 | 0 | -2.433228 | -1.706975 | 1.136924 |

**C**

SCF Done: E(RB+HF-LYP) = -2783.46069709 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.475134 | 1.893974 | -1.890625 |
| 2 | 7 | 0 | -1.489843 | 0.949605 | -0.948017 |
| 3 | 6 | 0 | -2.704286 | 0.508916 | -0.508128 |
| 4 | 6 | 0 | -3.933010 | 1.006633 | -1.005046 |
| 5 | 6 | 0 | -3.874334 | 2.004957 | -2.001578 |
| 6 | 6 | 0 | -2.641678 | 2.447577 | -2.443279 |
| 7 | 29 | 0 | -0.000004 | 0.000102 | -0.000002 |
| 8 | 7 | 0 | 1.489743 | -0.948483 | -0.949113 |
| 9 | 6 | 0 | 2.704235 | -0.508469 | -0.508685 |
| 10 | 6 | 0 | 3.932902 | -1.005935 | -1.005992 |
| 11 | 6 | 0 | 3.874114 | -2.003345 | -2.003432 |
| 12 | 6 | 0 | 2.641408 | -2.445319 | -2.445640 |
| 13 | 6 | 0 | 1.474925 | -1.891965 | -1.892603 |
| 14 | 6 | 0 | 5.162841 | -0.482057 | -0.481933 |
| 15 | 6 | 0 | 5.162887 | 0.481746 | 0.481896 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 6 | 0 | 3.932998 | 1.005790 | 1.005907 |
| 17 | 6 | 0 | 2.704284 | 0.508491 | 0.508551 |
| 18 | 7 | 0 | 1.489834 | 0.948662 | 0.948936 |
| 19 | 6 | 0 | 1.475106 | 1.892147 | 1.892427 |
| 20 | 6 | 0 | 2.641642 | 2.445337 | 2.445514 |
| 21 | 6 | 0 | 3.874306 | 2.003199 | 2.003353 |
| 22 | 1 | 0 | 0.496390 | 2.224687 | 2.225099 |
| 23 | 1 | 0 | 2.559275 | 3.210194 | 3.210368 |
| 24 | 1 | 0 | 4.793952 | 2.412162 | 2.412324 |
| 25 | 1 | 0 | 0.496178 | -2.224358 | -2.225329 |
| 26 | 1 | 0 | 2.558969 | -3.210170 | -3.210492 |
| 27 | 1 | 0 | 4.793721 | -2.412441 | -2.412359 |
| 28 | 1 | 0 | 6.099119 | 0.871146 | 0.871373 |
| 29 | 1 | 0 | 6.099036 | -0.871589 | -0.871367 |
| 30 | 6 | 0 | -5.162892 | 0.482091 | -0.481519 |
| 31 | 1 | 0 | -4.793988 | 2.414240 | -2.410212 |
| 32 | 1 | 0 | -2.559324 | 3.213127 | -3.207441 |
| 33 | 1 | 0 | -0.496423 | 2.226872 | -2.222954 |
| 34 | 6 | 0 | -2.704224 | -0.509017 | 0.508134 |
| 35 | 6 | 0 | -3.932885 | -1.006862 | 1.005077 |
| 36 | 6 | 0 | -3.874086 | -2.005036 | 2.001751 |
| 37 | 6 | 0 | -2.641375 | -2.447385 | 2.443571 |
| 38 | 6 | 0 | -1.474899 | -1.893703 | 1.890852 |
| 39 | 7 | 0 | -1.489726 | -0.949489 | 0.948092 |
| 40 | 6 | 0 | -5.162833 | -0.482540 | 0.481482 |
| 41 | 1 | 0 | -4.793689 | -2.414408 | 2.410411 |
| 42 | 1 | 0 | -2.558927 | -3.212793 | 3.207866 |
| 43 | 1 | 0 | -0.496147 | -2.226437 | 2.223226 |
| 44 | 1 | 0 | -6.099020 | -0.872409 | 0.870597 |
| 45 | 1 | 0 | -6.099128 | 0.871811 | -0.870668 |

**D**

SCF Done: E(RB+HF-LYP) = -2254.13883598 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.636212 | 0.860269 | 0.357938 |
| 2 | 6 | 0 | -2.605508 | -0.445629 | -0.201355 |
| 3 | 6 | 0 | -3.812351 | -1.188561 | -0.155548 |
| 4 | 6 | 0 | -4.966625 | -0.656600 | 0.412760 |
| 5 | 6 | 0 | -4.978104 | 0.632025 | 0.959145 |
| 6 | 6 | 0 | -3.795253 | 1.380485 | 0.921724 |
| 7 | 8 | 0 | -1.522342 | -0.963434 | -0.744078 |
| 8 | 29 | 0 | -0.000349 | -0.004422 | -0.738991 |
| 9 | 8 | 0 | 1.519974 | 0.957010 | -0.747639 |
| 10 | 6 | 0 | 2.604635 | 0.444237 | -0.203167 |
| 11 | 6 | 0 | 3.810076 | 1.189732 | -0.162478 |
| 12 | 6 | 0 | 4.965852 | 0.663122 | 0.407779 |
| 13 | 6 | 0 | 4.980265 | -0.622414 | 0.961294 |
| 14 | 6 | 0 | 3.798796 | -1.373327 | 0.929079 |
| 15 | 6 | 0 | 2.638304 | -0.858451 | 0.363403 |
| 16 | 1 | 0 | 1.712579 | -1.429172 | 0.325484 |
| 17 | 1 | 0 | 3.782804 | -2.377287 | 1.352558 |
| 18 | 1 | 0 | 5.886661 | -1.027890 | 1.405363 |
| 19 | 1 | 0 | 5.873843 | 1.266302 | 0.420975 |
| 20 | 1 | 0 | 3.804251 | 2.188993 | -0.591683 |
| 21 | 1 | 0 | -3.808774 | -2.190185 | -0.579233 |
| 22 | 1 | 0 | -5.875755 | -1.257958 | 0.430080 |
| 23 | 1 | 0 | -5.883342 | 1.041674 | 1.401745 |
| 24 | 1 | 0 | -3.776971 | 2.386752 | 1.339595 |
| 25 | 1 | 0 | -1.709482 | 1.429075 | 0.316155 |

**CPd**

SCF Done: E(RB+HF-LYP) = -5057.50424187 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.609089 | 2.129475 | -0.302446 |
| 2 | 6 | 0 | 0.227071 | 1.942163 | -0.078145 |
| 3 | 6 | 0 | -0.387302 | 2.573450 | 1.025637 |
| 4 | 6 | 0 | 0.401540 | 3.224069 | 1.968201 |
| 5 | 6 | 0 | 1.785641 | 3.338009 | 1.793061 |
| 6 | 6 | 0 | 2.379369 | 2.783131 | 0.654960 |
| 7 | 29 | 0 | -0.029290 | -0.053419 | 0.075599 |
| 8 | 35 | 0 | -0.903511 | 1.756789 | -1.738052 |
| 9 | 8 | 0 | -1.568511 | -0.145459 | 1.149690 |
| 10 | 6 | 0 | -2.579745 | -0.907341 | 0.786946 |
| 11 | 6 | 0 | -3.757387 | -0.950459 | 1.578132 |
| 12 | 6 | 0 | -4.842432 | -1.745587 | 1.222088 |
| 13 | 6 | 0 | -4.810545 | -2.536232 | 0.067667 |
| 14 | 6 | 0 | -3.657651 | -2.507745 | -0.724687 |
| 15 | 6 | 0 | -2.565479 | -1.716770 | -0.380982 |
| 16 | 8 | 0 | 1.282508 | -0.912471 | -0.945288 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 6 | 0 | 2.341877 | -1.503573 | -0.440641 |
| 18 | 6 | 0 | 2.569261 | -1.637075 | 0.955438 |
| 19 | 6 | 0 | 3.704351 | -2.273966 | 1.448506 |
| 20 | 6 | 0 | 4.666930 | -2.806651 | 0.584250 |
| 21 | 6 | 0 | 4.460965 | -2.686047 | -0.795262 |
| 22 | 6 | 0 | 3.330361 | -2.051939 | -1.300595 |
| 23 | 1 | 0 | 3.172367 | -1.961407 | -2.372811 |
| 24 | 1 | 0 | 5.195853 | -3.094799 | -1.488839 |
| 25 | 1 | 0 | 5.552693 | -3.302735 | 0.974424 |
| 26 | 1 | 0 | 3.838825 | -2.357057 | 2.526578 |
| 27 | 1 | 0 | 1.819648 | -1.232889 | 1.633602 |
| 28 | 1 | 0 | -1.674081 | -1.701935 | -1.005858 |
| 29 | 1 | 0 | -3.606844 | -3.114618 | -1.628200 |
| 30 | 1 | 0 | -5.660928 | -3.156008 | -0.207592 |
| 31 | 1 | 0 | -5.728802 | -1.750750 | 1.856701 |
| 32 | 1 | 0 | -3.784347 | -0.338002 | 2.476621 |
| 33 | 1 | 0 | -1.453692 | 2.459952 | 1.172017 |
| 34 | 1 | 0 | -0.074535 | 3.656449 | 2.845628 |
| 35 | 1 | 0 | 2.391990 | 3.855802 | 2.531819 |
| 36 | 1 | 0 | 3.452481 | 2.867891 | 0.500454 |
| 37 | 1 | 0 | 2.064199 | 1.693610 | -1.183069 |

**TSd**

SCF Done: E(RB+HF-LYP) = -5057.50369017 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.478182 | 1.285595 | 1.644762 |
| 2 | 6 | 0 | 2.474889 | 1.059527 | 0.664880 |
| 3 | 6 | 0 | 2.810818 | 1.390131 | -0.675672 |
| 4 | 6 | 0 | 4.061875 | 1.903545 | -1.004596 |
| 5 | 6 | 0 | 5.037430 | 2.115749 | -0.024304 |
| 6 | 6 | 0 | 4.725206 | 1.799665 | 1.303030 |
| 7 | 8 | 0 | 1.301629 | 0.583878 | 1.017360 |
| 8 | 29 | 0 | -0.053350 | -0.073832 | -0.139126 |
| 9 | 8 | 0 | -1.606983 | 0.526890 | -1.020389 |
| 10 | 6 | 0 | -2.360136 | 1.499774 | -0.550252 |
| 11 | 6 | 0 | -2.003083 | 2.288443 | 0.575979 |
| 12 | 6 | 0 | -2.832820 | 3.307330 | 1.034723 |
| 13 | 6 | 0 | -4.048180 | 3.593748 | 0.402645 |
| 14 | 6 | 0 | -4.414045 | 2.829441 | -0.710949 |
| 15 | 6 | 0 | -3.594327 | 1.807426 | -1.180660 |
| 16 | 1 | 0 | -3.880143 | 1.215725 | -2.047420 |
| 17 | 1 | 0 | -5.354998 | 3.033955 | -1.222084 |
| 18 | 1 | 0 | -4.691990 | 4.390901 | 0.767659 |
| 19 | 1 | 0 | -2.523024 | 3.890602 | 1.901355 |
| 20 | 1 | 0 | -1.054061 | 2.080975 | 1.066619 |
| 21 | 1 | 0 | 2.058334 | 1.231168 | -1.445417 |
| 22 | 1 | 0 | 4.278618 | 2.144630 | -2.044958 |
| 23 | 1 | 0 | 6.013641 | 2.516940 | -0.287124 |
| 24 | 1 | 0 | 5.467835 | 1.957899 | 2.085194 |
| 25 | 1 | 0 | 3.237988 | 1.042509 | 2.677422 |
| 26 | 6 | 0 | -0.467619 | -1.976916 | 0.100397 |
| 27 | 35 | 0 | 0.999747 | -1.992870 | -1.401690 |
| 28 | 6 | 0 | -0.001264 | -2.267509 | 1.397263 |
| 29 | 6 | 0 | -0.858800 | -2.885627 | 2.307538 |
| 30 | 6 | 0 | -2.140392 | -3.285165 | 1.923653 |
| 31 | 6 | 0 | -2.569009 | -3.050702 | 0.610727 |
| 32 | 6 | 0 | -1.732465 | -2.434692 | -0.312245 |
| 33 | 1 | 0 | 0.990177 | -1.944603 | 1.690820 |
| 34 | 1 | 0 | -0.510200 | -3.064528 | 3.322280 |
| 35 | 1 | 0 | -2.798659 | -3.777107 | 2.635129 |
| 36 | 1 | 0 | -3.565583 | -3.356464 | 0.299969 |
| 37 | 1 | 0 | -2.066627 | -2.235756 | -1.322937 |

**PDd**

SCF Done: E(RB+HF-LYP) = -5057.53464023 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.989746 | -1.639846 | 1.536612 |
| 2 | 6 | 0 | 1.796129 | -0.975426 | 0.325072 |
| 3 | 6 | 0 | 2.897180 | -0.604007 | -0.445284 |
| 4 | 6 | 0 | 4.191937 | -0.893780 | -0.000211 |
| 5 | 6 | 0 | 4.389414 | -1.557348 | 1.210864 |
| 6 | 6 | 0 | 3.283153 | -1.928975 | 1.978647 |
| 7 | 29 | 0 | 0.038697 | -0.487046 | -0.195364 |
| 8 | 35 | 0 | -0.163002 | -2.540256 | -1.178500 |
| 9 | 8 | 0 | -1.606869 | 0.120621 | -0.867726 |
| 10 | 6 | 0 | -2.710491 | 0.127178 | -0.148690 |
| 11 | 6 | 0 | -3.852193 | 0.813461 | -0.637707 |
| 12 | 6 | 0 | -5.047648 | 0.826981 | 0.072521 |
| 13 | 6 | 0 | -5.166299 | 0.166597 | 1.300828 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | -4.050583 | -0.511922 | 1.799183 |
| 15 | 6 | 0 | -2.847966 | -0.537355 | 1.097518 |
| 16 | 8 | 0 | 0.263357 | 1.017076 | 0.846225 |
| 17 | 6 | 0 | 0.719444 | 2.135228 | 0.296593 |
| 18 | 6 | 0 | 0.827081 | 2.346659 | -1.097770 |
| 19 | 6 | 0 | 1.307944 | 3.553686 | -1.600988 |
| 20 | 6 | 0 | 1.688121 | 4.592187 | -0.747512 |
| 21 | 6 | 0 | 1.577681 | 4.396550 | 0.633568 |
| 22 | 6 | 0 | 1.109649 | 3.193397 | 1.150978 |
| 23 | 1 | 0 | 1.028469 | 3.037207 | 2.223044 |
| 24 | 1 | 0 | 1.866819 | 5.192047 | 1.319042 |
| 25 | 1 | 0 | 2.059950 | 5.532355 | -1.147675 |
| 26 | 1 | 0 | 1.376593 | 3.684756 | -2.679759 |
| 27 | 1 | 0 | 0.499743 | 1.563260 | -1.775315 |
| 28 | 1 | 0 | -1.996893 | -1.081404 | 1.501350 |
| 29 | 1 | 0 | -4.115840 | -1.034592 | 2.752844 |
| 30 | 1 | 0 | -6.102321 | 0.182092 | 1.854368 |
| 31 | 1 | 0 | -5.902236 | 1.364373 | -0.337977 |
| 32 | 1 | 0 | -3.761337 | 1.328087 | -1.590744 |
| 33 | 1 | 0 | 2.761796 | -0.084921 | -1.390291 |
| 34 | 1 | 0 | 5.045708 | -0.597409 | -0.606809 |
| 35 | 1 | 0 | 5.396468 | -1.784143 | 1.554380 |
| 36 | 1 | 0 | 3.424518 | -2.448623 | 2.924646 |
| 37 | 1 | 0 | 1.135705 | -1.940971 | 2.138634 |

**E**

SCF Done: E(RB+HF-LYP) = -2211.72108209 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.816433 | 0.433495 | 0.000000 |
| 2 | 6 | 0 | 2.293915 | 1.690709 | 0.000000 |
| 3 | 6 | 0 | 0.875050 | 1.898862 | 0.000000 |
| 4 | 6 | 0 | 0.000000 | 0.788098 | 0.000000 |
| 5 | 6 | 0 | 0.558587 | -0.555993 | 0.000000 |
| 6 | 6 | 0 | 1.963205 | -0.719161 | 0.000000 |
| 7 | 6 | 0 | 0.300030 | 3.192454 | 0.000000 |
| 8 | 6 | 0 | -1.071528 | 3.333458 | 0.000000 |
| 9 | 6 | 0 | -1.873087 | 2.179700 | 0.000000 |
| 10 | 7 | 0 | -1.367321 | 0.947144 | 0.000000 |
| 11 | 6 | 0 | 2.474522 | -2.039264 | 0.000000 |
| 12 | 6 | 0 | 1.607083 | -3.110923 | 0.000000 |
| 13 | 6 | 0 | 0.223854 | -2.865362 | 0.000000 |
| 14 | 7 | 0 | -0.293152 | -1.637447 | 0.000000 |
| 15 | 29 | 0 | -1.989843 | -0.826980 | 0.000000 |
| 16 | 1 | 0 | -2.955113 | 2.255981 | 0.000000 |
| 17 | 1 | 0 | -1.541421 | 4.310707 | 0.000000 |
| 18 | 1 | 0 | 0.948603 | 4.063811 | 0.000000 |
| 19 | 1 | 0 | -0.485296 | -3.686155 | 0.000000 |
| 20 | 1 | 0 | 1.968392 | -4.133295 | 0.000000 |
| 21 | 1 | 0 | 3.549659 | -2.194223 | 0.000000 |
| 22 | 1 | 0 | 2.944107 | 2.560271 | 0.000000 |
| 23 | 1 | 0 | 3.891447 | 0.280993 | 0.000000 |

**CPe**

SCF Done: E(RB+HF-LYP) = -5015.14926088 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.076815 | 1.182414 | 0.601514 |
| 2 | 6 | 0 | -2.560018 | -0.023739 | 0.072558 |
| 3 | 6 | 0 | -2.289241 | -1.149297 | 0.905819 |
| 4 | 6 | 0 | -2.458863 | -0.977392 | 2.306371 |
| 5 | 6 | 0 | -2.882091 | 0.231176 | 2.829328 |
| 6 | 6 | 0 | -3.207246 | 1.305575 | 1.973210 |
| 7 | 29 | 0 | -0.610552 | -0.321873 | 0.055844 |
| 8 | 35 | 0 | -2.602581 | -0.319515 | -1.845289 |
| 9 | 7 | 0 | 0.619999 | 1.258234 | -0.053358 |
| 10 | 6 | 0 | 1.914145 | 0.832921 | -0.023976 |
| 11 | 6 | 0 | 3.014122 | 1.719901 | -0.062463 |
| 12 | 6 | 0 | 2.726359 | 3.102205 | -0.139823 |
| 13 | 6 | 0 | 1.411462 | 3.523911 | -0.170945 |
| 14 | 6 | 0 | 0.383864 | 2.565203 | -0.125948 |
| 15 | 6 | 0 | 4.346328 | 1.185753 | -0.023001 |
| 16 | 6 | 0 | 4.563245 | -0.158447 | 0.049766 |
| 17 | 6 | 0 | 3.466580 | -1.084356 | 0.089225 |
| 18 | 6 | 0 | 2.143510 | -0.587496 | 0.057252 |
| 19 | 7 | 0 | 1.048982 | -1.400177 | 0.089482 |
| 20 | 6 | 0 | 1.237683 | -2.717068 | 0.149043 |
| 21 | 6 | 0 | 2.514839 | -3.302448 | 0.183899 |
| 22 | 6 | 0 | 3.629554 | -2.487027 | 0.156409 |
| 23 | 1 | 0 | 0.344455 | -3.333767 | 0.169079 |
| 24 | 1 | 0 | 2.606576 | -4.381989 | 0.231133 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 1 | 0 | 4.629219 | -2.911507 | 0.182759 |
| 26 | 1 | 0 | -0.659775 | 2.864126 | -0.142500 |
| 27 | 1 | 0 | 1.158621 | 4.576885 | -0.229903 |
| 28 | 1 | 0 | 3.541165 | 3.820017 | -0.173397 |
| 29 | 1 | 0 | 5.574935 | -0.552158 | 0.077105 |
| 30 | 1 | 0 | 5.183206 | 1.877141 | -0.053367 |
| 31 | 1 | 0 | -2.279351 | -2.154977 | 0.494438 |
| 32 | 1 | 0 | -2.291448 | -1.827160 | 2.961849 |
| 33 | 1 | 0 | -3.013448 | 0.340965 | 3.901162 |
| 34 | 1 | 0 | -3.587584 | 2.232832 | 2.391376 |
| 35 | 1 | 0 | -3.357586 | 1.989817 | -0.066404 |

**TSe**

SCF Done: E(RB+HF-LYP) = -5015.14312082 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.578007 | 1.218293 | -0.403454 |
| 2 | 6 | 0 | 1.885768 | 0.922320 | -0.164732 |
| 3 | 6 | 0 | 2.916161 | 1.886825 | -0.243974 |
| 4 | 6 | 0 | 2.539475 | 3.207117 | -0.581377 |
| 5 | 6 | 0 | 1.209100 | 3.498159 | -0.813163 |
| 6 | 6 | 0 | 0.254696 | 2.471112 | -0.710275 |
| 7 | 6 | 0 | 4.270558 | 1.486849 | 0.016170 |
| 8 | 6 | 0 | 4.574711 | 0.196043 | 0.334138 |
| 9 | 6 | 0 | 3.549798 | -0.805684 | 0.421718 |
| 10 | 6 | 0 | 2.207387 | -0.440261 | 0.171826 |
| 11 | 7 | 0 | 1.177175 | -1.327352 | 0.237764 |
| 12 | 6 | 0 | 1.444368 | -2.595744 | 0.541120 |
| 13 | 6 | 0 | 2.747170 | -3.052620 | 0.805828 |
| 14 | 6 | 0 | 3.799337 | -2.158889 | 0.746880 |
| 15 | 29 | 0 | -0.574101 | -0.423494 | -0.195786 |
| 16 | 1 | 0 | 0.596945 | -3.274308 | 0.574223 |
| 17 | 1 | 0 | 2.907898 | -4.096722 | 1.050892 |
| 18 | 1 | 0 | 4.816247 | -2.485016 | 0.946518 |
| 19 | 1 | 0 | -0.800820 | 2.667683 | -0.872991 |
| 20 | 1 | 0 | 0.889092 | 4.501452 | -1.072236 |
| 21 | 1 | 0 | 3.298519 | 3.980949 | -0.654396 |
| 22 | 1 | 0 | 5.602799 | -0.095457 | 0.527318 |
| 23 | 1 | 0 | 5.053465 | 2.236703 | -0.047368 |
| 24 | 6 | 0 | -2.396427 | 0.104664 | 0.170680 |
| 25 | 35 | 0 | -2.222318 | -1.750872 | -1.029922 |
| 26 | 6 | 0 | -2.511838 | -0.101503 | 1.551670 |
| 27 | 6 | 0 | -3.172272 | 0.868433 | 2.314851 |
| 28 | 6 | 0 | -3.772161 | 1.963407 | 1.694523 |
| 29 | 6 | 0 | -3.715601 | 2.102402 | 0.301475 |
| 30 | 6 | 0 | -3.050556 | 1.158192 | -0.478516 |
| 31 | 1 | 0 | -2.099514 | -0.987378 | 2.024355 |
| 32 | 1 | 0 | -3.242929 | 0.738842 | 3.390743 |
| 33 | 1 | 0 | -4.311123 | 2.694516 | 2.288884 |
| 34 | 1 | 0 | -4.211287 | 2.938372 | -0.183825 |
| 35 | 1 | 0 | -3.033565 | 1.240700 | -1.560271 |

**PDe**

SCF Done: E(RB+HF-LYP) = -5015.15201249 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.872361 | 0.616773 | -1.211537 |
| 2 | 6 | 0 | -2.290373 | 0.268893 | 0.002227 |
| 3 | 6 | 0 | -2.845117 | 0.612542 | 1.230067 |
| 4 | 6 | 0 | -3.989956 | 1.419062 | 1.233725 |
| 5 | 6 | 0 | -4.571202 | 1.823936 | 0.030489 |
| 6 | 6 | 0 | -4.016972 | 1.423475 | -1.186829 |
| 7 | 29 | 0 | -0.541595 | -0.468403 | -0.012614 |
| 8 | 35 | 0 | -1.656787 | -2.391808 | -0.008784 |
| 9 | 7 | 0 | 0.391290 | 1.271109 | -0.012983 |
| 10 | 6 | 0 | 1.748683 | 1.126292 | -0.004734 |
| 11 | 6 | 0 | 2.639121 | 2.221713 | -0.002780 |
| 12 | 6 | 0 | 2.066271 | 3.514350 | -0.010437 |
| 13 | 6 | 0 | 0.691168 | 3.649203 | -0.019235 |
| 14 | 6 | 0 | -0.120055 | 2.501312 | -0.020051 |
| 15 | 6 | 0 | 4.052078 | 1.962461 | 0.006497 |
| 16 | 6 | 0 | 4.536811 | 0.686205 | 0.013141 |
| 17 | 6 | 0 | 3.649435 | -0.442756 | 0.010940 |
| 18 | 6 | 0 | 2.258231 | -0.209569 | 0.001965 |
| 19 | 7 | 0 | 1.336219 | -1.207869 | -0.000884 |
| 20 | 6 | 0 | 1.753901 | -2.469718 | 0.004540 |
| 21 | 6 | 0 | 3.121551 | -2.801796 | 0.013738 |
| 22 | 6 | 0 | 4.067912 | -1.794576 | 0.016961 |
| 23 | 1 | 0 | 0.975605 | -3.226888 | 0.001682 |
| 24 | 1 | 0 | 3.413310 | -3.846201 | 0.018055 |
| 25 | 1 | 0 | 5.128397 | -2.030316 | 0.023970 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | -1.201151 | 2.576726 | -0.026574 |
| 27 | 1 | 0 | 0.221921 | 4.626686 | -0.025423 |
| 28 | 1 | 0 | 2.709611 | 4.389751 | -0.009451 |
| 29 | 1 | 0 | 5.607554 | 0.506037 | 0.020088 |
| 30 | 1 | 0 | 4.733051 | 2.808166 | 0.008079 |
| 31 | 1 | 0 | -2.416603 | 0.268143 | 2.166448 |
| 32 | 1 | 0 | -4.431634 | 1.709000 | 2.182877 |
| 33 | 1 | 0 | -5.469253 | 2.434104 | 0.041608 |
| 34 | 1 | 0 | -4.479751 | 1.716623 | -2.124873 |
| 35 | 1 | 0 | -2.464588 | 0.275654 | -2.158318 |

**$TS_{met1}$**
SCF Done: E(RB+HF-LYP) = -5322.16600479 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 1.104068 | 2.175943 | -1.067800 |
| 2 | 6 | 0 | 1.623137 | 1.646856 | 0.128016 |
| 3 | 6 | 0 | 2.408448 | 2.475756 | 0.949400 |
| 4 | 6 | 0 | 2.650961 | 3.798838 | 0.586251 |
| 5 | 6 | 0 | 2.117515 | 4.322792 | -0.595275 |
| 6 | 6 | 0 | 1.342705 | 3.502855 | -1.419878 |
| 7 | 8 | 0 | 1.385529 | 0.364961 | 0.472901 |
| 8 | 29 | 0 | -0.254957 | -0.628018 | 0.121359 |
| 9 | 7 | 0 | -1.703890 | -0.426480 | -1.244434 |
| 10 | 6 | 0 | -2.901944 | -0.131184 | -0.660912 |
| 11 | 6 | 0 | -4.097098 | 0.064587 | -1.394957 |
| 12 | 6 | 0 | -4.032926 | -0.096423 | -2.794470 |
| 13 | 6 | 0 | -2.822745 | -0.430187 | -3.379166 |
| 14 | 6 | 0 | -1.685969 | -0.581478 | -2.571091 |
| 15 | 6 | 0 | -5.294943 | 0.420993 | -0.686385 |
| 16 | 6 | 0 | -5.295397 | 0.571783 | 0.668676 |
| 17 | 6 | 0 | -4.103437 | 0.357343 | 1.441164 |
| 18 | 6 | 0 | -2.911325 | -0.007591 | 0.769825 |
| 19 | 6 | 0 | -4.045094 | 0.479619 | 2.844962 |
| 20 | 6 | 0 | -2.847024 | 0.233054 | 3.493888 |
| 21 | 6 | 0 | -1.723349 | -0.147625 | 2.744402 |
| 22 | 7 | 0 | -1.741438 | -0.278005 | 1.416318 |
| 23 | 1 | 0 | -0.776358 | -0.365403 | 3.229332 |
| 24 | 1 | 0 | -2.766075 | 0.316046 | 4.572957 |
| 25 | 1 | 0 | -4.935480 | 0.761321 | 3.400719 |
| 26 | 1 | 0 | -0.721336 | -0.827266 | -3.006222 |
| 27 | 1 | 0 | -2.735756 | -0.563276 | -4.452747 |
| 28 | 1 | 0 | -4.926632 | 0.043149 | -3.396752 |
| 29 | 1 | 0 | -6.207012 | 0.850215 | 1.190864 |
| 30 | 1 | 0 | -6.206382 | 0.576553 | -1.257607 |
| 31 | 1 | 0 | 2.817122 | 2.060329 | 1.865147 |
| 32 | 1 | 0 | 3.258572 | 4.428737 | 1.232008 |
| 33 | 1 | 0 | 2.304762 | 5.357349 | -0.870098 |
| 34 | 1 | 0 | 0.926717 | 3.897792 | -2.344112 |
| 35 | 1 | 0 | 0.513824 | 1.519797 | -1.701894 |
| 36 | 6 | 0 | 2.934161 | -0.802769 | 0.110167 |
| 37 | 35 | 0 | 1.274727 | -2.397827 | -0.084957 |
| 38 | 6 | 0 | 3.678192 | -0.950977 | 1.273780 |
| 39 | 6 | 0 | 5.062790 | -0.778669 | 1.190865 |
| 40 | 6 | 0 | 5.677792 | -0.471745 | -0.025873 |
| 41 | 6 | 0 | 4.892232 | -0.327788 | -1.171244 |
| 42 | 6 | 0 | 3.504898 | -0.493109 | -1.116578 |
| 43 | 1 | 0 | 3.193867 | -1.192423 | 2.213129 |
| 44 | 1 | 0 | 5.660186 | -0.890796 | 2.092967 |
| 45 | 1 | 0 | 6.755002 | -0.344540 | -0.079563 |
| 46 | 1 | 0 | 5.354227 | -0.087271 | -2.126019 |
| 47 | 1 | 0 | 2.888214 | -0.377397 | -2.001024 |

**$TS_{met2}$**
SCF Done: E(RB+HF-LYP) = -5057.45969073 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.279832 | 2.197595 | 0.809825 |
| 2 | 6 | 0 | 1.134091 | 1.645286 | 0.203820 |
| 3 | 6 | 0 | 0.287906 | 2.493511 | -0.540152 |
| 4 | 6 | 0 | 0.574181 | 3.849907 | -0.658714 |
| 5 | 6 | 0 | 1.717451 | 4.394855 | -0.064812 |
| 6 | 6 | 0 | 2.563291 | 3.555635 | 0.664894 |
| 7 | 8 | 0 | 0.815550 | 0.342637 | 0.316531 |
| 8 | 29 | 0 | -0.805585 | -0.405090 | -0.442047 |
| 9 | 8 | 0 | -2.412641 | 0.359054 | -0.955495 |
| 10 | 6 | 0 | -3.501939 | 0.165022 | -0.249863 |
| 11 | 6 | 0 | -4.720715 | 0.801472 | -0.604119 |
| 12 | 6 | 0 | -5.882374 | 0.600456 | 0.134839 |
| 13 | 6 | 0 | -5.894029 | -0.240022 | 1.255009 |
| 14 | 6 | 0 | -4.702999 | -0.878637 | 1.618643 |

| | | | | | |
|---|---|---|---|---|---|
| 15 | 6 | 0 | -3.535004 | -0.684112 | 0.889328 |
| 16 | 35 | 0 | 0.562159 | -2.238899 | -0.705894 |
| 17 | 1 | 0 | 2.935075 | 1.556355 | 1.389241 |
| 18 | 1 | 0 | 3.455034 | 3.963684 | 1.138355 |
| 19 | 1 | 0 | 1.941935 | 5.454346 | -0.165058 |
| 20 | 1 | 0 | -0.102216 | 4.487024 | -1.225656 |
| 21 | 1 | 0 | -0.603405 | 2.056855 | -0.981729 |
| 22 | 1 | 0 | -2.606355 | -1.183889 | 1.160954 |
| 23 | 1 | 0 | -4.684467 | -1.539183 | 2.485183 |
| 24 | 1 | 0 | -6.805574 | -0.391491 | 1.828689 |
| 25 | 1 | 0 | -6.798540 | 1.107936 | -0.167679 |
| 26 | 1 | 0 | -4.717142 | 1.455041 | -1.473424 |
| 27 | 6 | 0 | 2.309268 | -0.947633 | 0.140165 |
| 28 | 6 | 0 | 2.731675 | -1.360015 | 1.402527 |
| 29 | 6 | 0 | 4.100192 | -1.379312 | 1.679677 |
| 30 | 6 | 0 | 5.034992 | -0.997070 | 0.710993 |
| 31 | 6 | 0 | 4.581273 | -0.588283 | -0.545676 |
| 32 | 6 | 0 | 3.215519 | -0.559708 | -0.842401 |
| 33 | 1 | 0 | 2.002872 | -1.647282 | 2.153386 |
| 34 | 1 | 0 | 4.435413 | -1.696150 | 2.666148 |
| 35 | 1 | 0 | 6.098810 | -1.016935 | 0.933671 |
| 36 | 1 | 0 | 5.293706 | -0.286657 | -1.311782 |
| 37 | 1 | 0 | 2.862322 | -0.237794 | -1.816844 |

**(phen)Cu(II)(OPh)$^{+}$**

SCF Done: E(UB+HF-LYP) = -2518.64747048 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 29 | 0 | -0.530416 | -0.000825 | -0.405350 |
| 2 | 7 | 0 | 0.894663 | -1.331436 | -0.176951 |
| 3 | 6 | 0 | 2.096842 | -0.717510 | 0.010060 |
| 4 | 6 | 0 | 2.096302 | 0.717992 | 0.009985 |
| 5 | 7 | 0 | 0.893634 | 1.331001 | -0.176950 |
| 6 | 6 | 0 | 0.852472 | 2.662651 | -0.187987 |
| 7 | 6 | 0 | 2.002753 | 3.452578 | -0.012381 |
| 8 | 6 | 0 | 3.225741 | 2.837904 | 0.179824 |
| 9 | 6 | 0 | 3.303016 | 1.425567 | 0.195377 |
| 10 | 6 | 0 | 4.518582 | 0.683605 | 0.383974 |
| 11 | 6 | 0 | 4.519087 | -0.681277 | 0.384109 |
| 12 | 6 | 0 | 3.304072 | -1.424169 | 0.195618 |
| 13 | 6 | 0 | 3.227826 | -2.836561 | 0.180310 |
| 14 | 6 | 0 | 0.854466 | -2.663125 | -0.187765 |
| 15 | 1 | 0 | -0.118423 | -3.118758 | -0.342389 |
| 16 | 1 | 0 | 1.916352 | -4.532738 | -0.030037 |
| 17 | 1 | 0 | 4.129525 | -3.426527 | 0.318402 |
| 18 | 1 | 0 | 5.445375 | -1.229618 | 0.526900 |
| 19 | 1 | 0 | 5.444467 | 1.232659 | 0.526645 |
| 20 | 1 | 0 | 4.127021 | 3.428548 | 0.317750 |
| 21 | 1 | 0 | 1.912994 | 4.533075 | -0.030737 |
| 22 | 1 | 0 | -0.120778 | 3.117557 | -0.342490 |
| 23 | 8 | 0 | -2.228608 | -0.000934 | -0.898052 |
| 24 | 6 | 0 | -3.410558 | -0.000517 | -0.298079 |
| 25 | 6 | 0 | -4.579831 | -0.000224 | -1.094787 |
| 26 | 6 | 0 | -5.829514 | 0.000203 | -0.490013 |
| 27 | 6 | 0 | -5.940378 | 0.000358 | 0.906821 |
| 28 | 6 | 0 | -4.785910 | 0.000071 | 1.703942 |
| 29 | 6 | 0 | -3.531684 | -0.000382 | 1.112345 |
| 30 | 1 | 0 | -4.470043 | -0.000352 | -2.174600 |
| 31 | 1 | 0 | -6.725229 | 0.000419 | -1.103980 |
| 32 | 1 | 0 | -6.920440 | 0.000693 | 1.373806 |
| 33 | 1 | 0 | -4.874249 | 0.000177 | 2.786408 |
| 34 | 1 | 0 | -2.625222 | -0.000639 | 1.714372 |
| 35 | 6 | 0 | 2.005301 | -3.452171 | -0.011881 |

**PhBr $^{\bullet-}$**

SCF Done: E(UB+HF-LYP) = -2803.34183894 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 35 | 0 | 2.271476 | 0.000039 | -0.003051 |
| 2 | 6 | 0 | -0.484807 | 0.001299 | 0.016798 |
| 3 | 6 | 0 | -1.176310 | 1.207229 | 0.009684 |
| 4 | 6 | 0 | -2.578618 | 1.209171 | -0.003480 |
| 5 | 6 | 0 | -3.280652 | -0.001271 | -0.009944 |
| 6 | 6 | 0 | -2.576395 | -1.210398 | -0.003415 |
| 7 | 6 | 0 | -1.174087 | -1.205903 | 0.009654 |
| 8 | 1 | 0 | -0.629184 | 2.150453 | 0.014395 |
| 9 | 1 | 0 | -3.128039 | 2.152545 | -0.008771 |
| 10 | 1 | 0 | -4.369988 | -0.002286 | -0.020326 |
| 11 | 1 | 0 | -3.124098 | -2.154772 | -0.008696 |
| 12 | 1 | 0 | -0.625154 | -2.148063 | 0.014390 |

**CPb(triplet)**
SCF Done: E(UB+HF-LYP) = -5322.18088269 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.085014 | -1.560204 | 1.140217 |
| 2 | 6 | 0 | -2.904237 | -1.651859 | -0.261303 |
| 3 | 6 | 0 | -4.059793 | -1.680846 | -1.073634 |
| 4 | 6 | 0 | -5.327874 | -1.609602 | -0.507739 |
| 5 | 6 | 0 | -5.492820 | -1.496230 | 0.878643 |
| 6 | 6 | 0 | -4.362178 | -1.471401 | 1.695706 |
| 7 | 8 | 0 | -1.693321 | -1.726029 | -0.809241 |
| 8 | 29 | 0 | -0.341925 | -0.792279 | 0.029871 |
| 9 | 7 | 0 | 1.035906 | -0.347443 | 1.307378 |
| 10 | 6 | 0 | 2.290075 | -0.723117 | 0.832894 |
| 11 | 6 | 0 | 3.483410 | -0.518144 | 1.581815 |
| 12 | 6 | 0 | 3.379647 | 0.077690 | 2.840760 |
| 13 | 6 | 0 | 2.096398 | 0.438989 | 3.323745 |
| 14 | 6 | 0 | 0.979438 | 0.215174 | 2.544433 |
| 15 | 6 | 0 | 2.329539 | -1.344809 | -0.421037 |
| 16 | 6 | 0 | 3.557418 | -1.779617 | -1.005110 |
| 17 | 6 | 0 | 4.758232 | -1.547121 | -0.249697 |
| 18 | 6 | 0 | 4.720712 | -0.949797 | 0.976770 |
| 19 | 6 | 0 | 3.495772 | -2.407382 | -2.250203 |
| 20 | 6 | 0 | 2.250608 | -2.596528 | -2.874607 |
| 21 | 6 | 0 | 1.093105 | -2.143294 | -2.243362 |
| 22 | 7 | 0 | 1.117105 | -1.519990 | -1.060218 |
| 23 | 6 | 0 | -0.548031 | 2.754202 | -0.436696 |
| 24 | 6 | 0 | 0.570573 | 3.153790 | 0.288422 |
| 25 | 6 | 0 | 1.391027 | 4.145698 | -0.254303 |
| 26 | 6 | 0 | 1.087164 | 4.719659 | -1.489850 |
| 27 | 6 | 0 | -0.041936 | 4.300582 | -2.195877 |
| 28 | 6 | 0 | -0.872151 | 3.307276 | -1.672683 |
| 29 | 35 | 0 | -1.717159 | 1.391107 | 0.279149 |
| 30 | 1 | 0 | 0.107059 | -2.281994 | -2.676697 |
| 31 | 1 | 0 | 2.175987 | -3.095328 | -3.834661 |
| 32 | 1 | 0 | 4.409301 | -2.755141 | -2.726060 |
| 33 | 1 | 0 | -0.012806 | 0.479795 | 2.899844 |
| 34 | 1 | 0 | 1.979112 | 0.887658 | 4.304745 |
| 35 | 1 | 0 | 4.268048 | 0.248871 | 3.441555 |
| 36 | 1 | 0 | 5.707356 | -1.865206 | -0.674380 |
| 37 | 1 | 0 | 5.641547 | -0.792162 | 1.533190 |
| 38 | 1 | 0 | -1.749270 | 2.970643 | -2.214656 |
| 39 | 1 | 0 | -0.281736 | 4.742056 | -3.159021 |
| 40 | 1 | 0 | 1.730241 | 5.491249 | -1.903133 |
| 41 | 1 | 0 | 2.270637 | 4.466123 | 0.296644 |
| 42 | 1 | 0 | 0.807437 | 2.701111 | 1.244527 |
| 43 | 1 | 0 | -3.926604 | -1.756617 | -2.149090 |
| 44 | 1 | 0 | -6.202244 | -1.635641 | -1.154420 |
| 45 | 1 | 0 | -6.487186 | -1.437331 | 1.311886 |
| 46 | 1 | 0 | -4.471501 | -1.401554 | 2.775632 |
| 47 | 1 | 0 | -2.208004 | -1.597561 | 1.787611 |

**Cu(II)$(OPh)_2$**
SCF Done: E(UB+HF-LYP) = -2254.05058606 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.896142 | 0.926734 | 0.215388 |
| 2 | 6 | 0 | -2.685707 | -0.443652 | -0.051320 |
| 3 | 6 | 0 | -3.800966 | -1.302052 | -0.130609 |
| 4 | 6 | 0 | -5.085150 | -0.796092 | 0.041185 |
| 5 | 6 | 0 | -5.286254 | 0.563920 | 0.302125 |
| 6 | 6 | 0 | -4.182917 | 1.420621 | 0.390720 |
| 7 | 8 | 0 | -1.461714 | -0.953641 | -0.218107 |
| 8 | 29 | 0 | -0.000034 | -0.000325 | -0.263885 |
| 9 | 8 | 0 | 1.461539 | 0.953179 | -0.218709 |
| 10 | 6 | 0 | 2.685642 | 0.443558 | -0.051639 |
| 11 | 6 | 0 | 3.800662 | 1.302286 | -0.130753 |
| 12 | 6 | 0 | 5.084964 | 0.796721 | 0.041327 |
| 13 | 6 | 0 | 5.286424 | -0.563220 | 0.302361 |
| 14 | 6 | 0 | 4.183326 | -1.420250 | 0.390765 |
| 15 | 6 | 0 | 2.896438 | -0.926756 | 0.215154 |
| 16 | 1 | 0 | 2.027660 | -1.578282 | 0.291402 |
| 17 | 1 | 0 | 4.329925 | -2.476858 | 0.598746 |
| 18 | 1 | 0 | 6.291630 | -0.951377 | 0.438207 |
| 19 | 1 | 0 | 5.937811 | 1.467123 | -0.026316 |
| 20 | 1 | 0 | 3.627982 | 2.354945 | -0.332449 |
| 21 | 1 | 0 | -3.628562 | -2.354772 | -0.332223 |
| 22 | 1 | 0 | -5.938186 | -1.466241 | -0.026602 |
| 23 | 1 | 0 | -6.291372 | 0.952383 | 0.437757 |
| 24 | 1 | 0 | -4.329241 | 2.477279 | 0.598642 |
| 25 | 1 | 0 | -2.027180 | 1.577994 | 0.291806 |

**CPd(triplet)**
SCF Done: E(UB+HF-LYP) = -5057.51176022 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.718422 | -1.567716 | -0.276397 |
| 2 | 6 | 0 | -1.444002 | -1.575964 | 0.292677 |
| 3 | 6 | 0 | -1.190003 | -2.385027 | 1.401871 |
| 4 | 6 | 0 | -2.205150 | -3.183941 | 1.938981 |
| 5 | 6 | 0 | -3.479062 | -3.180542 | 1.364943 |
| 6 | 6 | 0 | -3.734111 | -2.370665 | 0.256438 |
| 7 | 29 | 0 | 0.033432 | -0.477825 | -0.464138 |
| 8 | 35 | 0 | 1.354725 | -2.030004 | -1.593089 |
| 9 | 8 | 0 | 0.974988 | 0.088360 | 1.098329 |
| 10 | 6 | 0 | 2.209968 | 0.540906 | 0.977081 |
| 11 | 6 | 0 | 3.276859 | -0.112754 | 1.642280 |
| 12 | 6 | 0 | 4.564395 | 0.410067 | 1.605625 |
| 13 | 6 | 0 | 4.837844 | 1.580949 | 0.888176 |
| 14 | 6 | 0 | 3.798213 | 2.224927 | 0.206179 |
| 15 | 6 | 0 | 2.502578 | 1.722888 | 0.249208 |
| 16 | 8 | 0 | -0.771687 | 1.067910 | -1.133093 |
| 17 | 6 | 0 | -1.490311 | 2.047454 | -0.615276 |
| 18 | 6 | 0 | -2.033980 | 2.003661 | 0.692077 |
| 19 | 6 | 0 | -2.789523 | 3.065386 | 1.181125 |
| 20 | 6 | 0 | -3.040201 | 4.198145 | 0.399282 |
| 21 | 6 | 0 | -2.510149 | 4.252158 | -0.894012 |
| 22 | 6 | 0 | -1.746014 | 3.202718 | -1.395290 |
| 23 | 1 | 0 | -1.330163 | 3.238972 | -2.398807 |
| 24 | 1 | 0 | -2.692657 | 5.124941 | -1.519660 |
| 25 | 1 | 0 | -3.634207 | 5.021133 | 0.789814 |
| 26 | 1 | 0 | -3.192403 | 3.005477 | 2.190986 |
| 27 | 1 | 0 | -1.848171 | 1.125353 | 1.300960 |
| 28 | 1 | 0 | 1.687436 | 2.212769 | -0.275278 |
| 29 | 1 | 0 | 4.002873 | 3.131394 | -0.360579 |
| 30 | 1 | 0 | 5.848758 | 1.980452 | 0.853370 |
| 31 | 1 | 0 | 5.368289 | -0.102532 | 2.131277 |
| 32 | 1 | 0 | 3.050450 | -1.028842 | 2.180253 |
| 33 | 1 | 0 | -0.199014 | -2.389559 | 1.849287 |
| 34 | 1 | 0 | -1.999607 | -3.811001 | 2.805549 |
| 35 | 1 | 0 | -4.268734 | -3.803556 | 1.780909 |
| 36 | 1 | 0 | -4.726092 | -2.357527 | -0.193013 |
| 37 | 1 | 0 | -2.931619 | -0.926480 | -1.128665 |

**(phen)Cu(II)(OPh)(Br)**
SCF Done: E(UB+HF-LYP) = -5090.60827696 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -1.029261 | 1.373714 | -0.337542 |
| 2 | 6 | 0 | -2.283839 | 0.975963 | -0.024964 |
| 3 | 6 | 0 | -3.392036 | 1.851213 | 0.001033 |
| 4 | 6 | 0 | -3.134467 | 3.207753 | -0.301135 |
| 5 | 6 | 0 | -1.842720 | 3.608362 | -0.590728 |
| 6 | 6 | 0 | -0.805059 | 2.655881 | -0.594594 |
| 7 | 6 | 0 | -4.684201 | 1.315331 | 0.329062 |
| 8 | 6 | 0 | -4.847858 | -0.009949 | 0.613266 |
| 9 | 6 | 0 | -3.733607 | -0.917761 | 0.606416 |
| 10 | 6 | 0 | -2.452340 | -0.415816 | 0.287560 |
| 11 | 6 | 0 | -3.820457 | -2.296695 | 0.903066 |
| 12 | 6 | 0 | -2.677580 | -3.073624 | 0.863721 |
| 13 | 6 | 0 | -1.444652 | -2.480305 | 0.532484 |
| 14 | 7 | 0 | -1.333535 | -1.182534 | 0.269307 |
| 15 | 29 | 0 | 0.357591 | -0.144988 | -0.238359 |
| 16 | 35 | 0 | 1.439064 | -1.897374 | -1.294631 |
| 17 | 8 | 0 | 1.636222 | 1.121108 | 0.169540 |
| 18 | 6 | 0 | 2.919490 | 0.909991 | 0.462333 |
| 19 | 6 | 0 | 3.313006 | 0.038731 | 1.500753 |
| 20 | 6 | 0 | 4.655851 | -0.113983 | 1.831259 |
| 21 | 6 | 0 | 5.643308 | 0.601625 | 1.146507 |
| 22 | 6 | 0 | 5.265904 | 1.468680 | 0.116824 |
| 23 | 6 | 0 | 3.925106 | 1.620312 | -0.225756 |
| 24 | 1 | 0 | 0.230671 | 2.915147 | -0.789430 |
| 25 | 1 | 0 | -1.616117 | 4.645137 | -0.815969 |
| 26 | 1 | 0 | -3.951317 | 3.924809 | -0.297850 |
| 27 | 1 | 0 | -0.525745 | -3.053464 | 0.455320 |
| 28 | 1 | 0 | -2.714808 | -4.135913 | 1.080634 |
| 29 | 1 | 0 | -4.782627 | -2.733974 | 1.156855 |
| 30 | 1 | 0 | -5.536836 | 1.988657 | 0.344897 |
| 31 | 1 | 0 | -5.831987 | -0.400581 | 0.857183 |
| 32 | 1 | 0 | 3.623958 | 2.286383 | -1.029955 |
| 33 | 1 | 0 | 6.024623 | 2.027130 | -0.427271 |
| 34 | 1 | 0 | 6.690988 | 0.481725 | 1.408921 |

| | | | | | |
|---|---|---|---|---|---|
| 35 | 1 | 0 | 4.936219 | -0.795068 | 2.631826 |
| 36 | 1 | 0 | 2.542316 | -0.518626 | 2.028034 |

**Ph$^{\bullet}$**
SCF Done: E(UB+HF-LYP) = -231.561280804 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000000 | 0.000000 | 1.400175 |
| 2 | 6 | 0 | 0.000000 | 1.226379 | 0.771790 |
| 3 | 6 | 0 | 0.000000 | 1.214189 | -0.632604 |
| 4 | 6 | 0 | 0.000000 | 0.000000 | -1.324732 |
| 5 | 6 | 0 | 0.000000 | -1.214189 | -0.632604 |
| 6 | 6 | 0 | 0.000000 | -1.226379 | 0.771790 |
| 7 | 1 | 0 | 0.000000 | 2.162893 | 1.323295 |
| 8 | 1 | 0 | 0.000000 | 2.154667 | -1.179088 |
| 9 | 1 | 0 | 0.000000 | 0.000000 | -2.411295 |
| 10 | 1 | 0 | 0.000000 | -2.154667 | -1.179088 |
| 11 | 1 | 0 | 0.000000 | -2.162893 | 1.323295 |

**Cu(II)(OPh)$_2$(Br)$^-$**
SCF Done: E(UB+HF-LYP) = -4825.91844730 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.755973 | -0.392335 | 1.049556 |
| 2 | 6 | 0 | 2.561438 | -0.131802 | 0.337705 |
| 3 | 6 | 0 | 2.585691 | 0.895346 | -0.634855 |
| 4 | 6 | 0 | 3.754595 | 1.613705 | -0.875385 |
| 5 | 6 | 0 | 4.933232 | 1.343193 | -0.172390 |
| 6 | 6 | 0 | 4.917352 | 0.331737 | 0.792862 |
| 7 | 8 | 0 | 1.484795 | -0.858740 | 0.604705 |
| 8 | 29 | 0 | -0.183797 | -0.971080 | -0.132359 |
| 9 | 8 | 0 | -0.615320 | 0.641973 | -0.941434 |
| 10 | 6 | 0 | -1.478748 | 1.466136 | -0.368171 |
| 11 | 6 | 0 | -1.699726 | 2.745215 | -0.933464 |
| 12 | 6 | 0 | -2.602799 | 3.637289 | -0.363812 |
| 13 | 6 | 0 | -3.321495 | 3.298921 | 0.788034 |
| 14 | 6 | 0 | -3.115196 | 2.038489 | 1.355706 |
| 15 | 6 | 0 | -2.216327 | 1.135379 | 0.794322 |
| 16 | 35 | 0 | -1.634927 | -2.739107 | -0.175461 |
| 17 | 1 | 0 | 3.740059 | -1.179294 | 1.799307 |
| 18 | 1 | 0 | 5.821955 | 0.103628 | 1.355704 |
| 19 | 1 | 0 | 5.840985 | 1.908962 | -0.369737 |
| 20 | 1 | 0 | 3.742889 | 2.402015 | -1.627159 |
| 21 | 1 | 0 | 1.665898 | 1.119960 | -1.166087 |
| 22 | 1 | 0 | -2.082537 | 0.148721 | 1.231134 |
| 23 | 1 | 0 | -3.665199 | 1.748685 | 2.249811 |
| 24 | 1 | 0 | -4.023758 | 4.000575 | 1.231846 |
| 25 | 1 | 0 | -2.746909 | 4.613795 | -0.824853 |
| 26 | 1 | 0 | -1.140554 | 3.009537 | -1.827245 |

**$Cs_2CO_3$**
SCF Done: E(RB+HF-LYP) = -303.615196532 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.054078 | 0.006224 | 0.006627 |
| 2 | 8 | 0 | -0.310993 | -0.036086 | 1.318560 |
| 3 | 8 | 0 | 1.171023 | 0.030760 | -0.395123 |
| 4 | 55 | 0 | 2.469161 | -0.012354 | 2.073990 |
| 5 | 8 | 0 | -1.036537 | 0.021270 | -0.828196 |
| 6 | 55 | 0 | -3.167655 | -0.088783 | 0.972538 |

**$CsHCO_3$**
SCF Done: E(RB+HF-LYP) = -284.324205756 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 2.215030 | -0.179121 | 0.000478 |
| 2 | 8 | 0 | 1.519359 | 1.131070 | 0.002472 |
| 3 | 8 | 0 | 3.440876 | -0.092562 | -0.003062 |
| 4 | 1 | 0 | 2.262792 | 1.753888 | -0.000734 |
| 5 | 8 | 0 | 1.404014 | -1.131537 | 0.002520 |
| 6 | 55 | 0 | -1.208490 | 0.001183 | -0.000320 |

**CsBr**
SCF Done: E(RB+HF-LYP) = -2591.65907613 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 55 | 0 | 0.000000 | 0.000000 | 1.273312 |
| 2 | 35 | 0 | 0.000000 | 0.000000 | -2.000919 |

**(phen)Cu(I)(O-Ph-*p*-Me)**
SCF Done: E(RB+HF-LYP) = -2558.14958460 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.998595 | 3.482181 | -0.271337 |
| 2 | 6 | 0 | -3.253163 | 2.994785 | 0.049407 |
| 3 | 6 | 0 | -3.435976 | 1.600589 | 0.171873 |
| 4 | 6 | 0 | -2.314885 | 0.767514 | -0.052907 |
| 5 | 7 | 0 | -1.068949 | 1.258347 | -0.353720 |
| 6 | 6 | 0 | -0.935787 | 2.588811 | -0.459180 |
| 7 | 6 | 0 | -4.692871 | 0.997016 | 0.519619 |
| 8 | 6 | 0 | -4.819890 | -0.354569 | 0.646100 |
| 9 | 6 | 0 | -3.701090 | -1.224942 | 0.422443 |
| 10 | 6 | 0 | -2.452217 | -0.661674 | 0.062195 |
| 11 | 6 | 0 | -3.761247 | -2.631486 | 0.535014 |
| 12 | 6 | 0 | -2.624922 | -3.382531 | 0.296490 |
| 13 | 6 | 0 | -1.433693 | -2.723411 | -0.064630 |
| 14 | 7 | 0 | -1.346996 | -1.405813 | -0.186105 |
| 15 | 29 | 0 | 0.262181 | -0.016150 | -0.573643 |
| 16 | 8 | 0 | 1.737758 | -1.046690 | -0.666587 |
| 17 | 6 | 0 | 2.940048 | -0.611731 | -0.299455 |
| 18 | 6 | 0 | 4.091845 | -1.384220 | -0.563983 |
| 19 | 6 | 0 | 5.352683 | -0.948789 | -0.167463 |
| 20 | 6 | 0 | 5.538946 | 0.264863 | 0.512068 |
| 21 | 6 | 0 | 4.395148 | 1.027178 | 0.784337 |
| 22 | 6 | 0 | 3.128667 | 0.604478 | 0.392132 |
| 23 | 1 | 0 | 0.059827 | 2.948728 | -0.692232 |
| 24 | 1 | 0 | -1.818417 | 4.547452 | -0.371660 |
| 25 | 1 | 0 | -4.091660 | 3.666432 | 0.211506 |
| 26 | 1 | 0 | -5.546303 | 1.648174 | 0.688530 |
| 27 | 1 | 0 | -5.775933 | -0.794714 | 0.917270 |
| 28 | 1 | 0 | -4.698781 | -3.108923 | 0.808553 |
| 29 | 1 | 0 | -2.640183 | -4.464892 | 0.375215 |
| 30 | 1 | 0 | -0.518523 | -3.275232 | -0.264062 |
| 31 | 1 | 0 | 3.969281 | -2.329070 | -1.087132 |
| 32 | 1 | 0 | 6.219742 | -1.569920 | -0.390266 |
| 33 | 6 | 0 | 6.917790 | 0.737381 | 0.913494 |
| 34 | 1 | 0 | 4.498897 | 1.970499 | 1.319513 |
| 35 | 1 | 0 | 2.238036 | 1.191957 | 0.612026 |
| 36 | 1 | 0 | 6.863680 | 1.519234 | 1.679807 |
| 37 | 1 | 0 | 7.525937 | -0.081000 | 1.318967 |
| 38 | 1 | 0 | 7.475949 | 1.156756 | 0.063765 |

**(phen)Cu(II)(O-Ph-*p*-Me)(Br)**
SCF Done: E(UB+HF-LYP) = -5129.92566108 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.659402 | 1.544381 | -0.448905 |
| 2 | 6 | 0 | 2.670965 | 0.861906 | 0.288023 |
| 3 | 6 | 0 | 3.101254 | 0.002009 | 1.320657 |
| 4 | 6 | 0 | 4.454109 | -0.165511 | 1.592445 |
| 5 | 6 | 0 | 5.439318 | 0.514912 | 0.860518 |
| 6 | 6 | 0 | 5.010117 | 1.374243 | -0.160720 |
| 7 | 8 | 0 | 1.379358 | 1.090023 | 0.050894 |
| 8 | 29 | 0 | 0.070160 | -0.161692 | -0.300608 |
| 9 | 35 | 0 | 1.080825 | -1.934132 | -1.393938 |
| 10 | 7 | 0 | -1.301584 | 1.373928 | -0.355819 |
| 11 | 6 | 0 | -2.545384 | 0.995949 | 0.018425 |
| 12 | 6 | 0 | -3.639668 | 1.886407 | 0.087452 |
| 13 | 6 | 0 | -3.378759 | 3.236729 | -0.238517 |
| 14 | 6 | 0 | -2.096667 | 3.617387 | -0.591131 |
| 15 | 6 | 0 | -1.073073 | 2.650853 | -0.634368 |
| 16 | 6 | 0 | -4.922309 | 1.371001 | 0.479427 |
| 17 | 6 | 0 | -5.090394 | 0.050459 | 0.782310 |
| 18 | 6 | 0 | -3.989795 | -0.872525 | 0.732506 |
| 19 | 6 | 0 | -2.717701 | -0.390741 | 0.351519 |
| 20 | 7 | 0 | -1.610958 | -1.172587 | 0.290571 |
| 21 | 6 | 0 | -1.727676 | -2.466710 | 0.568900 |
| 22 | 6 | 0 | -2.952248 | -3.040614 | 0.959923 |
| 23 | 6 | 0 | -4.081622 | -2.247676 | 1.044591 |
| 24 | 1 | 0 | -0.044289 | 2.894882 | -0.879220 |
| 25 | 1 | 0 | -1.867168 | 4.649050 | -0.836114 |
| 26 | 1 | 0 | -4.185196 | 3.964680 | -0.204030 |
| 27 | 1 | 0 | -0.820940 | -3.053165 | 0.455488 |

| | | | | | |
|---|---|---|---|---|---|
| 28 | 1 | 0 | -2.993928 | -4.100624 | 1.187017 |
| 29 | 1 | 0 | -5.037090 | -2.669566 | 1.345425 |
| 30 | 1 | 0 | -5.764259 | 2.056092 | 0.528467 |
| 31 | 1 | 0 | -6.067446 | -0.324710 | 1.074291 |
| 32 | 1 | 0 | 3.339543 | 2.209785 | -1.246446 |
| 33 | 1 | 0 | 5.751055 | 1.917835 | -0.744806 |
| 34 | 6 | 0 | 6.908504 | 0.302753 | 1.142823 |
| 35 | 1 | 0 | 4.755903 | -0.837427 | 2.394372 |
| 36 | 1 | 0 | 2.349738 | -0.533530 | 1.896095 |
| 37 | 1 | 0 | 7.506244 | 1.166473 | 0.830271 |
| 38 | 1 | 0 | 7.094118 | 0.136282 | 2.210540 |
| 39 | 1 | 0 | 7.302891 | -0.573209 | 0.608438 |

**(phen)Cu(I)(O-Ph-*p*-OMe)**

SCF Done: E(RB+HF-LYP) = -2633.35171713 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.199212 | 3.508533 | -0.359509 |
| 2 | 6 | 0 | -3.470087 | 3.071400 | -0.029395 |
| 3 | 6 | 0 | -3.696298 | 1.688555 | 0.139154 |
| 4 | 6 | 0 | -2.600570 | 0.813762 | -0.050098 |
| 5 | 7 | 0 | -1.338889 | 1.254957 | -0.365210 |
| 6 | 6 | 0 | -1.164475 | 2.577097 | -0.513230 |
| 7 | 6 | 0 | -4.973533 | 1.136280 | 0.498248 |
| 8 | 6 | 0 | -5.144237 | -0.205741 | 0.668019 |
| 9 | 6 | 0 | -4.051917 | -1.117465 | 0.482139 |
| 10 | 6 | 0 | -2.783327 | -0.605240 | 0.114040 |
| 11 | 6 | 0 | -4.156610 | -2.516942 | 0.639996 |
| 12 | 6 | 0 | -3.042642 | -3.310473 | 0.435046 |
| 13 | 6 | 0 | -1.828370 | -2.700552 | 0.064257 |
| 14 | 7 | 0 | -1.699720 | -1.390952 | -0.097929 |
| 15 | 29 | 0 | -0.052744 | -0.067079 | -0.554598 |
| 16 | 8 | 0 | 1.357560 | -1.175554 | -0.682082 |
| 17 | 6 | 0 | 2.608123 | -0.808959 | -0.403416 |
| 18 | 6 | 0 | 3.690673 | -1.652941 | -0.740490 |
| 19 | 6 | 0 | 5.000647 | -1.300109 | -0.443503 |
| 20 | 6 | 0 | 5.287792 | -0.093607 | 0.209402 |
| 21 | 6 | 0 | 4.234331 | 0.755623 | 0.560951 |
| 22 | 6 | 0 | 2.919838 | 0.394668 | 0.256936 |
| 23 | 1 | 0 | -0.158229 | 2.897958 | -0.757043 |
| 24 | 1 | 0 | -1.985629 | 4.563700 | -0.495066 |
| 25 | 1 | 0 | -4.288235 | 3.773630 | 0.104488 |
| 26 | 1 | 0 | -5.807118 | 1.819095 | 0.639048 |
| 27 | 1 | 0 | -6.115616 | -0.606410 | 0.945859 |
| 28 | 1 | 0 | -5.110542 | -2.955934 | 0.921214 |
| 29 | 1 | 0 | -3.092507 | -4.388703 | 0.548584 |
| 30 | 1 | 0 | -0.928879 | -3.285877 | -0.109542 |
| 31 | 1 | 0 | 3.475444 | -2.589964 | -1.247006 |
| 32 | 1 | 0 | 5.828309 | -1.951674 | -0.710803 |
| 33 | 8 | 0 | 6.622432 | 0.157253 | 0.457098 |
| 34 | 1 | 0 | 4.418982 | 1.694358 | 1.073374 |
| 35 | 1 | 0 | 2.087060 | 1.041270 | 0.529513 |
| 36 | 6 | 0 | 6.948404 | 1.364250 | 1.110176 |
| 37 | 1 | 0 | 8.036845 | 1.375325 | 1.207849 |
| 38 | 1 | 0 | 6.631081 | 2.243748 | 0.530358 |
| 39 | 1 | 0 | 6.497751 | 1.424303 | 2.112029 |

**(phen)Cu(II)(O-Ph-*p*-OMe)(Br)**

SCF Done: E(UB+HF-LYP) = -5205.12914883 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.415353 | 1.361909 | 0.503571 |
| 2 | 6 | 0 | -2.423163 | 0.755997 | -0.287989 |
| 3 | 6 | 0 | -2.851318 | -0.080556 | -1.344531 |
| 4 | 6 | 0 | -4.198047 | -0.294974 | -1.590868 |
| 5 | 6 | 0 | -5.173089 | 0.323748 | -0.793266 |
| 6 | 6 | 0 | -4.773495 | 1.156049 | 0.258583 |
| 7 | 8 | 0 | -1.133971 | 1.022270 | -0.080042 |
| 8 | 29 | 0 | 0.209089 | -0.188514 | 0.291734 |
| 9 | 35 | 0 | -0.747822 | -1.981782 | 1.400587 |
| 10 | 7 | 0 | 1.539923 | 1.383403 | 0.353857 |
| 11 | 6 | 0 | 2.793691 | 1.039794 | -0.020905 |
| 12 | 6 | 0 | 3.864397 | 1.959207 | -0.084603 |
| 13 | 6 | 0 | 3.567780 | 3.301168 | 0.244697 |
| 14 | 6 | 0 | 2.275470 | 3.646928 | 0.596164 |
| 15 | 6 | 0 | 1.278241 | 2.653269 | 0.635648 |
| 16 | 6 | 0 | 5.161570 | 1.479296 | -0.473754 |
| 17 | 6 | 0 | 5.366035 | 0.164355 | -0.778291 |
| 18 | 6 | 0 | 4.290242 | -0.787693 | -0.734585 |
| 19 | 6 | 0 | 3.003846 | -0.340899 | -0.358438 |
| 20 | 7 | 0 | 1.917942 | -1.151886 | -0.305823 |

| | | | | | |
|---|---|---|---|---|---|
| 21 | 6 | 0 | 2.071306 | -2.441968 | -0.585146 |
| 22 | 6 | 0 | 3.312700 | -2.982460 | -0.970491 |
| 23 | 6 | 0 | 4.420692 | -2.159164 | -1.048697 |
| 24 | 1 | 0 | 0.243493 | 2.869992 | 0.881051 |
| 25 | 1 | 0 | 2.018479 | 4.671472 | 0.843858 |
| 26 | 1 | 0 | 4.355042 | 4.049995 | 0.213926 |
| 27 | 1 | 0 | 1.180266 | -3.053142 | -0.478041 |
| 28 | 1 | 0 | 3.383966 | -4.040589 | -1.199102 |
| 29 | 1 | 0 | 5.388606 | -2.554488 | -1.345851 |
| 30 | 1 | 0 | 5.984980 | 2.186880 | -0.518504 |
| 31 | 1 | 0 | 6.353863 | -0.184098 | -1.067207 |
| 32 | 1 | 0 | -3.099688 | 2.000263 | 1.324196 |
| 33 | 1 | 0 | -5.505950 | 1.642008 | 0.894162 |
| 34 | 8 | 0 | -6.477371 | 0.050122 | -1.125488 |
| 35 | 1 | 0 | -4.525966 | -0.940828 | -2.400298 |
| 36 | 1 | 0 | -2.096664 | -0.565654 | -1.958611 |
| 37 | 6 | 0 | -7.495984 | 0.622161 | -0.328807 |
| 38 | 1 | 0 | -8.441712 | 0.271833 | -0.748513 |
| 39 | 1 | 0 | -7.423762 | 0.298124 | 0.718860 |
| 40 | 1 | 0 | -7.472236 | 1.720758 | -0.362518 |

**(phen)Cu(I)(O-Ph-*p*-F)**
SCF Done: E(RB+HF-LYP) = -2618.06580264 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.020299 | 3.476788 | -0.262191 |
| 2 | 6 | 0 | -3.272390 | 2.974956 | 0.044616 |
| 3 | 6 | 0 | -3.441574 | 1.578463 | 0.161447 |
| 4 | 6 | 0 | -2.309235 | 0.758238 | -0.053563 |
| 5 | 7 | 0 | -1.066047 | 1.263329 | -0.341292 |
| 6 | 6 | 0 | -0.946118 | 2.595148 | -0.442118 |
| 7 | 6 | 0 | -4.695709 | 0.960627 | 0.493561 |
| 8 | 6 | 0 | -4.809835 | -0.392680 | 0.613675 |
| 9 | 6 | 0 | -3.679447 | -1.250369 | 0.399407 |
| 10 | 6 | 0 | -2.432586 | -0.672836 | 0.055768 |
| 11 | 6 | 0 | -3.726135 | -2.658027 | 0.505871 |
| 12 | 6 | 0 | -2.579499 | -3.396195 | 0.277389 |
| 13 | 6 | 0 | -1.390999 | -2.723254 | -0.066997 |
| 14 | 7 | 0 | -1.316668 | -1.404322 | -0.181792 |
| 15 | 29 | 0 | 0.279178 | 0.001265 | -0.551481 |
| 16 | 8 | 0 | 1.763980 | -1.016801 | -0.643311 |
| 17 | 6 | 0 | 2.966511 | -0.581028 | -0.279010 |
| 18 | 6 | 0 | 4.118565 | -1.346844 | -0.564283 |
| 19 | 6 | 0 | 5.386845 | -0.917709 | -0.177124 |
| 20 | 6 | 0 | 5.520859 | 0.284153 | 0.508709 |
| 21 | 6 | 0 | 4.413796 | 1.066183 | 0.816575 |
| 22 | 6 | 0 | 3.150337 | 0.630912 | 0.424967 |
| 23 | 1 | 0 | 0.047364 | 2.966654 | -0.665794 |
| 24 | 1 | 0 | -1.850624 | 4.544156 | -0.358115 |
| 25 | 1 | 0 | -4.119731 | 3.637068 | 0.199738 |
| 26 | 1 | 0 | -5.557742 | 1.602164 | 0.655249 |
| 27 | 1 | 0 | -5.764111 | -0.843873 | 0.872512 |
| 28 | 1 | 0 | -4.661656 | -3.146290 | 0.766799 |
| 29 | 1 | 0 | -2.584324 | -4.478943 | 0.351701 |
| 30 | 1 | 0 | -0.467899 | -3.264742 | -0.257901 |
| 31 | 1 | 0 | 3.994717 | -2.282739 | -1.101657 |
| 32 | 1 | 0 | 6.272936 | -1.504621 | -0.401533 |
| 33 | 9 | 0 | 6.759540 | 0.703050 | 0.887838 |
| 34 | 1 | 0 | 4.549983 | 1.997824 | 1.358403 |
| 35 | 1 | 0 | 2.257696 | 1.211413 | 0.650895 |

**(phen)Cu(II)(O-Ph-*p*-F)(Br)**
SCF Done: E(UB+HF-LYP) = -5189.84181678 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.663666 | 1.502844 | -0.470378 |
| 2 | 6 | 0 | 2.687628 | 0.850686 | 0.311960 |
| 3 | 6 | 0 | 3.129190 | 0.016590 | 1.361867 |
| 4 | 6 | 0 | 4.485077 | -0.159431 | 1.620957 |
| 5 | 6 | 0 | 5.414799 | 0.508226 | 0.830533 |
| 6 | 6 | 0 | 5.022239 | 1.338553 | -0.213447 |
| 7 | 8 | 0 | 1.392628 | 1.080088 | 0.094431 |
| 8 | 29 | 0 | 0.080607 | -0.164124 | -0.279532 |
| 9 | 35 | 0 | 1.115935 | -1.939083 | -1.342887 |
| 10 | 7 | 0 | -1.282518 | 1.375180 | -0.342820 |
| 11 | 6 | 0 | -2.533532 | 0.999192 | 0.009321 |
| 12 | 6 | 0 | -3.625486 | 1.893173 | 0.066971 |
| 13 | 6 | 0 | -3.354748 | 3.244634 | -0.246248 |
| 14 | 6 | 0 | -2.066140 | 3.622856 | -0.576765 |
| 15 | 6 | 0 | -1.045383 | 2.652974 | -0.610135 |
| 16 | 6 | 0 | -4.915976 | 1.380092 | 0.435482 |

| | | | | | |
|---|---|---|---|---|---|
| 17 | 6 | 0 | -5.093585 | 0.058212 | 0.726916 |
| 18 | 6 | 0 | -3.995766 | -0.868539 | 0.687642 |
| 19 | 6 | 0 | -2.716241 | -0.389021 | 0.329769 |
| 20 | 7 | 0 | -1.611760 | -1.174816 | 0.279348 |
| 21 | 6 | 0 | -1.737421 | -2.470421 | 0.546651 |
| 22 | 6 | 0 | -2.970012 | -3.042307 | 0.915006 |
| 23 | 6 | 0 | -4.097489 | -2.245657 | 0.988183 |
| 24 | 1 | 0 | -0.012300 | 2.895023 | -0.837960 |
| 25 | 1 | 0 | -1.829212 | 4.655159 | -0.811670 |
| 26 | 1 | 0 | -4.158996 | 3.975293 | -0.219517 |
| 27 | 1 | 0 | -0.831207 | -3.059438 | 0.442815 |
| 28 | 1 | 0 | -3.019075 | -4.103754 | 1.133650 |
| 29 | 1 | 0 | -5.059006 | -2.666078 | 1.271202 |
| 30 | 1 | 0 | -5.756023 | 2.068020 | 0.475987 |
| 31 | 1 | 0 | -6.076388 | -0.315205 | 1.001197 |
| 32 | 1 | 0 | 3.329363 | 2.138806 | -1.284972 |
| 33 | 1 | 0 | 5.777921 | 1.838217 | -0.811971 |
| 34 | 9 | 0 | 6.737663 | 0.344878 | 1.085037 |
| 35 | 1 | 0 | 4.830483 | -0.802800 | 2.424466 |
| 36 | 1 | 0 | 2.384136 | -0.498843 | 1.962041 |

**(phen)Cu(I)(O-Ph-*p*-$CF_3$)**
SCF Done: E(RB+HF-LYP) = -2855.87731657 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.743333 | 3.502039 | -0.354731 |
| 2 | 6 | 0 | -3.990860 | 3.072777 | 0.058857 |
| 3 | 6 | 0 | -4.216888 | 1.690879 | 0.240334 |
| 4 | 6 | 0 | -3.142566 | 0.809670 | -0.023449 |
| 5 | 7 | 0 | -1.902918 | 1.243325 | -0.418012 |
| 6 | 6 | 0 | -1.727098 | 2.561906 | -0.577136 |
| 7 | 6 | 0 | -5.471437 | 1.147506 | 0.682228 |
| 8 | 6 | 0 | -5.639640 | -0.193953 | 0.858622 |
| 9 | 6 | 0 | -4.569075 | -1.112935 | 0.596277 |
| 10 | 6 | 0 | -3.324441 | -0.610121 | 0.145725 |
| 11 | 6 | 0 | -4.675280 | -2.512840 | 0.755106 |
| 12 | 6 | 0 | -3.585277 | -3.314203 | 0.471765 |
| 13 | 6 | 0 | -2.393703 | -2.712840 | 0.021009 |
| 14 | 7 | 0 | -2.264478 | -1.403477 | -0.143801 |
| 15 | 29 | 0 | -0.643063 | -0.096009 | -0.696690 |
| 16 | 8 | 0 | 0.795031 | -1.172625 | -0.930741 |
| 17 | 6 | 0 | 2.017953 | -0.796441 | -0.604470 |
| 18 | 6 | 0 | 3.131522 | -1.597227 | -0.953854 |
| 19 | 6 | 0 | 4.420558 | -1.220569 | -0.604758 |
| 20 | 6 | 0 | 4.655480 | -0.035232 | 0.106481 |
| 21 | 6 | 0 | 3.564906 | 0.767564 | 0.465737 |
| 22 | 6 | 0 | 2.275837 | 0.394978 | 0.117494 |
| 23 | 1 | 0 | -0.735812 | 2.875517 | -0.883946 |
| 24 | 1 | 0 | -2.531535 | 4.555763 | -0.502745 |
| 25 | 1 | 0 | -4.792960 | 3.780741 | 0.248355 |
| 26 | 1 | 0 | -6.288683 | 1.835570 | 0.880611 |
| 27 | 1 | 0 | -6.592895 | -0.589056 | 1.199616 |
| 28 | 1 | 0 | -5.611648 | -2.945050 | 1.098587 |
| 29 | 1 | 0 | -3.636196 | -4.392441 | 0.583983 |
| 30 | 1 | 0 | -1.514813 | -3.306820 | -0.216537 |
| 31 | 1 | 0 | 2.952140 | -2.511901 | -1.511575 |
| 32 | 1 | 0 | 5.261071 | -1.845662 | -0.893002 |
| 33 | 6 | 0 | 6.038326 | 0.326179 | 0.534676 |
| 34 | 1 | 0 | 3.734146 | 1.689094 | 1.015267 |
| 35 | 1 | 0 | 1.414773 | 1.006361 | 0.382175 |
| 36 | 9 | 0 | 6.193962 | 1.664465 | 0.700905 |
| 37 | 9 | 0 | 6.390944 | -0.240829 | 1.722057 |
| 38 | 9 | 0 | 6.976521 | -0.075703 | -0.360033 |

**(phen)Cu(II)(O-Ph-*p*-$CF_3$)(Br)**
SCF Done: E(UB+HF-LYP) = -5427.65077861 A.U.

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.935758 | 1.460906 | 0.844326 |
| 2 | 6 | 0 | -1.951741 | 0.788702 | 0.087297 |
| 3 | 6 | 0 | -2.386222 | -0.098582 | -0.922990 |
| 4 | 6 | 0 | -3.737596 | -0.300015 | -1.163836 |
| 5 | 6 | 0 | -4.701342 | 0.382071 | -0.410343 |
| 6 | 6 | 0 | -4.287365 | 1.264881 | 0.594380 |
| 7 | 8 | 0 | -0.666158 | 1.045302 | 0.296393 |
| 8 | 29 | 0 | 0.707204 | -0.187390 | 0.441301 |
| 9 | 35 | 0 | -0.193147 | -2.010957 | 1.538788 |
| 10 | 7 | 0 | 2.035307 | 1.378486 | 0.386851 |
| 11 | 6 | 0 | 3.249049 | 1.033628 | -0.101531 |
| 12 | 6 | 0 | 4.313215 | 1.949283 | -0.253261 |
| 13 | 6 | 0 | 4.054027 | 3.288156 | 0.119013 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | 2.801343 | 3.634368 | 0.591933 |
| 15 | 6 | 0 | 1.805309 | 2.645229 | 0.708183 |
| 16 | 6 | 0 | 5.564812 | 1.468867 | -0.770127 |
| 17 | 6 | 0 | 5.730845 | 0.157791 | -1.113010 |
| 18 | 6 | 0 | 4.658972 | -0.790226 | -0.978721 |
| 19 | 6 | 0 | 3.419299 | -0.343260 | -0.471065 |
| 20 | 7 | 0 | 2.340398 | -1.151459 | -0.317402 |
| 21 | 6 | 0 | 2.455579 | -2.437847 | -0.631147 |
| 22 | 6 | 0 | 3.648739 | -2.976688 | -1.148767 |
| 23 | 6 | 0 | 4.748548 | -2.157723 | -1.324118 |
| 24 | 1 | 0 | 0.797942 | 2.862310 | 1.048570 |
| 25 | 1 | 0 | 2.573281 | 4.656476 | 0.874935 |
| 26 | 1 | 0 | 4.838286 | 4.034772 | 0.025207 |
| 27 | 1 | 0 | 1.576483 | -3.046560 | -0.442494 |
| 28 | 1 | 0 | 3.690177 | -4.031341 | -1.399212 |
| 29 | 1 | 0 | 5.679451 | -2.553480 | -1.721724 |
| 30 | 1 | 0 | 6.384526 | 2.172941 | -0.883171 |
| 31 | 1 | 0 | 6.683910 | -0.190424 | -1.501395 |
| 32 | 1 | 0 | -2.607851 | 2.133442 | 1.631583 |
| 33 | 1 | 0 | -5.030453 | 1.787305 | 1.189304 |
| 34 | 6 | 0 | -6.155098 | 0.219124 | -0.721455 |
| 35 | 1 | 0 | -4.052836 | -0.993231 | -1.937789 |
| 36 | 1 | 0 | -1.637806 | -0.633507 | -1.501892 |
| 37 | 9 | 0 | -6.938189 | 0.406919 | 0.368672 |
| 38 | 9 | 0 | -6.589750 | 1.108347 | -1.655574 |
| 39 | 9 | 0 | -6.440086 | -1.011319 | -1.213441 |

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3. ***Table S1.*** Electronic Energies, Zero-Point Vibrational Energies, Thermal Corrections to Enthalpies and Gibbs Free Energies and Solvation Energies in Toluene.

| Complex | SP (a.u.) | ZPE (a.u.) | ΔH (a.u.) | ΔG (a.u.) | Gsol (kcal/mol) |
|---|---|---|---|---|---|
| PhBr | -2805.853714 | 0.090832 | 0.097468 | 0.059962 | -0.98 |
| PhOH | -307.558441 | 0.104812 | 0.11125 | 0.075845 | -2.43 |
| $Ph_2O$ | -538.653097 | 0.185647 | 0.196575 | 0.148291 | -0.9 |
| $Cs_2CO_3$ | -303.741772 | 0.015306 | 0.023545 | -0.022107 | -9.83 |
| $CsHCO_3$ | -284.438582 | 0.026995 | 0.033574 | -0.005203 | -7.56 |
| CsBr | -2594.112899 | 0.000315 | 0.004284 | -0.026242 | -7.55 |
| phen | -571.747801 | 0.170961 | 0.181059 | 0.1363 | -3.4 |
| *oxidative addition* | | | | | |
| **A** | -3343.354674 | 0.173268 | 0.187492 | 0.129347 | -3.83 |
| CPa | -6149.190652 | 0.265368 | 0.286697 | 0.213415 | -0.1 |
| TSa | -6149.183047 | 0.264484 | 0.285615 | 0.211479 | -0.23 |
| PDa | -6149.181123 | 0.265418 | 0.286948 | 0.212512 | 0.8 |
| **B** | -1076.110541 | 0.266723 | 0.285236 | 0.217949 | -3.43 |
| CPb | -3881.961068 | 0.358114 | 0.384481 | 0.295817 | 1.7 |
| TSb | -3881.939728 | 0.357531 | 0.383219 | 0.298824 | 1.25 |
| PDb | -3881.948034 | 0.359031 | 0.384897 | 0.300641 | 2.76 |
| TSrd | -3881.936094 | 0.358306 | 0.383658 | 0.30128 | 1.83 |
| PDrd | -3882.000485 | 0.359577 | 0.385783 | 0.297493 | 2.77 |
| **C** | -1340.765207 | 0.347203 | 0.369429 | 0.295893 | -13.5 |
| **D** | -811.395956 | 0.18727 | 0.201627 | 0.143447 | -21.7 |
| CPd | -3617.221226 | 0.277597 | 0.30012 | 0.220047 | -16.44 |
| TSd | -3617.214808 | 0.277338 | 0.29914 | 0.221704 | -16.59 |
| PDd | -3617.228831 | 0.278755 | 0.300619 | 0.223003 | -15.77 |
| **E** | -768.923874 | 0.173571 | 0.185251 | 0.136546 | -19.89 |
| CPe | -3574.811281 | 0.265521 | 0.284593 | 0.216816 | -15.92 |
| TSe | -3574.798473 | 0.265222 | 0.283736 | 0.218079 | -15.78 |
| PDe | -3574.800305 | 0.266276 | 0.285207 | 0.21825 | -16.93 |
| *Sigma-bond metathesis* | | | | | |
| $Ts_{met1}$ | -3881.919834 | 0.356861 | 0.382494 | 0.29768 | 2.9 |
| $Ts_{met2}$ | -3617.192035 | 0.276969 | 0.298646 | 0.222426 | -16.90 |
| *Single-electron transfer mechanism* | | | | | |
| $PhBr^{\bullet-}$ | -2805.867543 | 0.087071 | 0.09493 | 0.050833 | -30.12 |
| $(phen)Cu(II)(OPh)^{+}$ | -1075.906193 | 0.268468 | 0.286745 | 0.219359 | -16.87 |
| $Cu(II)(OPh)_2$ | -811.279652 | 0.188558 | 0.202897 | 0.143199 | 0.32 |
| CPb(triplet) | -3881.917691 | 0.357013 | 0.383149 | 0.296041 | 0.02 |
| CPd(triplet) | -3617.209507 | 0.277072 | 0.299813 | 0.217427 | -14.76 |

| | | | | | |
|---|---|---|---|---|---|
| *Halogen atom transfer mechanism* | | | | | |
| $Ph^{\bullet}$ | -231.622251 | 0.087625 | 0.092938 | 0.060236 | -0.92 |
| (phen)Cu(II)(OPh)(Br) | -3650.297662 | 0.268864 | 0.289203 | 0.216933 | -2.18 |
| $Cu(II)(OPh)_2(Br)^-$ | -3385.576998 | 0.188461 | 0.205083 | 0.139145 | -18.37 |
| *Substituent effect for (phen)Cu(OAr)* | | | | | |
| (phen)Cu(I)(O-Ph-*p*-Me) | -1115.437182 | 0.294281 | 0.314674 | 0.242613 | -2.81 |
| (phen)Cu(II)(O-Ph-*p*-Me)(Br) | -3689.624445 | 0.296347 | 0.318607 | 0.24118 | -2.12 |
| (phen)Cu(I)(O-Ph-*p*-OMe) | -1190.663666 | 0.299403 | 0.320542 | 0.246892 | -3.45 |
| (phen)Cu(II)(O-Ph-*p*-OMe)(Br) | -3764.852387 | 0.301511 | 0.324495 | 0.245848 | -2.6 |
| (phen)Cu(I)(O-Ph-*p*-F) | -1175.380076 | 0.258543 | 0.277915 | 0.208462 | -2.97 |
| (phen)Cu(II)(O-Ph-*p*-F)(Br) | -3749.566709 | 0.260656 | 0.281851 | 0.207315 | -2.27 |
| (phen)Cu(I)(O-Ph-*p*-CF3) | -1413.269349 | 0.271659 | 0.293816 | 0.217034 | -2.02 |
| (phen)Cu(II)(O-Ph-*p*-CF3)(Br) | -3987.452394 | 0.273814 | 0.297764 | 0.215804 | -1.63 |

Note: SP: Single point electronic energy; ZPE: Zero-point vibrational energy;
ΔH: Thermal correction to enthalpy; ΔG: Thermal correction to Gibbs free energy;
Gsol : Solvation energy in toluene.