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Supporting Information

Mercury Methylation by Cobalt Corrinoids: Relativistic Effects Dictate the Reaction Mechanism

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Supporting Information

Outline

Computational Methodologies

All nonrelativistic and relativistic results reported in this study were obtained from calculations performed using the Amsterdam density functional (ADF) program package.[1] Relativistic corrections were included using the spin-orbital relativistic zero-order regular approximation (SO-ZORA).[2] The geometries of the complexes studied were optimized using the BP86[3,4] functional together with Grimme's dispersion correction[5] (denoted as BP86-D3) and the all-electron ZORA-optimized TZ2P basis set.[6] Previous studies (see, for instance, refs [7-12]) showed that this triple-ξ double polarized basis set gives results close to the basis set limit. For all the closed-shell complexes the restricted DFT approach, whereas for all open-shell complexes the unrestricted DFT approach was used.

Geometry optimizations of the complexes used for the analysis of changes in Gibbs free energies of the reactions were followed by vibrational frequency analysis (analytically for the nonrelativistic calculations and numerically for the SO-ZORA calculations using BP86-D3/TZ2P) to verify that the optimized structures are minima and to obtain the thermal energy contributions to the free energies of the complexes. The thermodynamic energy contributions

from a few low frequencies, lower than 20 cm^{-1}, were also included in the final free energy analyses. In order to facilitate the convergence of the calculations, the augmented Roothaan-Hall direct inversion iterative subspace (ADIIS)[13] scheme was used. To mimic the biological reaction mechanisms, we used water as a solvent by employing the conductor-like screening model (COSMO)[14] as implemented in ADF.

Potential energy surface (PES) scans were performed using SO-ZORA/BP86-D3/TZ2P employing COSMO/H_2O to include SOC. The nonrelativistic PES scans were performed using BP86-D3/TZ2P employing COSMO/H_2O. The PES plots are run in unrestricted manner so that the bond breaking and forming processes remain realistic and geometry optimizations were performed at each scan step.

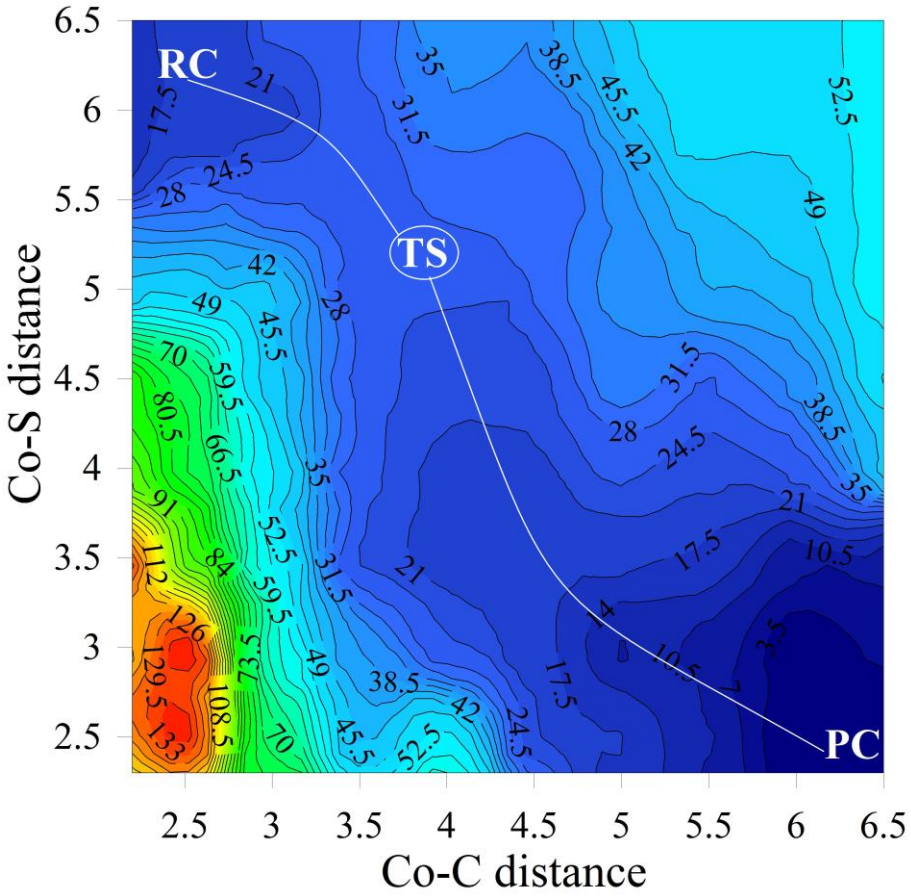

Figure S1. PESs corresponding to LERs employing the SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O) level of theory for B = Cys.

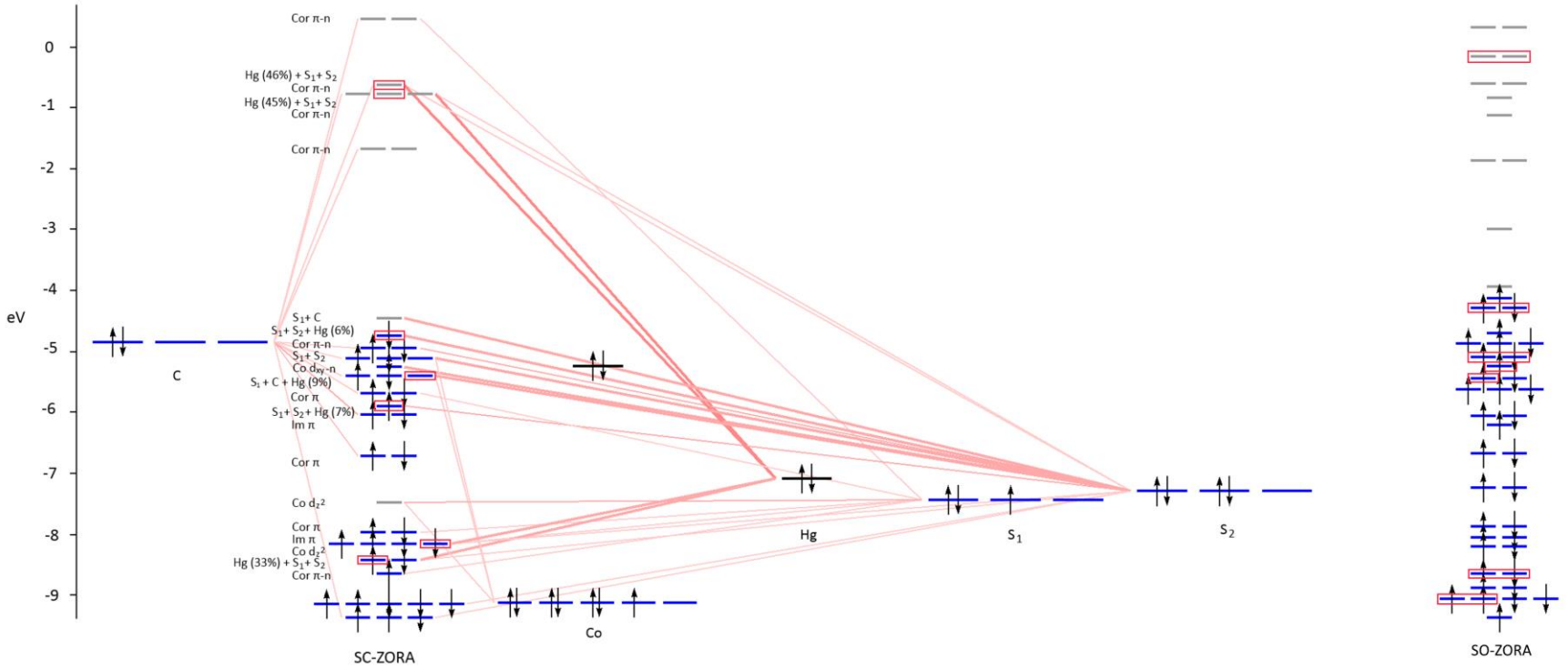

Figure S2. Frontier molecular orbitals for the transition state structure of the complex with an imidazole axial ligand; calculated with SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O). Orbitals with contributions from Hg are boxed in red.

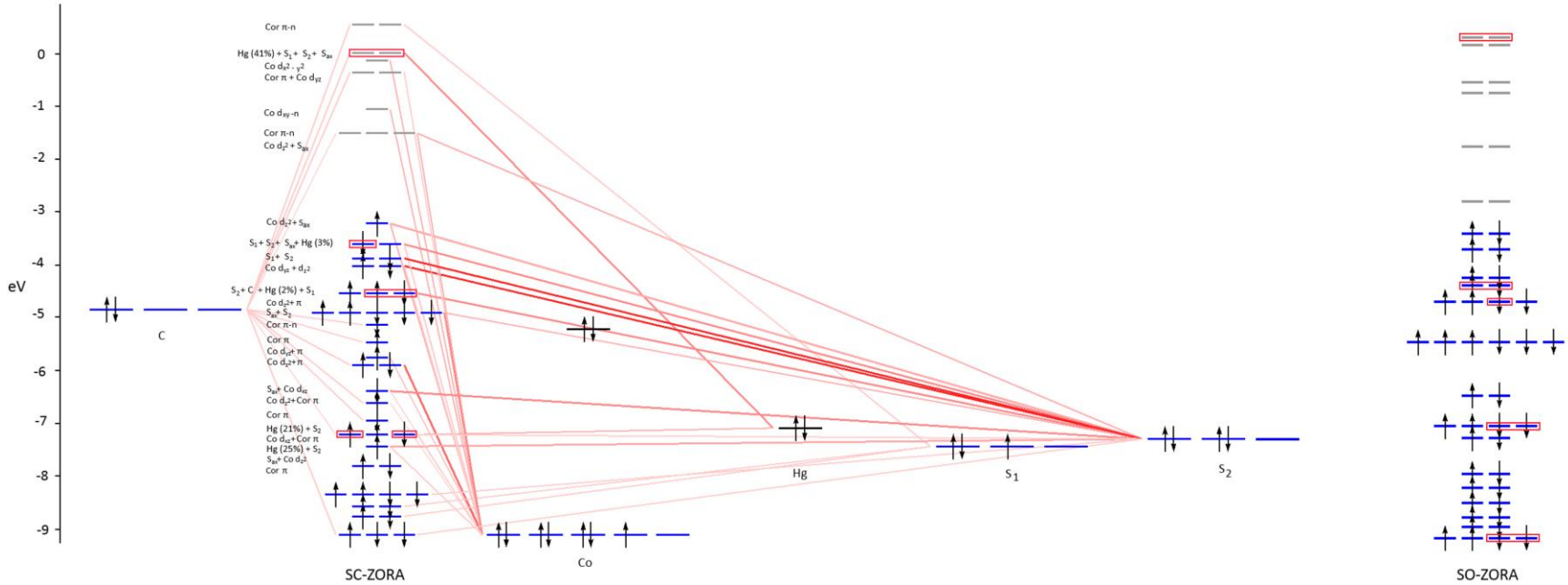

Figure S3. Frontier molecular orbitals for the transition state structure of the complex with a thiolate axial ligand; calculated with SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O). Orbitals with contributions from Hg are boxed in red.

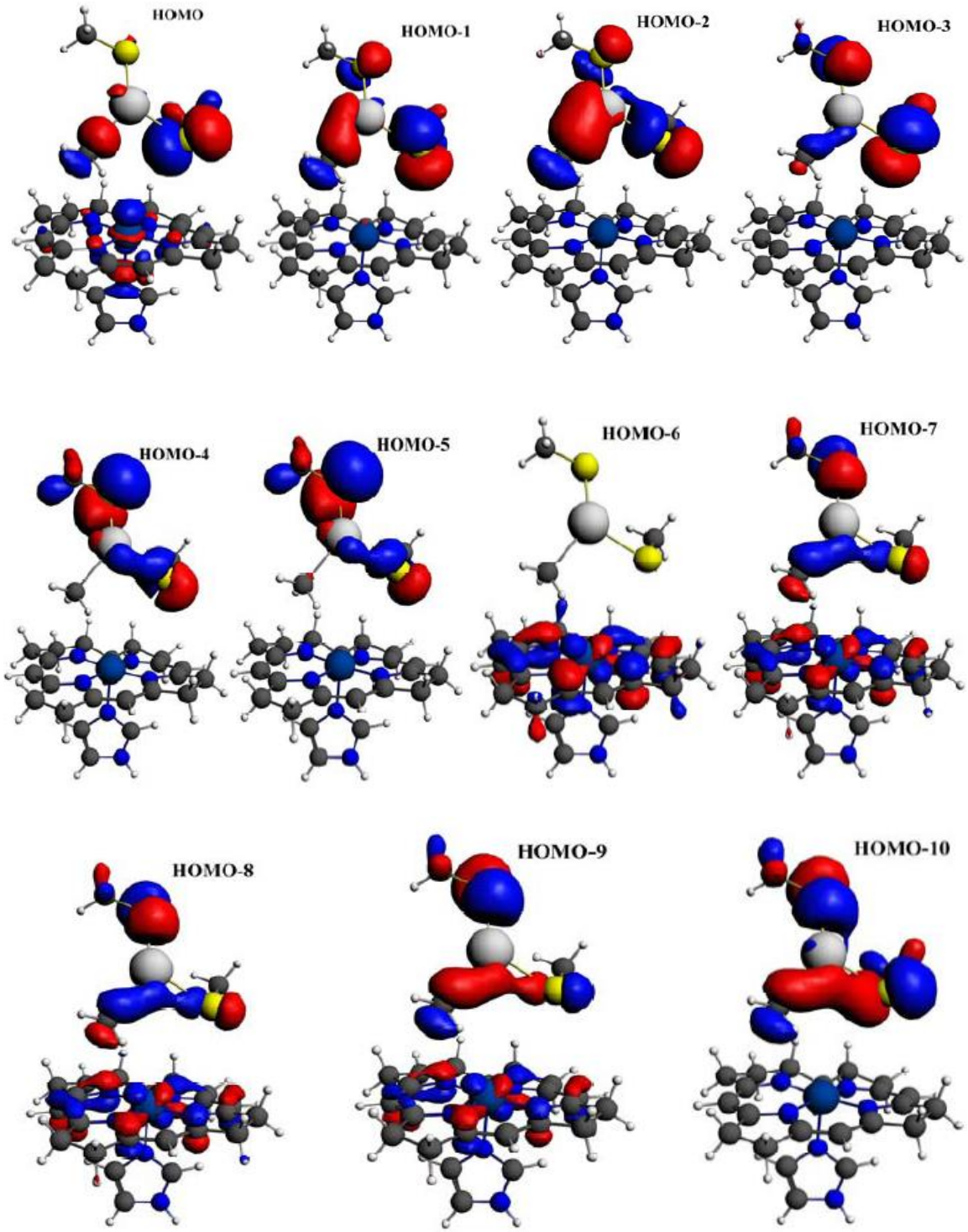

Figure S4. Frontier occupied molecular orbitals for the transition state structure of the complex with an imidazole axial ligand; calculated using SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O). Note that each orbital is occupied by a single electron.

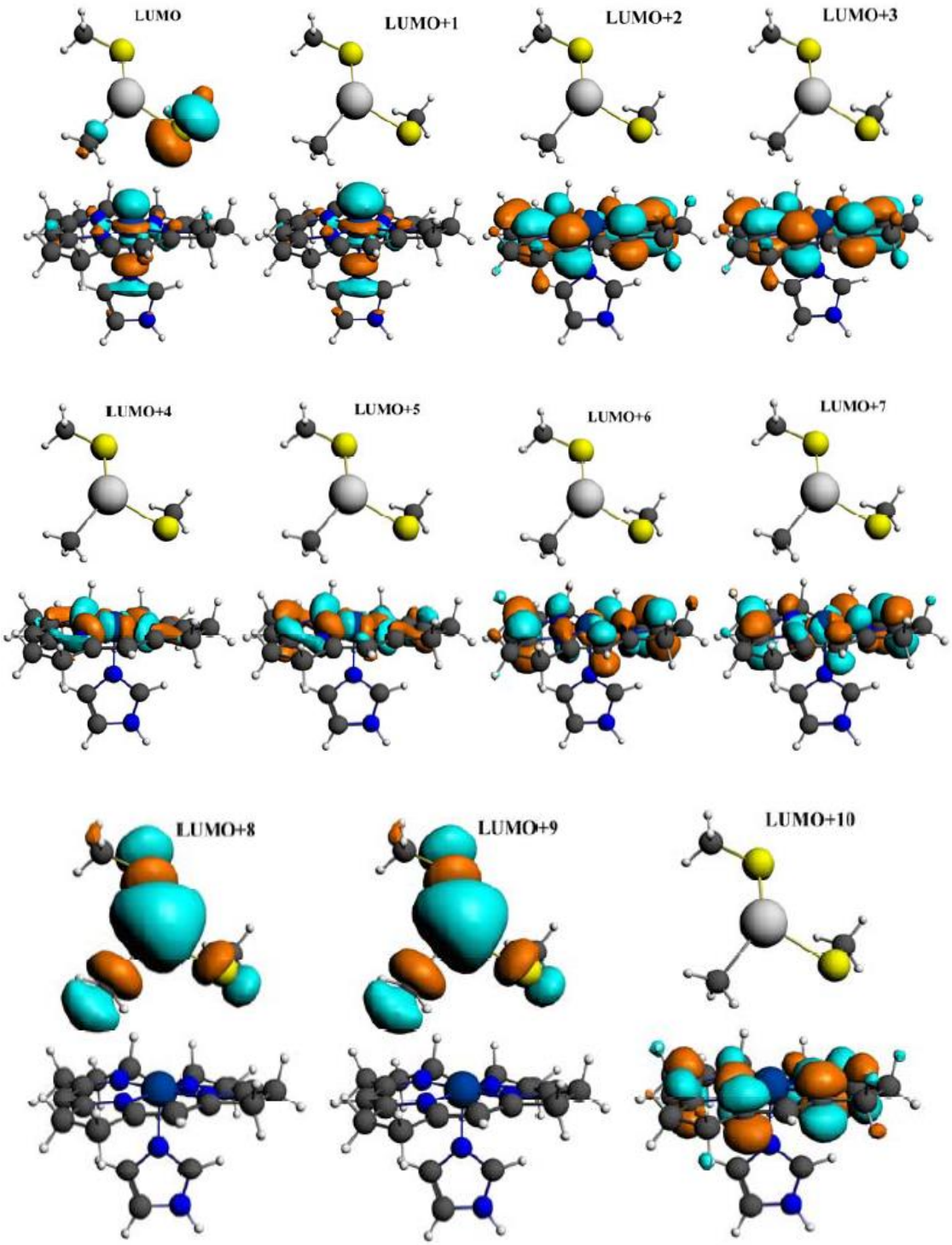

Figure S5. Frontier unoccupied molecular orbitals for the transition state structure of the complex with an imidazole axial ligand; calculated using SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O).

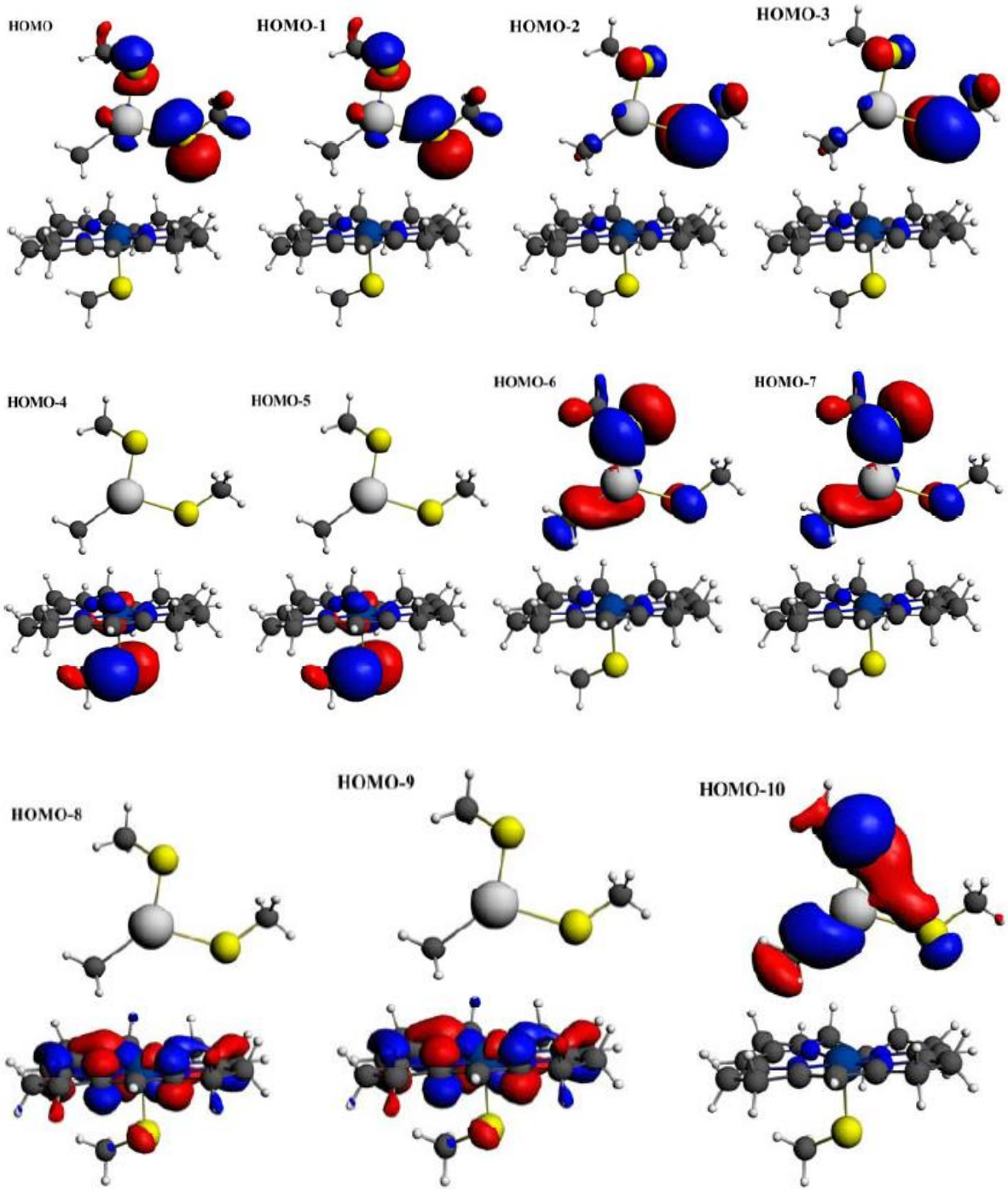

Figure S6. Frontier occupied molecular orbitals for the transition state structure of the complex with a thiolate axial ligand; calculated using SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O). Note that each orbital is occupied by a single electron.

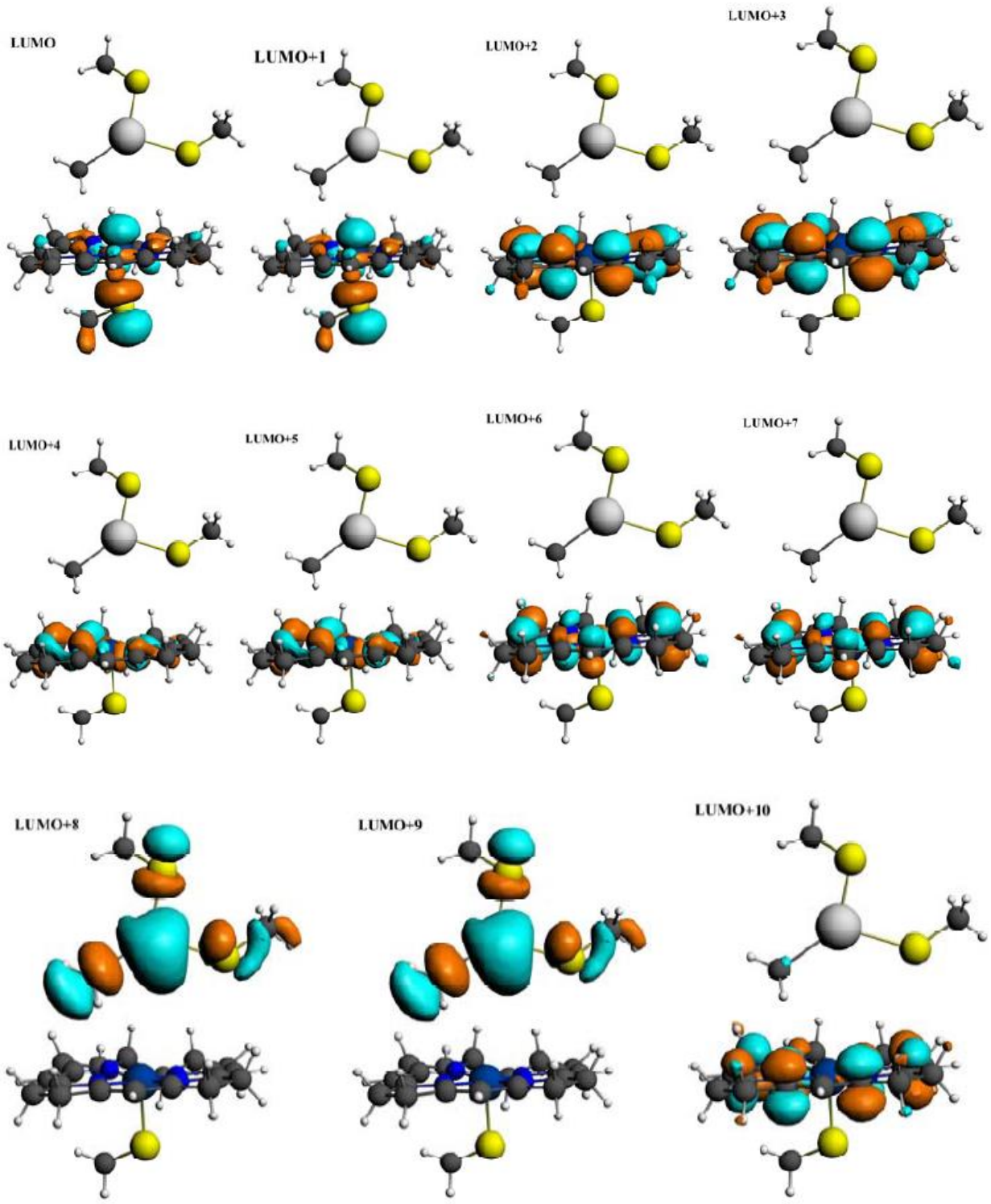

Figure S7. Frontier unoccupied molecular orbitals for the transition state structure of the complex with a thiolate axial ligand; calculated using SO-ZORA/BP86-D3/TZ2P (COSMO/H_2O).

References

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58
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N	0.483936000	0.292936000	-3.915854000
H	-2.065781000	1.061906000	-2.041653000
H	1.855609000	-0.447476000	-2.424936000
H	-1.336335000	1.127660000	-4.725246000
S	0.252672000	-0.214071000	2.457287000
C	-0.209089000	-1.924846000	2.900460000
H	0.489692000	-2.656759000	2.475472000
H	-1.228908000	-2.160942000	2.571459000
H	-0.166374000	-1.987117000	3.995737000
H	1.036605000	0.180011000	-4.757560000

```
54
6-Coordinated, Me and SMe, charge = 0, singlet, SO-ZORA/TZ2P/COSMO/H2O
optimized geometry.
Co      -0.028709000      0.130561000      0.145275000
N        1.812290000      0.426858000      0.217085000
N        0.220041000     -1.780140000      0.288224000
N       -1.942413000      0.023575000     -0.033750000
N       -0.082036000      1.994776000      0.143420000
C        2.271104000      1.804902000     -0.052825000
H        2.301099000      1.935616000     -1.148867000
C        3.677521000      1.846165000      0.555247000
H        4.345457000      2.543210000      0.039252000
H        3.612066000      2.143392000      1.611802000
C        4.132655000      0.372765000      0.448328000
H        4.661639000      0.176435000     -0.497811000
C        2.816232000     -0.373428000      0.451604000
C        2.646801000     -1.771345000      0.628337000
H        3.524396000     -2.377726000      0.842319000
C        1.430375000     -2.399749000      0.534255000
C        1.239334000     -3.887810000      0.732110000
H        1.880170000     -4.461773000      0.052991000
H        1.524955000     -4.167966000      1.754293000
C       -0.259788000     -4.096198000      0.475792000
H       -0.453015000     -4.674626000     -0.438245000
C       -0.780228000     -2.688936000      0.311165000
C       -2.132835000     -2.389016000      0.199184000
C       -2.664451000     -1.117122000      0.022270000
C       -4.143376000     -0.852344000     -0.124530000
H       -4.648797000     -1.046423000      0.832676000
H       -4.599810000     -1.516798000     -0.866818000
C       -4.191053000      0.632621000     -0.510534000
C       -2.773719000      1.101911000     -0.271842000
C       -2.388308000      2.418561000     -0.301280000
H       -3.146350000      3.174153000     -0.495970000
C       -1.054767000      2.840715000     -0.061079000
C       -0.571632000      4.271805000      0.035857000
H       -0.888039000      4.699979000      1.000286000
H       -0.990148000      4.906502000     -0.754004000
C        0.963685000      4.106948000     -0.039487000
H        1.509525000      4.867279000      0.528144000
C        1.169977000      2.689153000      0.503707000
H       -4.446587000      0.765562000     -1.570774000
H       -4.913265000      1.217045000      0.069613000
H        1.294061000      4.148728000     -1.087298000
H        4.793645000      0.051498000      1.261899000
H       -0.772991000     -4.614733000      1.294238000
H       -2.832631000     -3.221811000      0.233111000
H        1.247655000      2.687925000      1.605354000
C       -0.946580000     -1.177963000     -2.936846000
```

H	-1.984060000	-0.917136000	-2.685322000
S	0.214129000	0.114541000	-2.335174000
H	-0.864103000	-1.275976000	-4.027303000
C	-0.208757000	0.143787000	2.144880000
H	-0.910842000	-0.653380000	2.429529000
H	-0.595123000	1.117608000	2.478059000
H	0.778016000	-0.043355000	2.592717000

```
50
5-Coordinated, SMe, charge = 0, doublet, SO-ZORA/TZ2P/COSMO/H2O optimized
geometry.
Co       0.004078000      0.109757000     -0.048377000
N        1.824389000      0.417695000      0.128937000
N        0.241730000     -1.773609000      0.275282000
N       -1.905713000      0.001113000     -0.123055000
N       -0.077391000      1.962404000      0.094111000
C        2.282034000      1.810435000     -0.086272000
H        2.329938000      1.977020000     -1.175701000
C        3.674326000      1.848015000      0.553621000
H        4.346585000      2.562983000      0.068711000
H        3.583448000      2.119183000      1.614977000
C        4.145631000      0.382709000      0.424824000
H        4.694243000      0.213862000     -0.515235000
C        2.838760000     -0.375931000      0.381433000
C        2.676448000     -1.770390000      0.556161000
H        3.558164000     -2.374563000      0.761286000
C        1.456951000     -2.397075000      0.505081000
C        1.274473000     -3.885726000      0.696626000
H        1.721119000     -4.424220000     -0.150163000
H        1.780059000     -4.235128000      1.604018000
C       -0.250064000     -4.056188000      0.744761000
H       -0.627768000     -4.822511000      0.057388000
C       -0.761011000     -2.685323000      0.373779000
C       -2.107325000     -2.399935000      0.197610000
C       -2.636167000     -1.138659000     -0.043257000
C       -4.113242000     -0.875570000     -0.200752000
H       -4.620340000     -1.030844000      0.762655000
H       -4.570442000     -1.563479000     -0.921171000
C       -4.155780000      0.594944000     -0.638191000
C       -2.746232000      1.073872000     -0.382524000
C       -2.369302000      2.391954000     -0.400196000
H       -3.129526000      3.144681000     -0.600047000
C       -1.051600000      2.817706000     -0.105976000
C       -0.584479000      4.246311000      0.059148000
H       -0.908513000      4.629975000      1.039467000
H       -1.003235000      4.909661000     -0.706807000
C        0.951818000      4.097918000     -0.014903000
H        1.489136000      4.843422000      0.580215000
C        1.167290000      2.665780000      0.485174000
H       -4.382759000      0.687701000     -1.709524000
H       -4.893493000      1.196062000     -0.095776000
H        1.285583000      4.175805000     -1.059257000
H        4.793201000      0.052164000      1.245378000
H       -0.604731000     -4.323959000      1.750031000
H       -2.809214000     -3.228388000      0.281471000
H        1.237858000      2.636897000      1.586311000
C       -1.274634000     -0.789981000     -3.134664000
```

H	-2.155641000	-0.149293000	-2.996518000
S	0.247417000	0.045656000	-2.527352000
H	-1.170949000	-1.020480000	-4.203523000
H	-1.439483000	-1.724587000	-2.583411000

```
50
5-Coordinated, SMe, charge = 1, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized
geometry.
Co      -0.012337000      0.121578000     -0.044984000
N        1.809482000      0.425116000      0.138936000
N        0.221310000     -1.753482000      0.249098000
N       -1.921064000      0.029804000     -0.099179000
N       -0.083580000      1.977344000      0.094369000
C        2.273602000      1.811034000     -0.111880000
H        2.311351000      1.948262000     -1.207289000
C        3.675774000      1.839291000      0.501017000
H        4.340574000      2.551443000      0.003710000
H        3.607894000      2.105861000      1.564794000
C        4.133920000      0.371998000      0.351193000
H        4.649668000      0.202270000     -0.606928000
C        2.825988000     -0.381208000      0.337143000
C        2.661285000     -1.775023000      0.489336000
H        3.542025000     -2.387123000      0.667275000
C        1.439143000     -2.391919000      0.450100000
C        1.243284000     -3.870201000      0.674861000
H        1.864480000     -4.455173000     -0.012157000
H        1.556095000     -4.132271000      1.693593000
C       -0.260543000     -4.074344000      0.460274000
H       -0.482516000     -4.669935000     -0.435330000
C       -0.778688000     -2.674197000      0.274254000
C       -2.125451000     -2.379894000      0.132321000
C       -2.654987000     -1.111256000     -0.042737000
C       -4.128539000     -0.843033000     -0.185959000
H       -4.625156000     -1.019351000      0.778490000
H       -4.588140000     -1.521658000     -0.912468000
C       -4.174086000      0.633421000     -0.596852000
C       -2.761559000      1.104904000     -0.363082000
C       -2.374227000      2.417581000     -0.403618000
H       -3.126303000      3.173363000     -0.615960000
C       -1.052684000      2.833783000     -0.127476000
C       -0.572694000      4.259786000     -0.003528000
H       -0.892323000      4.665342000      0.968822000
H       -0.997501000      4.903601000     -0.781513000
C        0.961148000      4.101980000     -0.083883000
H        1.504343000      4.859718000      0.488471000
C        1.175280000      2.684565000      0.452973000
H       -4.423454000      0.750224000     -1.660506000
H       -4.895757000      1.229185000     -0.029124000
H        1.289001000      4.151337000     -1.131705000
H        4.803335000      0.028155000      1.147225000
H       -0.759914000     -4.567939000      1.301973000
H       -2.824266000     -3.212944000      0.162024000
H        1.250416000      2.679319000      1.553329000
```

C	-0.918210000	-1.177694000	-2.911661000
H	-1.973459000	-0.909675000	-2.780950000
S	0.200580000	0.098454000	-2.253004000
H	-0.691732000	-1.227676000	-3.985947000
H	-0.722022000	-2.160382000	-2.466341000
H	-0.715871000	-2.147474000	-2.475040000

```
55
6-Coordinated, 2SMe, charge = 0, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized
geometry.
Co      -0.008725000      0.057650000     -0.107824000
N       -1.868680000     -0.148794000     -0.169718000
N        0.266079000     -1.840335000     -0.357286000
N        1.866999000      0.464564000      0.090139000
N       -0.459801000      1.868614000      0.003823000
C       -2.674860000      1.041050000      0.166492000
H       -2.736485000      1.099552000      1.267789000
C       -4.042610000      0.730493000     -0.449923000
H       -4.870696000      1.203540000      0.087122000
H       -4.059540000      1.074421000     -1.493856000
C       -4.086933000     -0.814520000     -0.402225000
H       -4.534435000     -1.181562000      0.534980000
C       -2.619203000     -1.181306000     -0.432887000
C       -2.080385000     -2.472299000     -0.674167000
H       -2.765289000     -3.283362000     -0.911404000
C       -0.737870000     -2.751626000     -0.622800000
C       -0.152162000     -4.117348000     -0.903720000
H       -0.601448000     -4.879723000     -0.257459000
H       -0.369175000     -4.407120000     -1.940126000
C        1.351931000     -3.922717000     -0.662345000
H        1.710802000     -4.471318000      0.219355000
C        1.475180000     -2.437818000     -0.424787000
C        2.696784000     -1.790161000     -0.282662000
C        2.866827000     -0.436116000     -0.020374000
C        4.217227000      0.205410000      0.184228000
H        4.757066000      0.236147000     -0.773017000
H        4.835244000     -0.370869000      0.881575000
C        3.859424000      1.610613000      0.688815000
C        2.370416000      1.700940000      0.446012000
C        1.640083000      2.854805000      0.572303000
H        2.159885000      3.767358000      0.854825000
C        0.246854000      2.920549000      0.313860000
C       -0.601376000      4.172533000      0.303873000
H       -0.395937000      4.741522000     -0.616664000
H       -0.376934000      4.832051000      1.150189000
C       -2.037575000      3.601164000      0.316547000
H       -2.757349000      4.229096000     -0.217610000
C       -1.854714000      2.221389000     -0.325791000
H        4.059852000      1.715349000      1.764059000
H        4.401616000      2.414595000      0.180181000
H       -2.382495000      3.479834000      1.353316000
H       -4.644871000     -1.269175000     -1.228971000
H        1.974313000     -4.239046000     -1.507655000
H        3.594910000     -2.400982000     -0.350213000
H       -1.935655000      2.265729000     -1.425861000
C        1.182394000     -1.172930000      2.823891000
```

H	2.146655000	-0.678831000	2.645037000
S	-0.213720000	-0.146001000	2.232179000
H	1.055970000	-1.320726000	3.904557000
S	0.110626000	0.195701000	-2.449003000
C	0.784606000	1.849368000	-2.855398000
H	1.717564000	2.031713000	-2.306568000
H	0.069726000	2.649569000	-2.619453000
H	0.995266000	1.873933000	-3.932710000
H	1.187693000	-2.153270000	2.329936000

```
11
Hg(SMe)2, charge = 0, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
Hg      -0.000719000     -0.000064000     -0.256808000
S        0.418467000      2.311342000     -0.287094000
C       -0.839186000      2.938017000      0.912467000
H       -0.702294000      4.024734000      0.947848000
H       -0.671758000      2.515731000      1.907581000
H       -1.851980000      2.708174000      0.568935000
S       -0.415169000     -2.312397000     -0.288692000
C        0.841851000     -2.935057000      0.913718000
H        0.707111000     -4.021981000      0.949951000
H        0.671949000     -2.512051000      1.908096000
H        1.854736000     -2.703530000      0.571488000
```

```
15
MeHg(SMe)2, charge = -1, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
C       -0.195327000      2.701839000     -0.032124000
H        0.653474000      3.388213000     -0.140532000
H       -0.906967000      2.864304000     -0.852009000
H       -0.699213000      2.883707000      0.925986000
Hg       0.452355000      0.664945000     -0.082994000
S        1.854294000     -1.280849000     -0.406102000
C        1.068184000     -2.619259000      0.592773000
H        1.086157000     -3.548531000      0.012155000
H        0.030741000     -2.338623000      0.821208000
H        1.623001000     -2.763102000      1.526886000
S       -2.041695000     -0.677945000      0.511959000
C       -1.969639000     -1.544646000     -1.122438000
H       -2.803418000     -2.250932000     -1.222876000
H       -1.024773000     -2.096263000     -1.219191000
H       -2.024086000     -0.820492000     -1.945614000
```

15
MeHg(SMe)2, charge = 0, doublet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
C -0.273790000 2.599044000 0.327042000
H 0.575555000 3.281891000 0.448139000
H -0.903285000 2.915118000 -0.512926000
H -0.868334000 2.558868000 1.247338000
Hg 0.474813000 0.651655000 -0.079337000
S 1.667251000 -1.350196000 -0.573337000
C 1.311621000 -2.345564000 0.931455000
H 1.706660000 -3.351901000 0.757054000
H 0.227640000 -2.391342000 1.095303000
H 1.794624000 -1.904148000 1.809175000
S -2.034645000 -0.508252000 0.276312000
C -2.059714000 -1.742403000 -1.056670000
H -3.019971000 -2.272520000 -0.980942000
H -1.229064000 -2.449960000 -0.965664000
H -2.024522000 -1.245317000 -2.033590000

10
MeHgSMe, charge = 0, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
C -2.398031000 0.410501000 0.009015000
H -2.909676000 -0.246414000 -0.752745000
H -2.807100000 0.208290000 1.040916000
H -2.530604000 1.498553000 -0.259582000
Hg -0.336491000 -0.031277000 -0.000951000
S 1.982718000 -0.562339000 -0.011792000
C 2.738727000 1.126331000 0.026939000
H 3.824798000 0.982757000 0.028577000
H 2.442177000 1.663853000 0.933086000
H 2.450192000 1.701698000 -0.858836000

4
Me anion, charge = -1, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
C 1.140038000 0.174201000 -0.008160000
H 0.116655000 0.165290000 0.420343000
H 1.659760000 -0.707487000 0.420519000
H 1.644269000 1.064822000 0.420521000

4
Me radical, charge = 0, doublet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
C 1.140074000 0.174201000 0.079611000
H 0.053035000 0.164724000 0.072810000
H 1.691833000 -0.762422000 0.071319000
H 1.675392000 1.120328000 0.072175000

5
SMe anion, charge = -1, singlet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
S 1.979267000 -0.566436000 -0.011902000
C 2.747268000 1.128409000 0.027028000
H 3.843477000 1.061641000 0.030296000
H 2.436843000 1.677506000 0.926099000
H 2.444640000 1.714392000 -0.851159000

5
SMe radical, charge = 0, doublet, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
S 1.987873000 -0.544025000 -0.014631000
C 2.740652000 1.094063000 0.047453000
H 3.834929000 1.030732000 0.024149000
H 2.412884000 1.609146000 0.961342000
H 2.387098000 1.676998000 -0.815784000

69
Transition state structure for the complex with imidazole axial ligand, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
Co 4.745357116 11.030358680 -4.928582846
N 6.279557116 12.209158680 -5.075182846
C 7.583257116 11.780058680 -5.239982846
C 8.502157116 12.959358680 -5.450382846
C 7.543957116 14.157958680 -5.534482846
C 6.199057116 13.548358680 -5.225682846
C 8.004457116 10.471058680 -5.247482846
C 7.137757116 9.368358680 -5.055182846
N 5.851157116 9.507158680 -4.839982846
C 5.174357116 8.191058680 -4.707782846
C 6.193957116 7.193658680 -5.275882846
C 7.544457116 7.912658680 -5.069382846
C 3.854557116 8.376758680 -5.442082846
N 3.388957116 9.732058680 -5.085182846
C 2.087457116 9.829658680 -5.188682846
C 1.468757116 8.475658680 -5.472782846
C 2.630757116 7.502358680 -5.159782846
C 5.028257116 14.286958680 -5.082382846
C 3.751957116 13.763858680 -4.907382846
N 3.447857116 12.445258680 -4.919682846
C 2.079557116 12.258158680 -4.846082846
C 1.400857116 13.570558680 -4.549382846
C 2.510657116 14.611058680 -4.770582846
C 1.415557116 11.068658680 -5.051882846
H 4.980657116 8.012858680 -3.635182846
H 4.077357116 8.382158680 -6.527482846
H 5.114957116 15.371258680 -5.141682846
H 0.327557116 11.075558680 -5.022582846
H 9.064257116 10.274658680 -5.403082846
H 2.609657116 7.215858680 -4.098082846
H 2.602057116 6.589958680 -5.766982846
H 7.526957116 14.603058680 -6.540682846
H 0.561957116 8.288258680 -4.883782846
H 1.077757116 13.552858680 -3.496882846
H 1.182257116 8.423558680 -6.537182846
H 2.604957116 15.327458680 -3.944482846
H 6.011257116 7.056458680 -6.353082846
H 6.150557116 6.210858680 -4.792682846
H 8.004257116 7.653458680 -4.101182846
H 8.282957116 7.690658680 -5.850782846
H 0.510657116 13.732958680 -5.168482846
H 9.198357116 13.043958680 -4.603382846
H 2.356757116 15.191758680 -5.692982846
H 9.111157116 12.830458680 -6.354882846
H 7.794357116 14.960058680 -4.827282846
C 5.336757116 10.866158680 -9.130882846

C	5.772757116	10.713758680	-7.840082846
N	4.752357116	11.047858680	-6.968482846
C	3.709857116	11.396658680	-7.718482846
N	4.031357116	11.294758680	-9.031582846
H	6.747057116	10.395958680	-7.492682846
H	2.738557116	11.710958680	-7.360082846
H	5.824857116	10.710658680	-10.083682846
C	6.699761757	11.529684184	-1.238593570
H	6.322561757	12.359184184	-1.845693570
H	6.725061757	10.608084184	-1.837893570
H	7.722761757	11.773484184	-0.917793570
Hg	4.984988152	10.807694735	0.554759666
S	2.601894452	11.095335476	-0.842123889
C	1.827294452	9.503035476	-0.400523889
H	1.209794452	9.645035476	0.495476111
H	2.569594452	8.723935476	-0.185823889
H	1.176794452	9.166335476	-1.219223889
S	4.821735158	9.239720735	2.420436225
C	6.504635158	9.342520735	3.157336225
H	6.476635158	8.688520735	4.038336225
H	6.742635158	10.357820735	3.489036225
H	7.273935158	8.974120735	2.470236225
H	3.414357116	11.516358680	-9.807982846

65
Transition state structure for the complex with thiolate axial ligand, SO-ZORA/TZ2P/COSMO/H2O optimized geometry.
Co 8.316376184 11.103091387 -5.120998148
N 9.977339730 11.912936743 -4.563428398
N 8.875618448 9.438723223 -4.456081004
N 6.753188273 10.141014281 -5.511088680
N 7.421281098 12.778319169 -5.472435194
C 11.132941721 11.217850637 -4.150152624
C 12.312121257 12.169634013 -3.976031588
C 11.703717422 13.569090252 -4.252947428
C 10.266356713 13.263053975 -4.651803563
C 11.199995433 9.850995429 -3.919538117
C 10.068088095 8.992272363 -4.045159215
C 7.845803373 8.329888434 -4.384708206
C 8.699008691 7.036800407 -4.401995356
C 10.032092197 7.498364471 -3.729397860
C 6.878324056 8.636346304 -5.528316090
C 5.525810979 10.519392685 -5.874977681
C 4.607948843 9.319775558 -6.093956579
C 5.410261598 8.143573999 -5.448167934
C 9.353910363 14.250568627 -5.043650233
C 8.020092024 14.022127937 -5.412141802
C 6.071371399 12.929370487 -5.864568003
C 5.719200773 14.403227610 -6.044127182
C 7.058898997 15.141696427 -5.788953266
C 5.171174091 11.892436679 -6.046276370
C 8.594650930 11.200021388 -1.021069993
C 2.363553231 12.733909694 -1.593756789
C 5.970153497 11.768752510 2.868361484
C 10.359068671 9.682442292 -7.507464292
H 7.305294918 8.421724232 -3.414338780
H 7.346234257 8.357977676 -6.495640678
H 9.707269271 15.286121678 -5.053766017
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H 12.153821131 9.421148065 -3.601486620
H 5.112876587 8.016121037 -4.389729872
H 5.259849131 7.189518901 -5.978362982
H 12.225137007 14.111965628 -5.060539196
H 3.613518393 9.472922681 -5.641067703
H 4.936319231 14.700672662 -5.324111353
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H 8.887358966 6.710135281 -5.441917813
H 8.215729642 6.209518053 -3.858205725
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H 10.924592111 6.977973894 -4.116545863
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H 12.739538390 12.083404728 -2.962386144

H	7.424651810	15.673153196	-6.686154204
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H	11.724807928	14.220359175	-3.360471079
H	8.895277855	11.772396075	-1.918207730
H	8.362082851	10.153321038	-1.290495427
H	9.377051423	11.245281656	-0.241916895
H	2.144360266	13.671510086	-1.054279673
H	2.076987618	11.880218294	-0.955462858
H	1.757642610	12.705596414	-2.517194684
H	5.518002406	11.992960196	3.850269809
H	7.067064271	11.848844582	2.951281450
H	5.700648523	10.740500339	2.575220926
H	11.136883963	9.829676000	-6.741653490
H	9.943713686	8.665014357	-7.446030525
H	10.806922351	9.839049180	-8.505756132
Hg	6.344424703	12.211360243	-0.371950860
S	4.181019932	12.645603074	-2.034126085
S	5.288826658	13.005466409	1.634196835
S	9.006091689	10.990441222	-7.33099493