Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


**Supplementary Information**

# How does multi-reference computation change the catalysis chemistry? DFT and CASPT2 studies of the Cu-catalysed coupling reactions between aryl iodides and β-diketones

Nan He[1], Naoki Nakatani[1], Masahiko Hada[1]

[1]*Department of Chemistry, Faculty of Science, Tokyo Metropolitan University, 1-1 Minami-Osawa, Hachioji, Tokyo, 192-0397, Japan*

E-mail: naokin@tmu.ac.jp

## Contents

## 1. *ω*-B97XD calculated energy profiles.

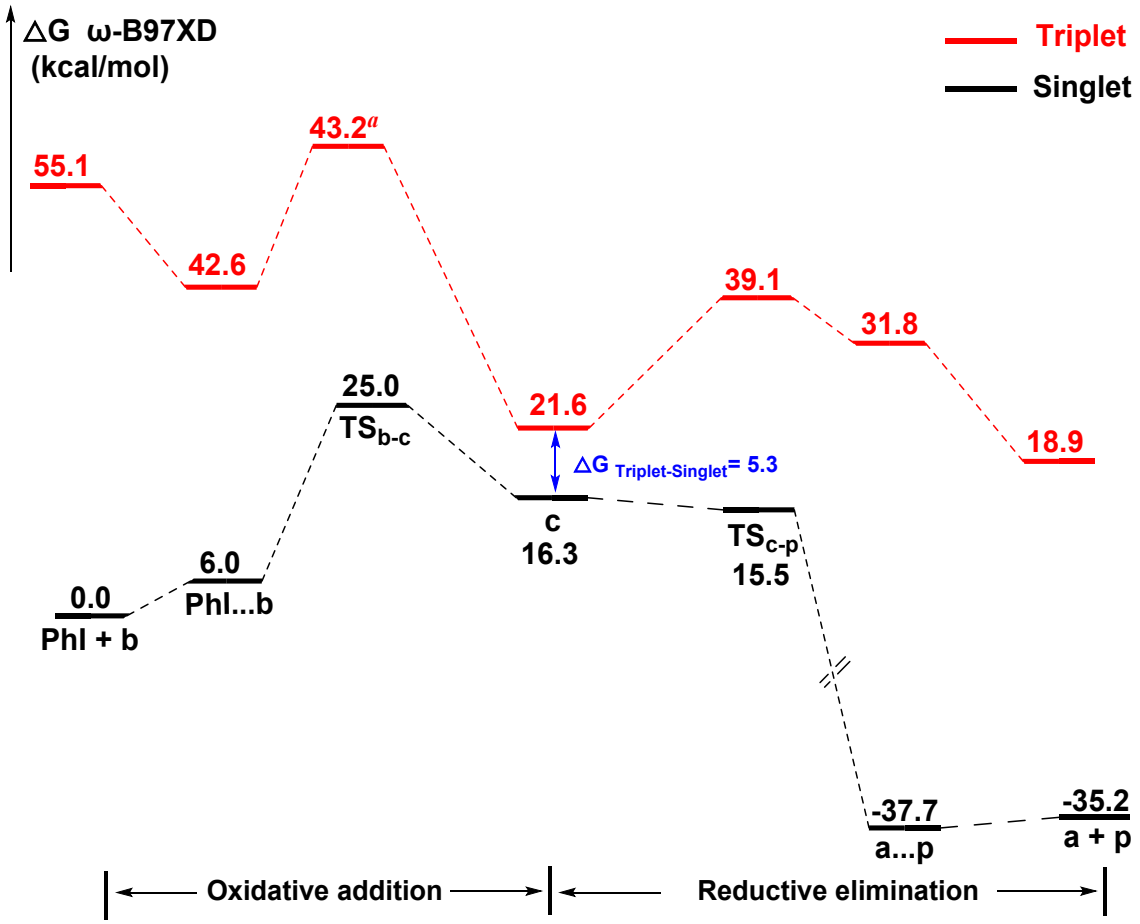


**Figure S1.** Gibbs free energy profiles of the OA-RE pathway in the singlet and the triple spin states. [a] We took the geometry of **TS$_{b-c}$** in the singlet spin state to evaluate the single-point energy in the triplet spin state, because **TS$_{b-c}$** in the triplet spin state could not be located.

**Table S1.** The DFT-calculated $\Delta E_{S-T}$ of complex **c** for several functionals. The CASPT2-calculated $\Delta E_{S-T}$ was also shown.

| Functional | $\Delta E_{S-T}$ (kacl/mol) |
|---|---|
| B3LYP-D3 | 15.1 |
| B3LYP*//B3LYP-D3 | 17.6 |
| *ω*-B97XD | 11.8 |
| PBE0 | 14.1 |
| TPSS | 19.6 |
| TPSSh | 17.7 |
| M06-L | 17.7 |
| MN15 | 14.1 |
| CASPT2//*ω*-B97XD | 36.2 |

The $\omega$-B97XD calculated Gibbs free energy profiles of the OA-RE pathway were shown in Figure S1. It is obvious that the triplet spin state is always higher in energy than the singlet spin state along the reaction coordinate. The smallest spin-energy gap ($\Delta E_{S\text{-}T}$) between these two spin states was found in the intermediate **c** (11.8 kcal/mol in electronic energy, and 5.3 kcal/mol in Gibbs free energy). We also examined several functionals to evaluate the $\Delta E_{S\text{-}T}$ and concluded that the intersystem crossing (ISC) never occurs in this reaction, as summarized in Table S1.

In the CASPT2 calculation, moreover, the $\Delta E_{S\text{-}T}$ was estimated to be 36.2 kcal/mol in electronic energy, which was much larger than that calculated by DFT method. Therefore, contribution of the triplet spin state was safely excluded from this catalytic reaction along the OA-RE pathway.

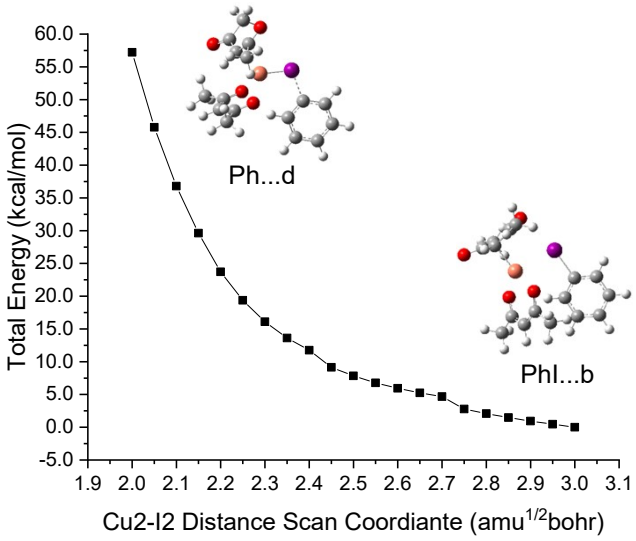


**Figure S2.** Scanned PEC for the Cu2-I2 stretching in the IAT pathway.

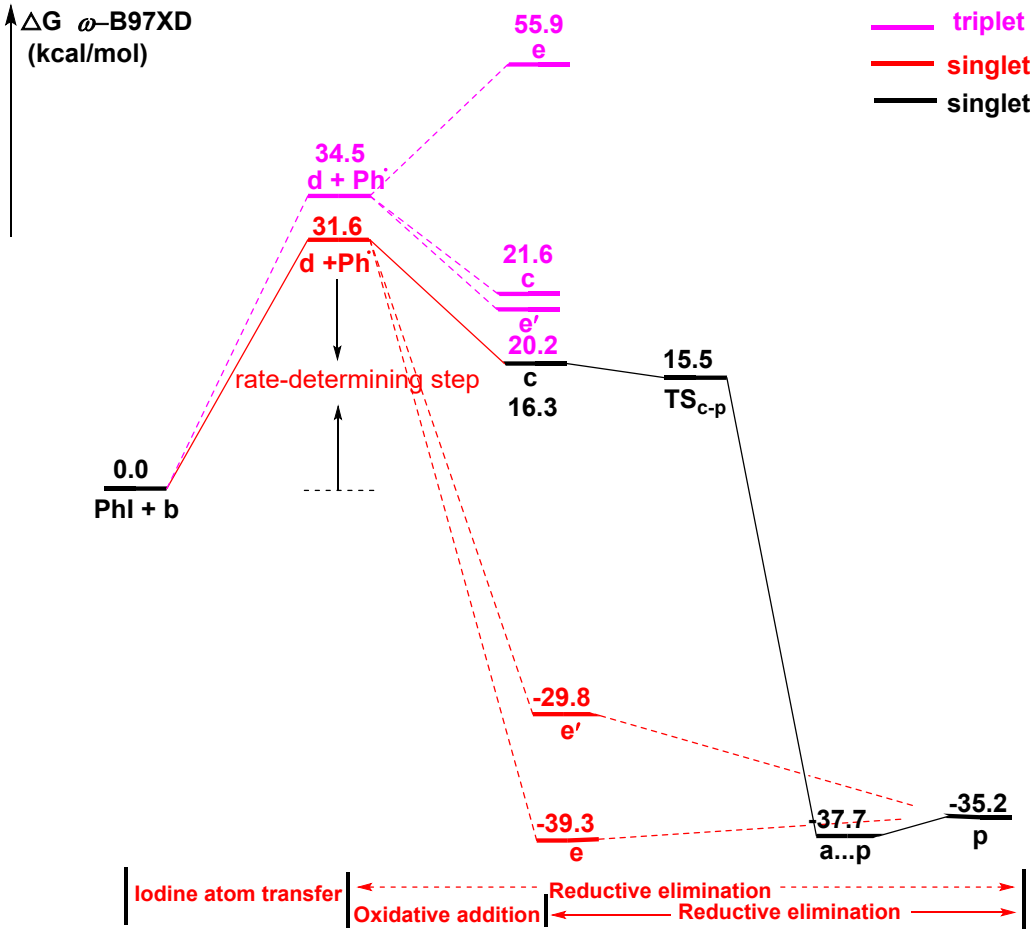


**Figure S3.** Gibbs free energy profiles for the IAT pathway in the singlet and the triplet spin states.

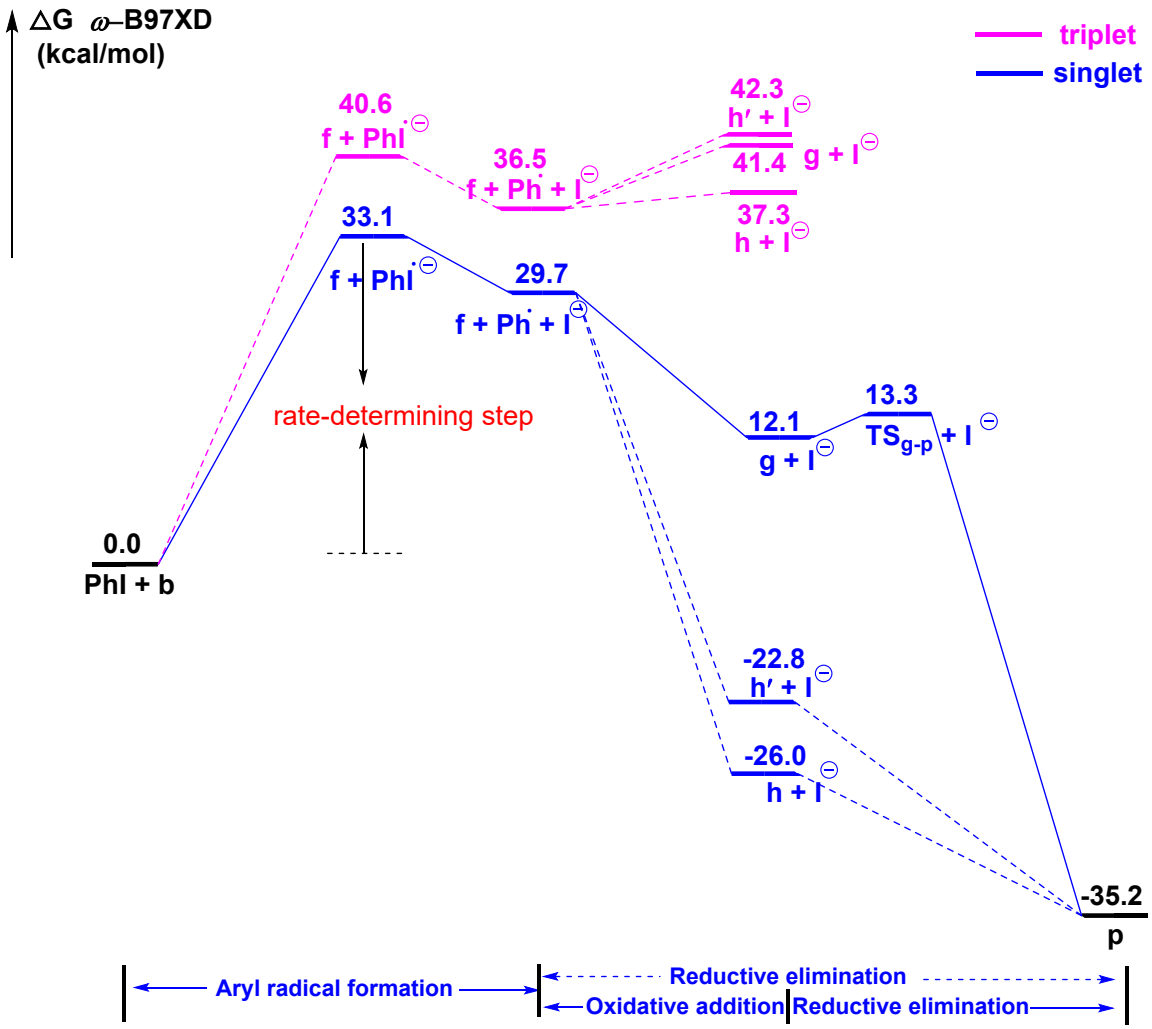


**Figure S4.** Gibbs free energy profiles for the SET pathway in the singlet and the triplet spin states.

The energies of precursory complexes **d**+Ph (IAT pathway) and **f**+PhI$^{-}$ (SET pathway) in the triplet spin state were computed to be 34.5 kcal/mol and 40.6 kcal/mol higher than the energy of a reactant **d**+Ph in the singlet spin state, respectively. Since **d**+Ph or **f**+PhI$^{-}$ consists of a pair of the doublet spin states, the singlet and the triplet spin states are degenerated. Thus, we also computed the triplet energies of intermediates **e**, **e'**, **h**, **h'** and **g**. Consequently, we found that these intermediates in the IAT and the SET pathways were less stable than those in the singlet spin state so that the catalytic reaction would occur neither by the IAT pathway nor by the SET pathway.

## 2. Active spaces for CASSCF/CASPT2 calculation.

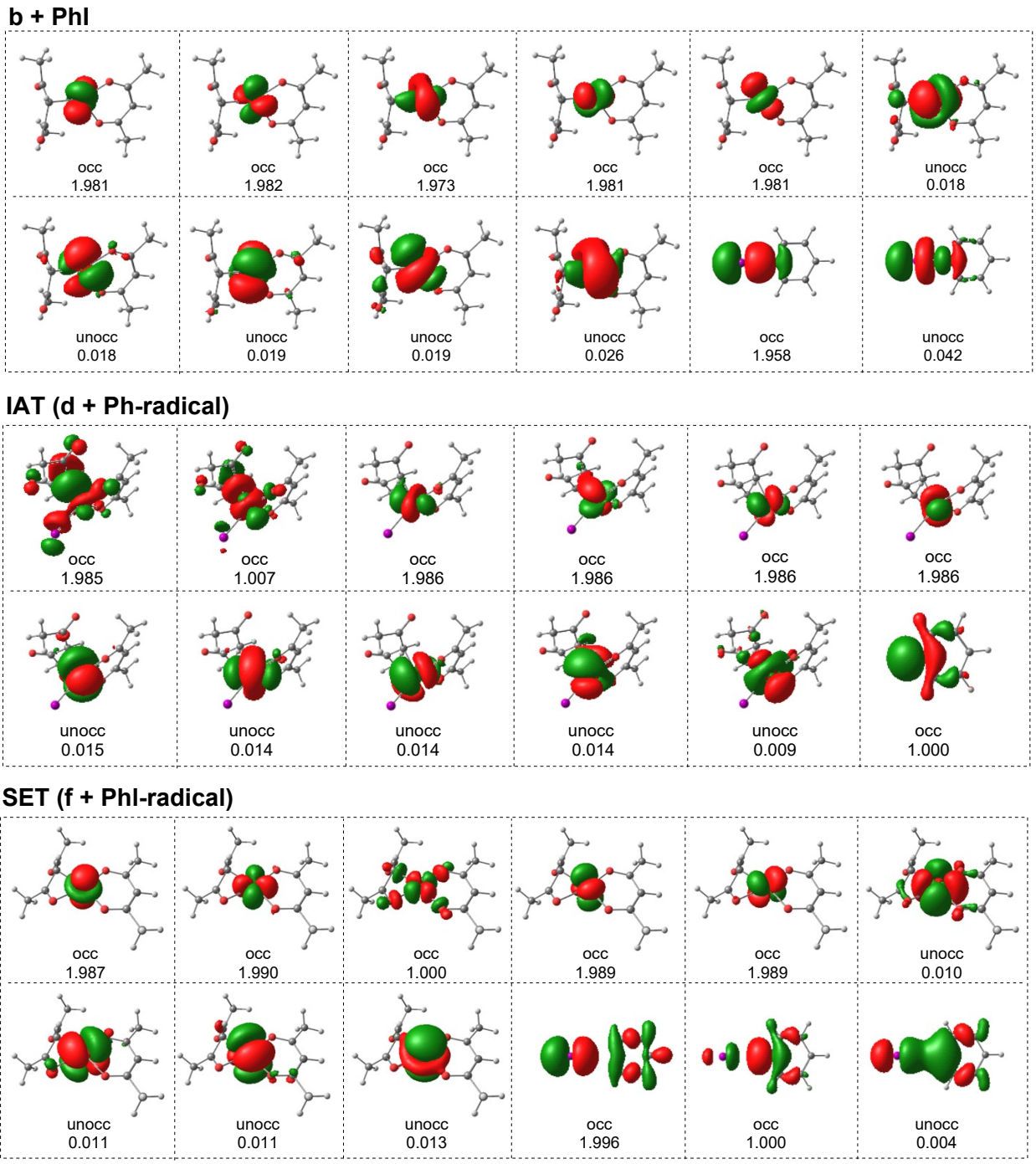


**Figure S5**. The active orbitals considered in the CASSCF/CASPT2 singlet-point calculations. Natural orbital occupation numbers of complexes **b + PhI**, **d** + Ph-radical, and **f** + PhI-radical were also shown.

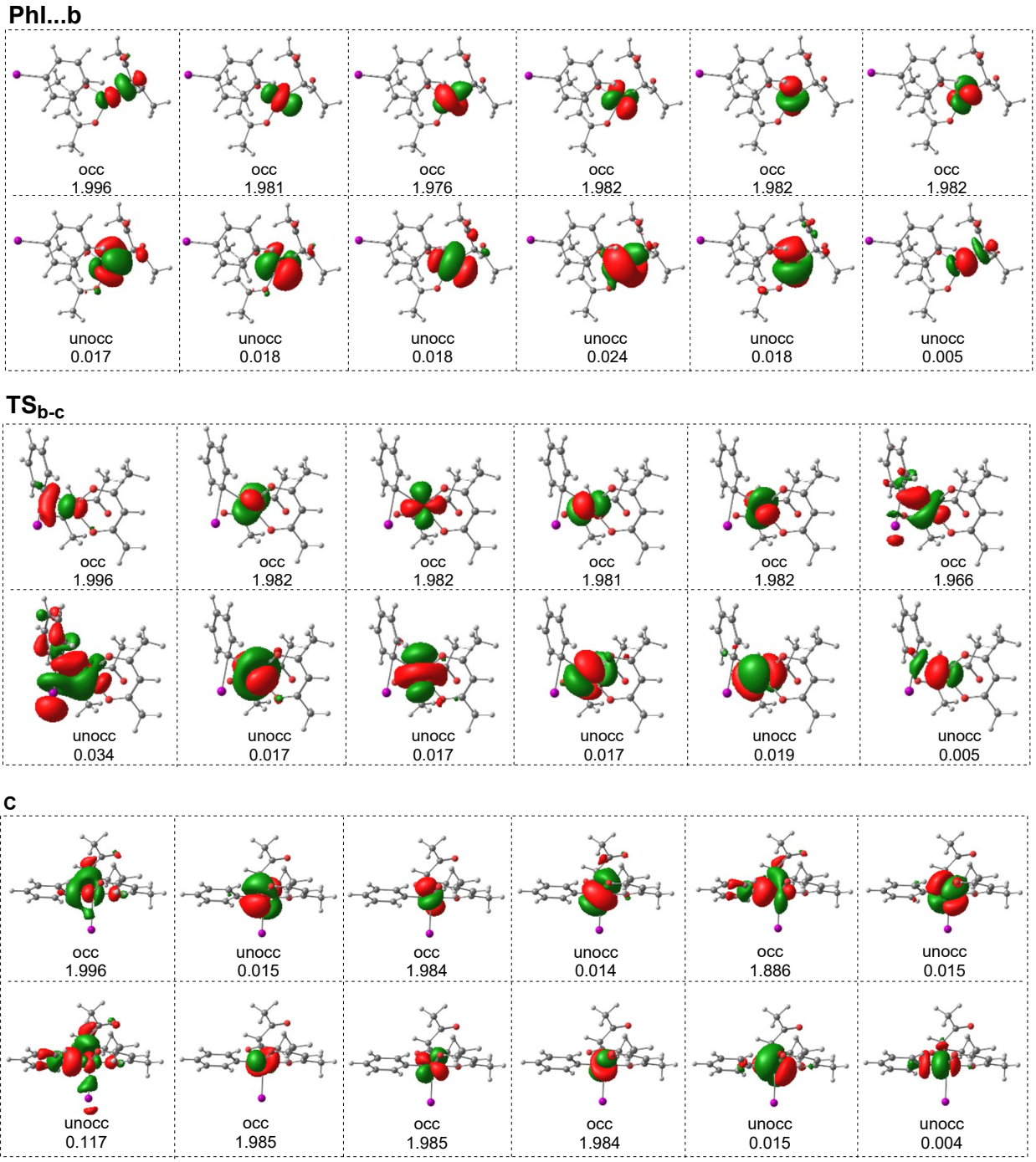


**Figure S6.** Active spaces and natural orbital occupation numbers of **PhI…b**, $\mathbf{TS_{b\text{-}c}}$, and **c**.

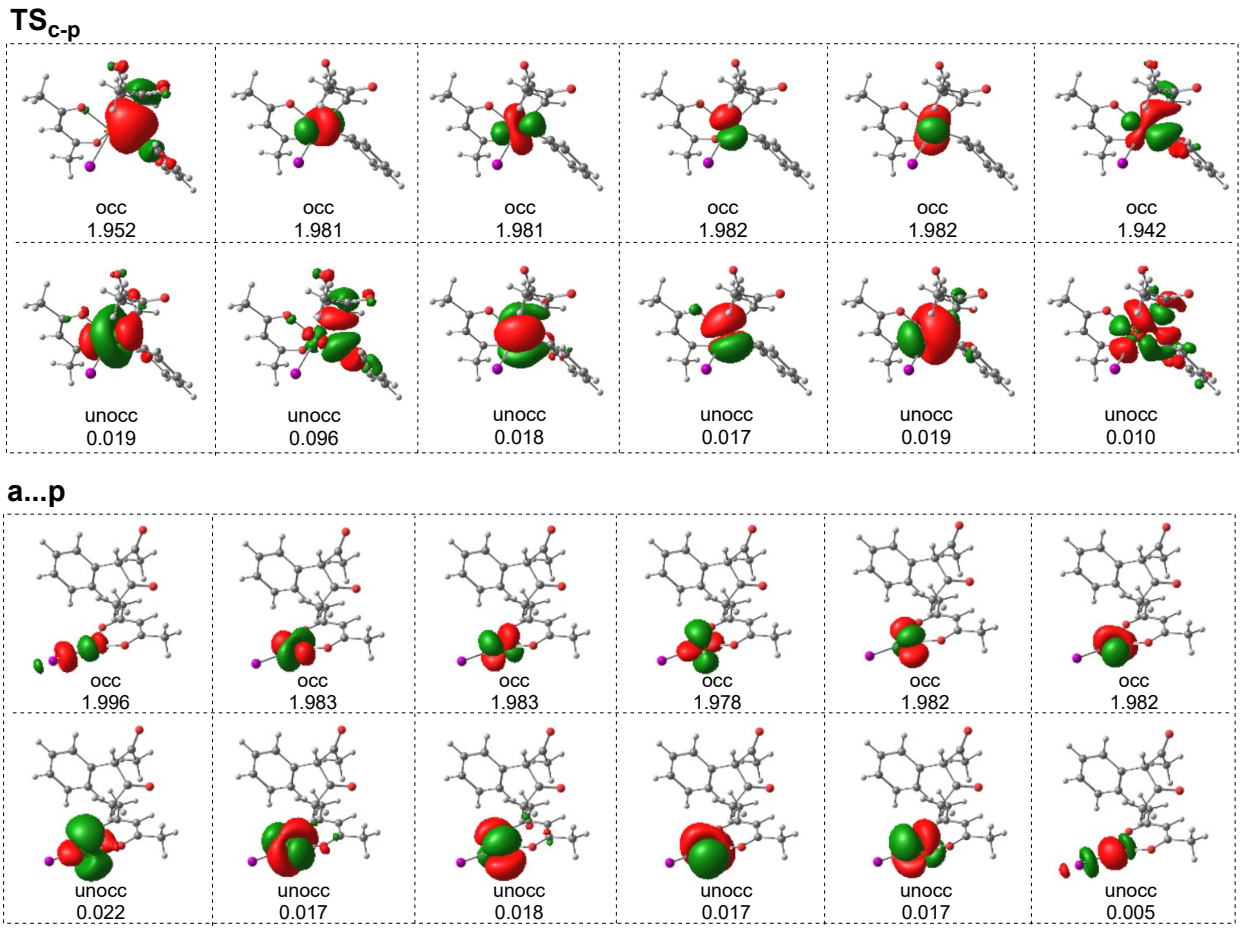


**Figure S7.** Active spaces and natural orbital occupation numbers of **TS$_{c-p}$**, and **a…p**.

The active space including 10 electrons in 10 orbitals (denoted as 10e in 10o) was considered for precursory complexes **b**, which consists of the five 3d orbitals and the corresponding five 3d' orbitals (Figure S5, top). Energy of PhI was evaluated by using active space (2e in 2o) comprising a C-I σ bond orbital and its corresponding one C-I σ* anti-bond orbital. On the other hand, the active space including 11 electrons in 11 orbitals (denoted as 11e in 11o) was considered for precursory complexes **d**, which involves the five 3d orbitals and the four 3d' orbitals corresponding the four doubly-occupied 3d orbitals (Figure S5, middle). Additionally, one Cu-ligand σ bond orbital (doubly occupied) is also involved in the active space. We performed the CASSCF(1e in 1o) calculations for Ph radicals, in which the active space only involves a singly-occupied orbital of the Ph radical. Furthermore, the active space including 9 electrons in 9 orbitals (denoted as 9e in 9o) was considered for precursory complexes **f**, which involves the five 3d orbitals and the four 3d' orbitals corresponding the four doubly-occupied 3d orbitals (Figure S5, bottom). We performed

the CASSCF(3e in 3o) calculations for PhI radicals, in which the active space involves a C-I σ bond orbital and its corresponding one C-I σ* anti-bond orbital, as well as a singly-occupied orbital of the Ph radical. In total, these choices of the active space were of the 12 electrons in 12 orbitals which were consistent with the latter reaction steps. However, it should be noted that CASSCF/CASPT2 method is not size-extensive in case where the strong electron correlation appears. Thus, the CASPT2 reaction energy of overall catalytic cycle is not quantitatively useful.

In the OA and RE steps, we performed the CASSCF(12e in 12o) calculation for each complex. Complex **PhI…b** is an optimised structure in which the PhI is weakly bound to complex **b**. The active space of complex **PhI…b** contains the five 3d orbitals and the corresponding five 3d' orbitals, in which one orbital includes the Cu-C σ-bonding orbital between the Cu centre and β-diketone group (Figure S6, top). Additionally, one 3p orbital of Cu and its corresponding unoccupied orbital are also involved in the active space. In the transition state $\mathbf{TS_{b\text{-}c}}$, the active space involves the five 3d orbitals and the corresponding the five 3d' orbitals , as well as one 3p orbital of Cu and its corresponding unoccupied orbital, in which the Cu-C σ-bonding orbital describes interaction between the Cu centre and the phenyl group (Figure S6, middle). This Cu-C σ-bonding orbital is essential for the OA reaction and the others are important for the strong electron correlation from Cu centre. In the intermediate complex **c**, the active space involves the five 3d orbitals and the corresponding five 3d' orbitals, in which the Cu-C σ-bonding orbital describes interaction between the Cu centre and the phenyl/diketone group (Figure S6, bottom). Additionally, one 3p orbital of Cu and its corresponding unoccupied orbital are also included in the active space, which also describes the weak σ bond orbital between the phenyl and diketone ligands. In the transition state $\mathbf{TS_{c\text{-}p}}$, the active space involves the five 3d orbitals and the corresponding the five 3d' orbitals , as well as one σ bond orbital and its corresponding unoccupied orbital between the phenyl and diketone ligands, in which the Cu-C σ-bonding orbital describes interaction between the Cu centre and the phenyl/diketone group (Figure S7, top). This Cu-C σ-bonding orbital is essential for the RE reaction and the others are important for the strong electron correlation from Cu centre. In the complex **a…p**, the active space involves the five 3d orbitals and the corresponding five 3d' orbitals, as well as the one 3p orbital of Cu and its corresponding unoccupied orbital (Figure S7, bottom).

To check the convergence of size of the active space, we performed CASSCF(10e in 10o) calculations and the corresponding CASPT2 calculations, in which the active space only included

five 3d and five 3d' orbitals of the Cu centre. As a result, the energy profile of the CASSCF(10e in 10o)/CASPT2 method was quantitatively the same as that of the CASSCF(12e in 12o)/CASPT2 method (see Figure S8). Thus, we concluded that size of the active space converged at the CASSCF(12e in 12o)/CASPT2 level of theory. This was because the multi-reference character less occurred in these Cu complexes. In fact, 90% or more of the CASSCF wavefunction consisted of Hartree-Fock configuration, as shown in Table S2, even though the reaction involved bond cleavage/formation processes. In case where the active space is insufficient, collapse of the perturbation correction (known as appearance of intruder states) occurs to see almost zero reference weight in CASPT2 calculation. In our calculation, obtained reference weights shown in Table S2 indicated that the intruder state problem was successfully excluded by employing the imaginary level shift of 0.1 a.u.

Furthermore, from the empirical relationship between the CASPT2 reference weight and number of correlated electrons (S. Langhoff, *Quantum Mechanical Electronic Structure Calculations with Chemical Accuracy*, **2012**, Springer, p.368), the CASPT2 reference weight of our system (134 correlated electrons) was estimated to be 27-51%. Thus, the reference weight of 45% in Table S2 showed that our CASPT2 results were reliable.

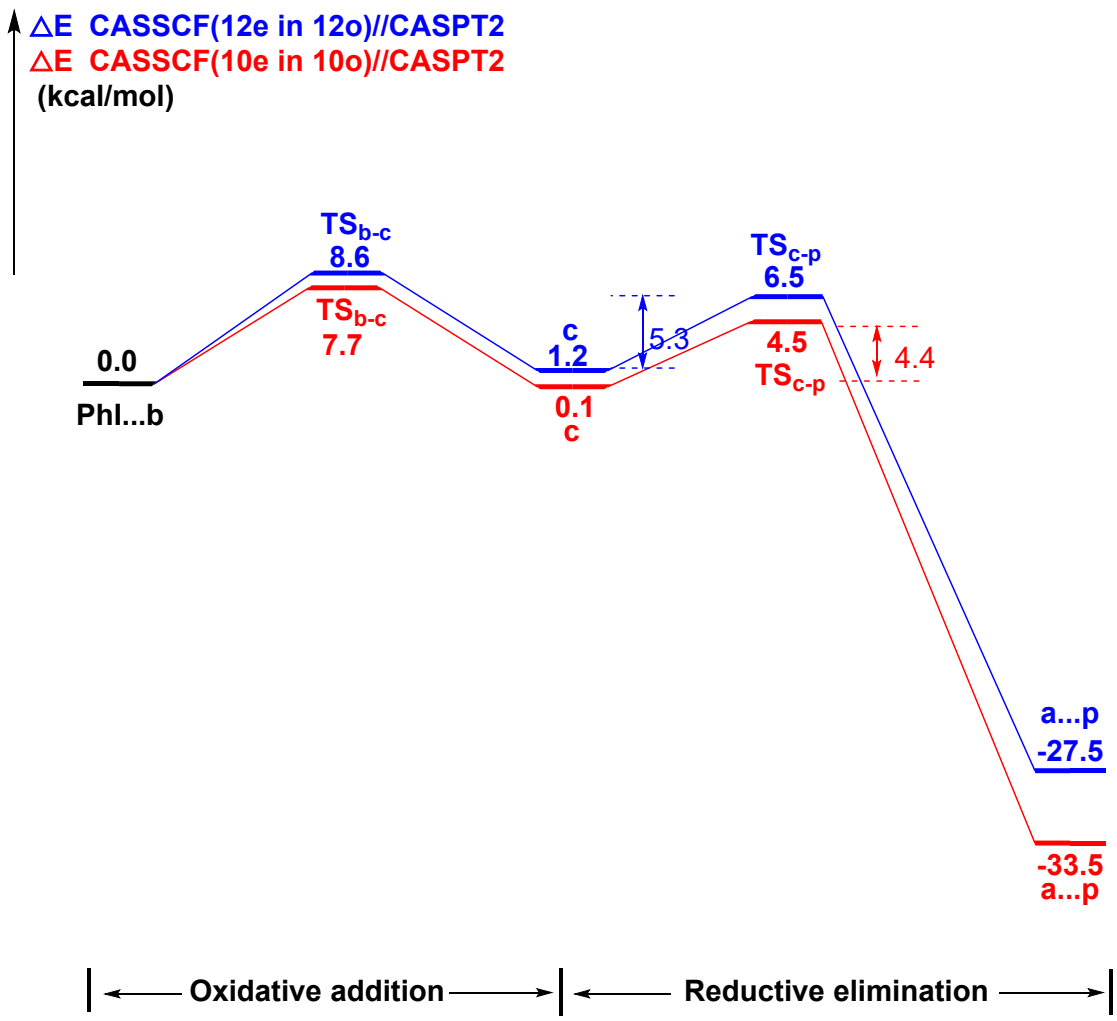


**Figure S8.** Electronic energy profile of the OA-RE mechanism calculated by the CASSCF(10e in 10o)/CASPT2 method (red line) and the CASSCF(12e in 12o)/CASPT2 method (blue line). The electronic energy of **PhI...b** was taken as the reference (energy zero).

**Table S2**. Weight of Hartree-Fock configuration in the CASSCF(12e in 12o) wavefunction, and the reference weight in the CASPT2 wavefunction.

| | **CASSCF** | **CASPT2** |
|---|---|---|
| **Complexes** | **Weight of Hartree-Fock config.** | **Reference weight** |
| **PhI…b** | 0.95206 | 0.46067 |
| **$TS_{b-c}$** | 0.94770 | 0.45429 |
| **c** | 0.91357 | 0.45651 |
| **$TS_{c-p}$** | 0.91490 | 0.45932 |
| **a…p** | 0.95393 | 0.46624 |

## 3. DFT-calculations for the OA-RE pathway

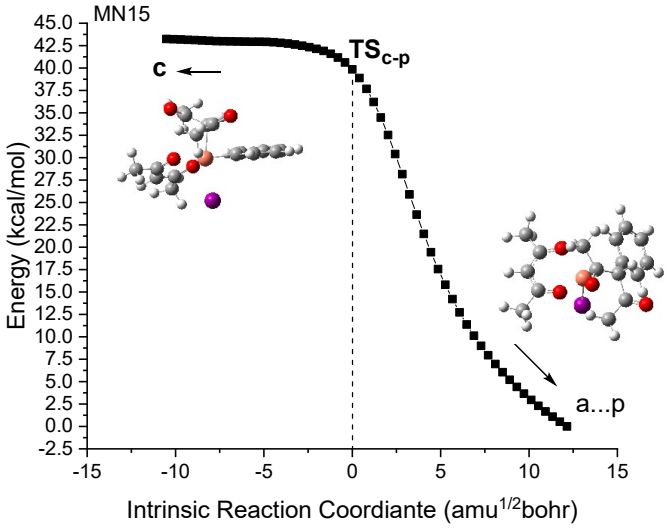


Figure S9. The PEC calculated by MN15 along the $\omega$-B97XD-optimised IRC in the RE step.

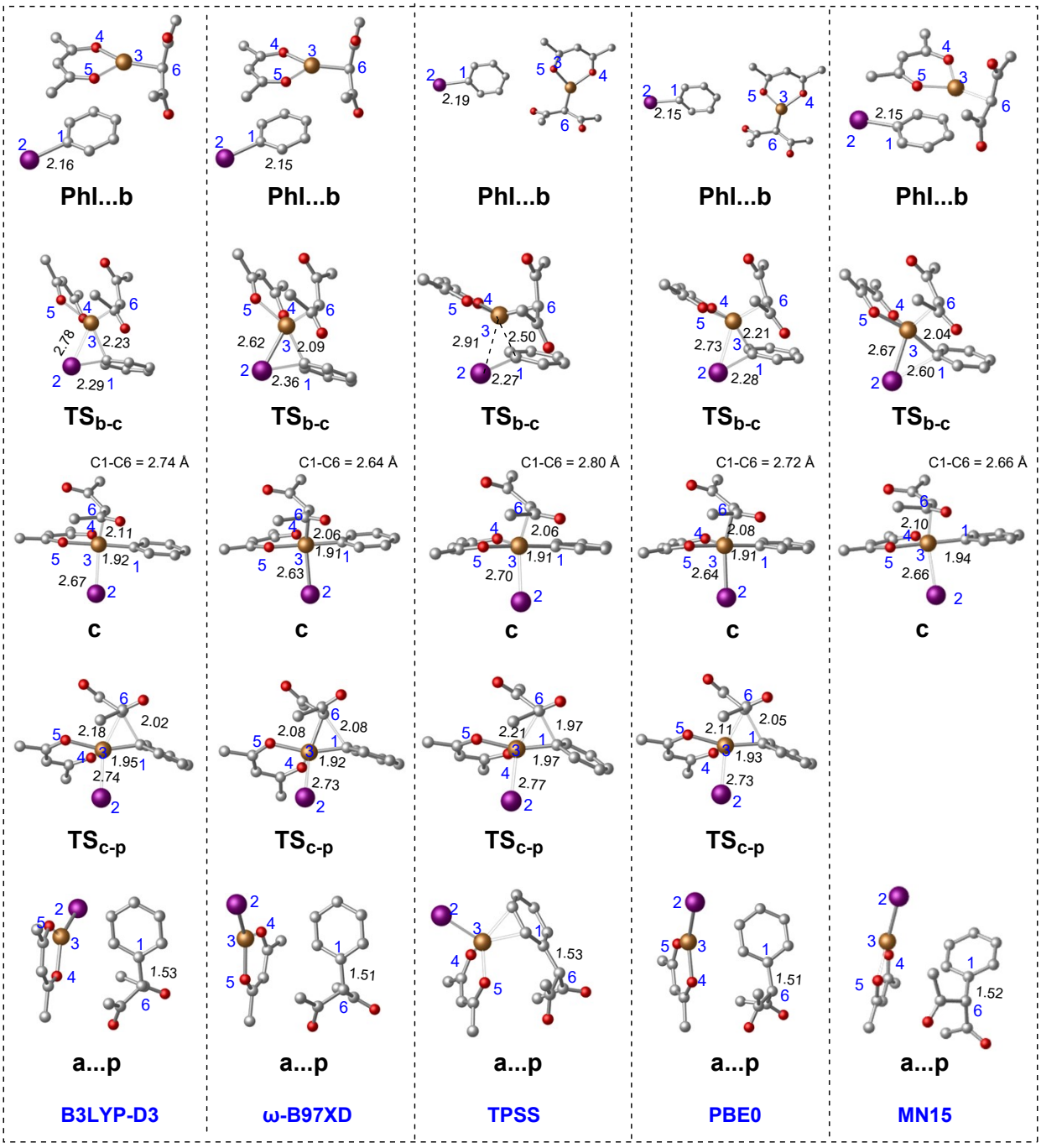


**Figure S10.** DFT-optimised geometries for the OA-RE pathway (hydrogen atoms were not displayed for the sake of simplicity). Numbers were interatomic distance in Å.

## 4. Dependency to the size of basis sets in CASPT2 calculation.

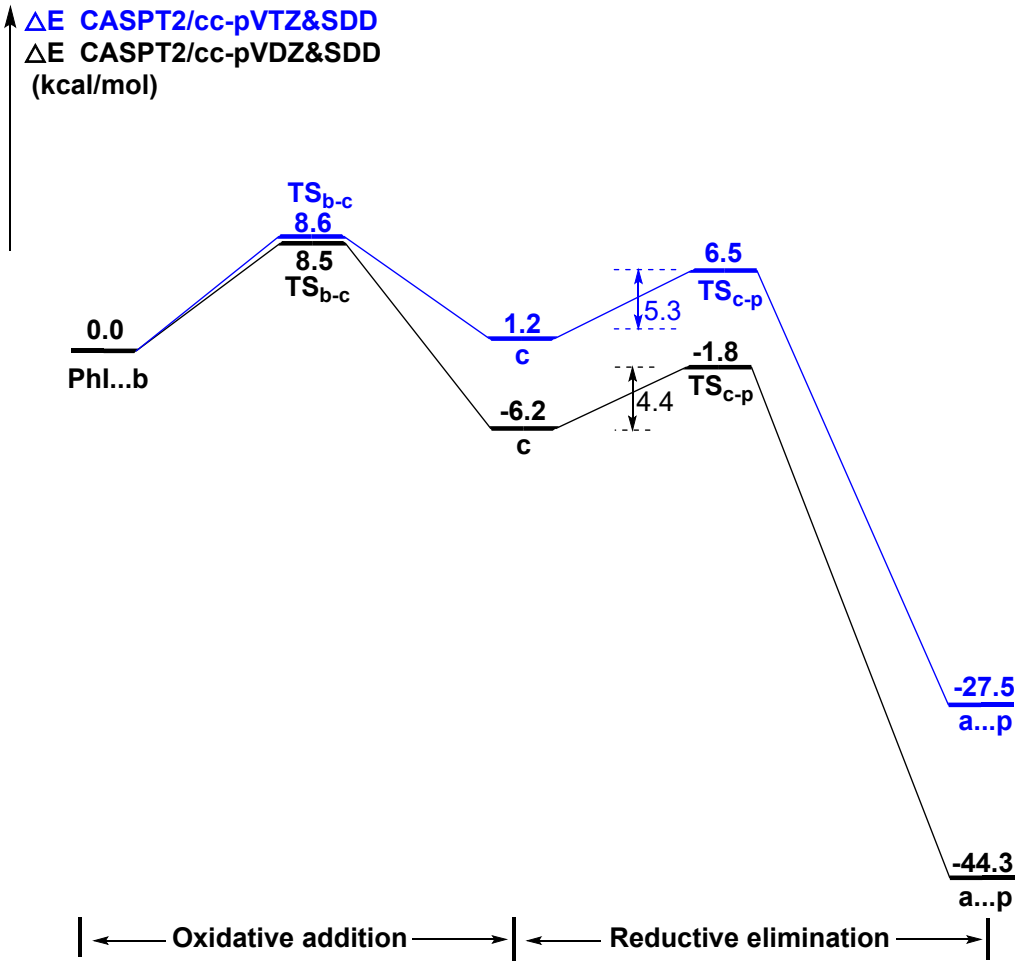


**Figure S11.** Electronic energy profiles of the OA-RE mechanism calculated by CASPT2//$\omega$-B97XD with SDD basis set for Cu and cc-pVTZ basis sets for the other atoms (blue line) and with SDD basis set for Cu and cc-pVDZ basis sets for the other atoms (black line). The electronic energy of **PhI...b** was taken as the reference (energy zero).

In general, electron correlation energy slowly converges with respect to size of basis sets. Thus, we examined dependency to the size of basis sets in CASPT2 calculation using the correlation-consistent valence double-ζ (cc-pVDZ) and the valence triple-ζ (cc-pVTZ) basis sets. Note that the SDD basis sets was employed for Cu atom in both cases. As a result, although the cc-pVDZ calculation gave the larger reaction energies both for the OA and the RE steps, the activation energies were less affected (errors were less than 1 kcal/mol), as shown in Figure S11. Thus, we employed the cc-pVTZ basis sets for the CASPT2 energy profile, but the cc-pVDZ basis sets for

the PEC calculation along the IRCs of the OA and the RE steps to save the computational resources.

## 7. Kohn-Sham molecular orbitals analysis

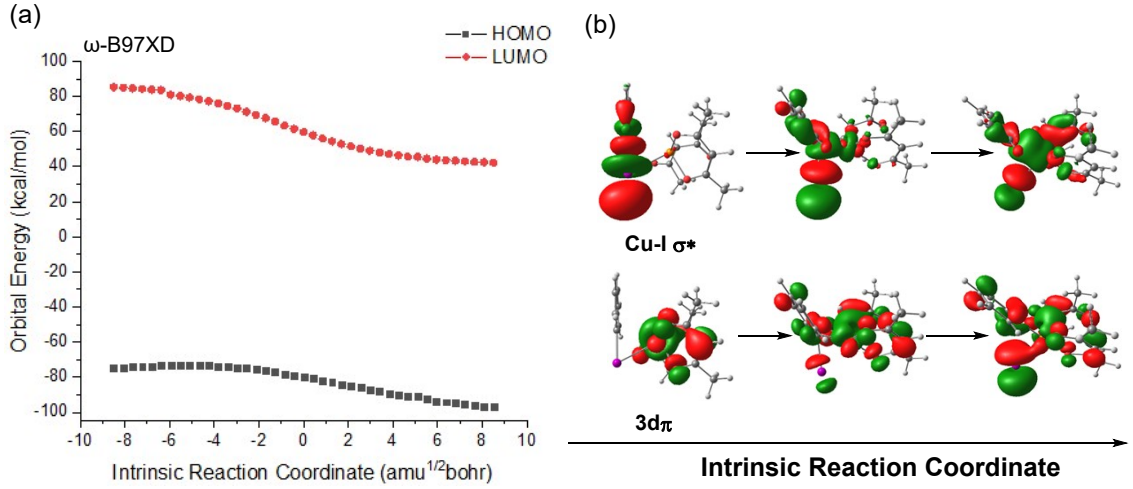


**Figure S12.** Change in the orbital energies of HOMO and LUMO calculated by ω-B97XD functional in the OA step.

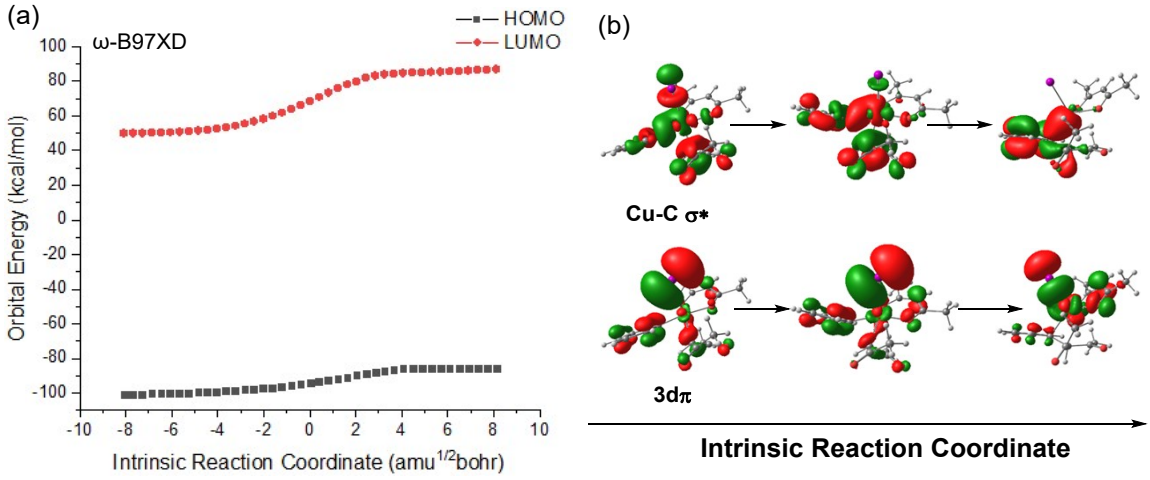


**Figure S13.** Change in the orbital energies of HOMO and LUMO calculated by *ω*-B97XD functional in the RE step.

To explain the role of the 3d orbitals, we analysed the change in Kohn-Sham molecular orbitals (MOs) along the intrinsic reaction coordinate (IRC). Changes in the orbital energies of HOMO and LUMO were shown in Figure S12(a) and Figure S13(a) for the OA and the RE steps, respectively. Orbital pictures from leftmost, mid, and rightmost-points were also displayed in Figure S12(b) and Figure S13(b) for the OA and the RE steps, respectively. From Figure S12(b), it is shown that the 3dπ orbital interacts with the C-I antibonding σ* orbital to result in bonding

interaction between Cu-C and Cu-I in the OA step. From Figure S13(b), on the other hand, it is shown that the 3dπ orbital interacts with the Cu-C antibonding σ* orbital to result in bonding interaction between C-C.

## 8. Potential energy curves (PECs) of the singlet and triplet spin states

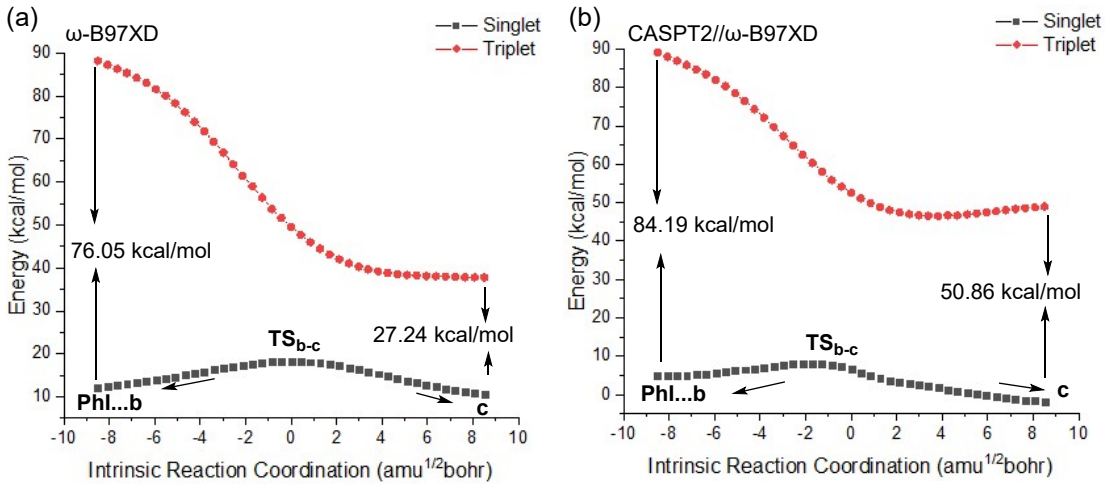


**Figure S14.** PECs along the IRC of **TS$_{b-c}$** optimised by $\omega$-B97XD functional. (a) PECs evaluated by $\omega$-B97XD functional and (b) by CASPT2 method, for the singlet and triplet spin states.

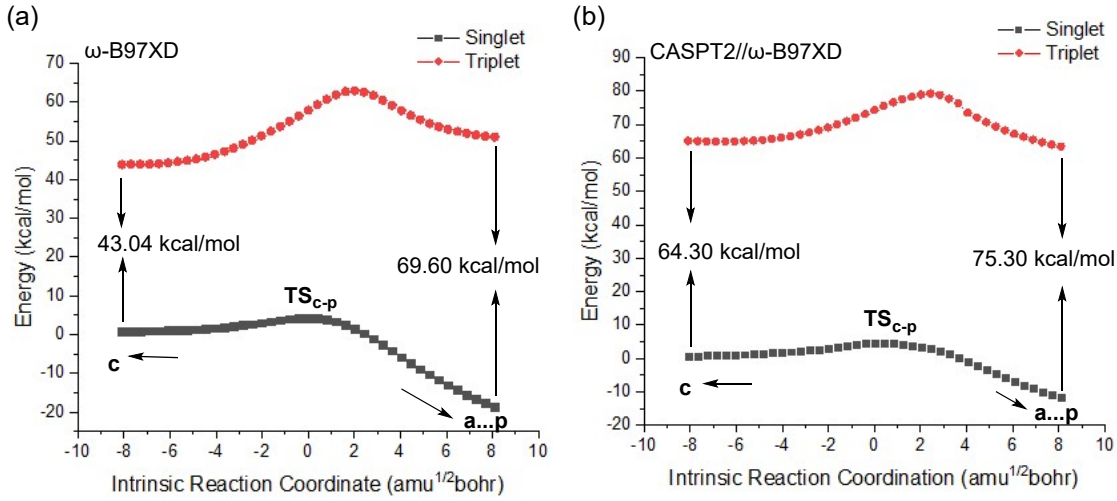


**Figure S15.** PECs along the IRC of **TS$_{c-p}$** optimised by $\omega$-B97XD functional. (a) PECs evaluated by $\omega$-B97XD functional and (b) by CASPT2 method, for the singlet and triplet spin states.

From Figure S14 and S15, a large singlet-triplet gap was found both in the OA and the RE steps, indicating that the ISC never occurs during the OA-RE pathway. It should be noted that the CASPT2 results were surprisingly close to the DFT($\omega$-B97XD) results, and CASSCF/CASPT2 calculated results.

## 9. Data for B3LYP-D3 and CASPT2//B3LYP-D3 calculations

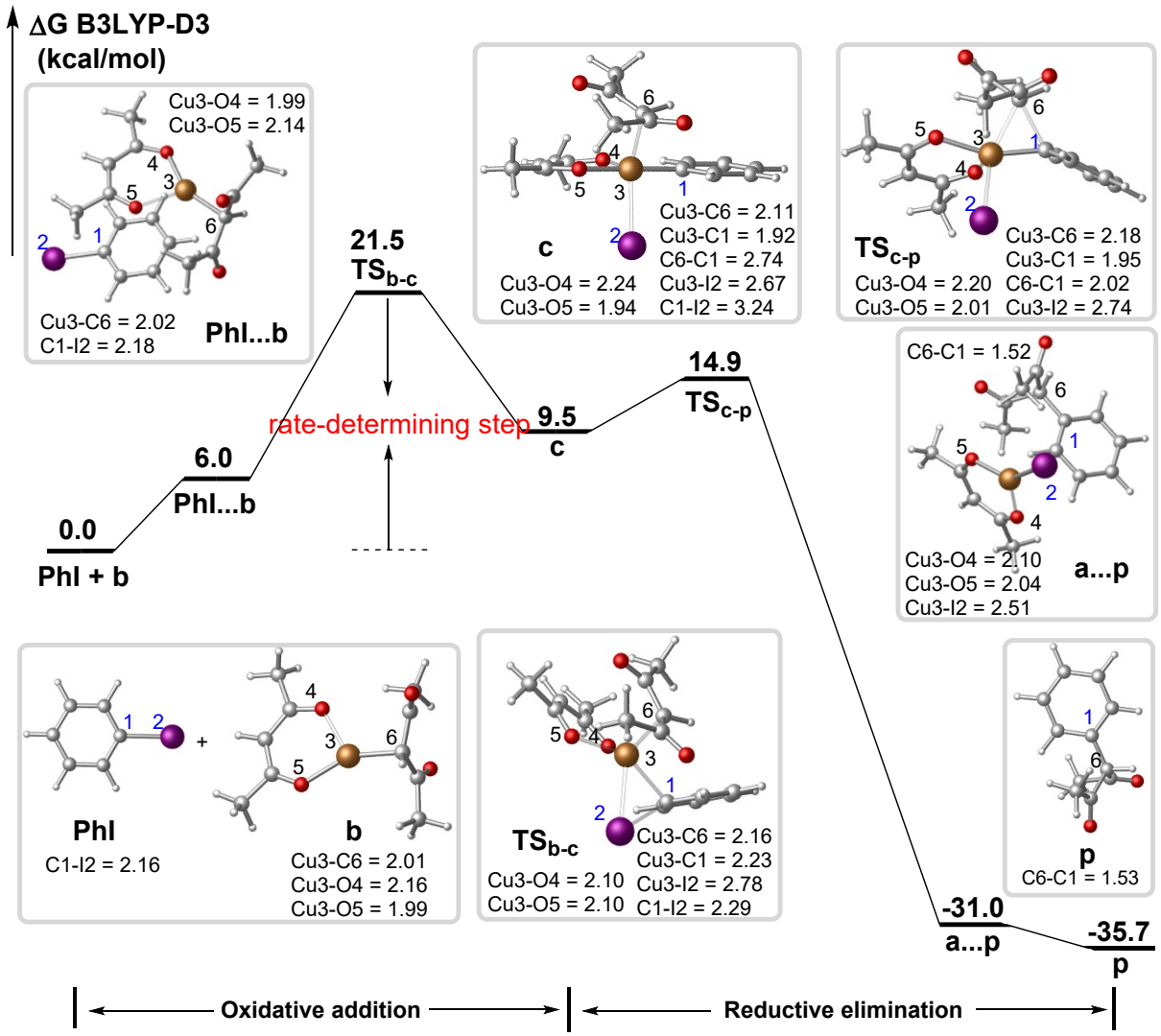


**Figure S16.** The Gibbs free energy profiles for the OA-RE pathway (H: small & white, C: gray, O: red, Cu: yellow, I: purple). Important bond lengths were displayed in Å.

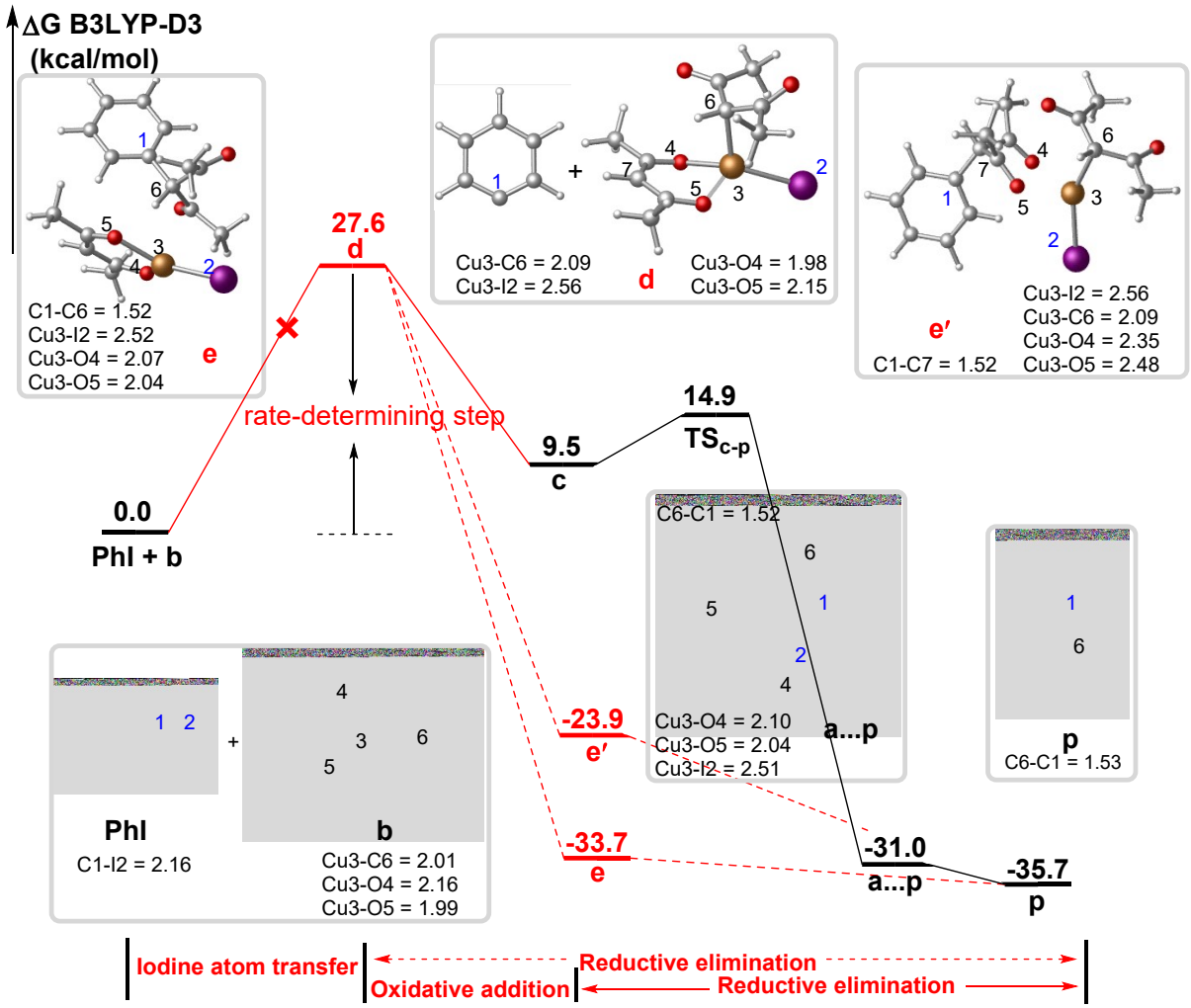


**Figure S17.** The Gibbs free energy profiles for the IAT pathway (H: small & white, C: gray, O: red, Cu: yellow, I: purple). Important bond lengths were displayed in Å.

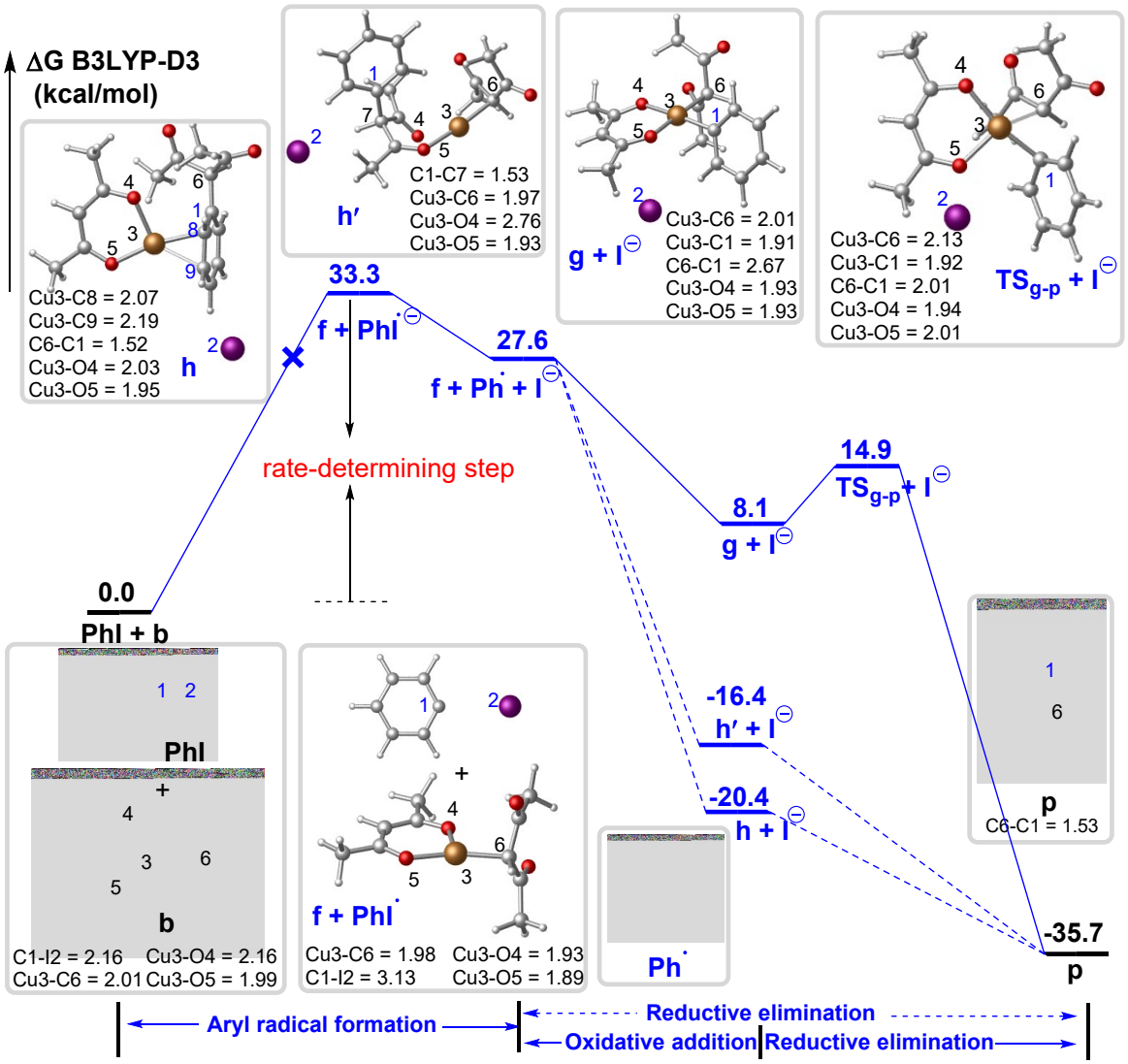


**Figure S18.** The Gibbs free energy profiles for the SET pathway (H: small & white, C: gray, O: red, Cu: yellow, I: purple). Important bond lengths were displayed in Å.

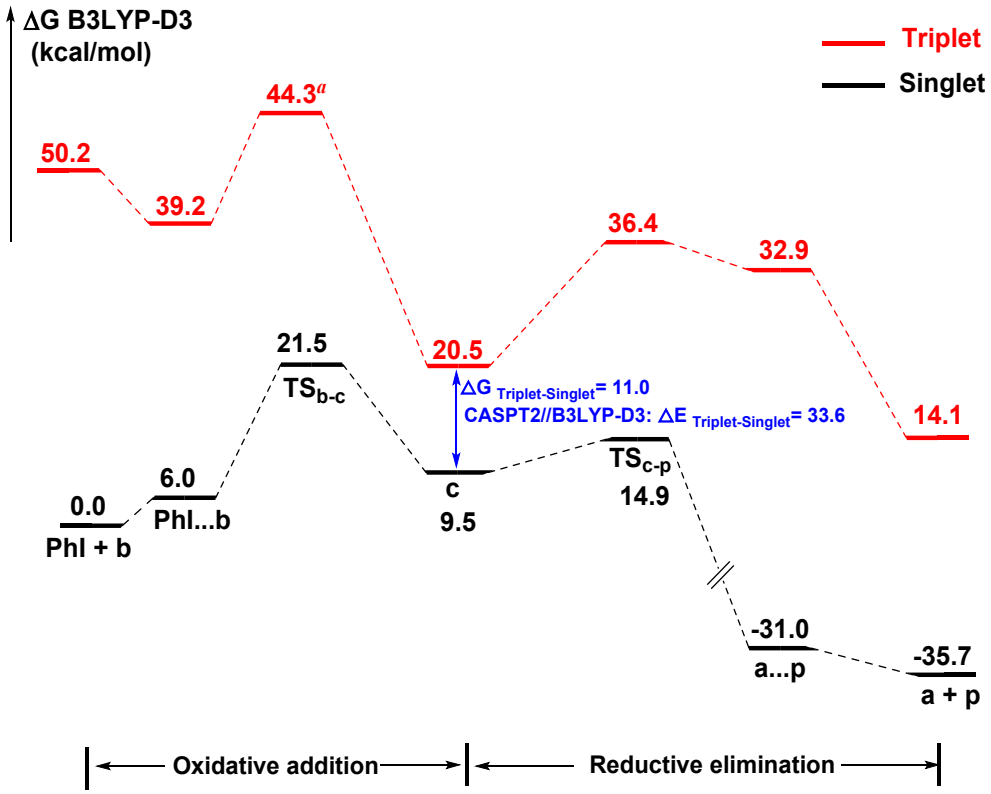


**Figure S19.** Gibbs free energy profiles for the OA-RE pathway in the singlet and the triple spin states. [a] We took the geometry of $\mathbf{TS_{b-c}}$ in the singlet spin state to evaluate the single-point energy in the triplet spin state, because $\mathbf{TS_{b-c}}$ in the triplet spin state could not be located.

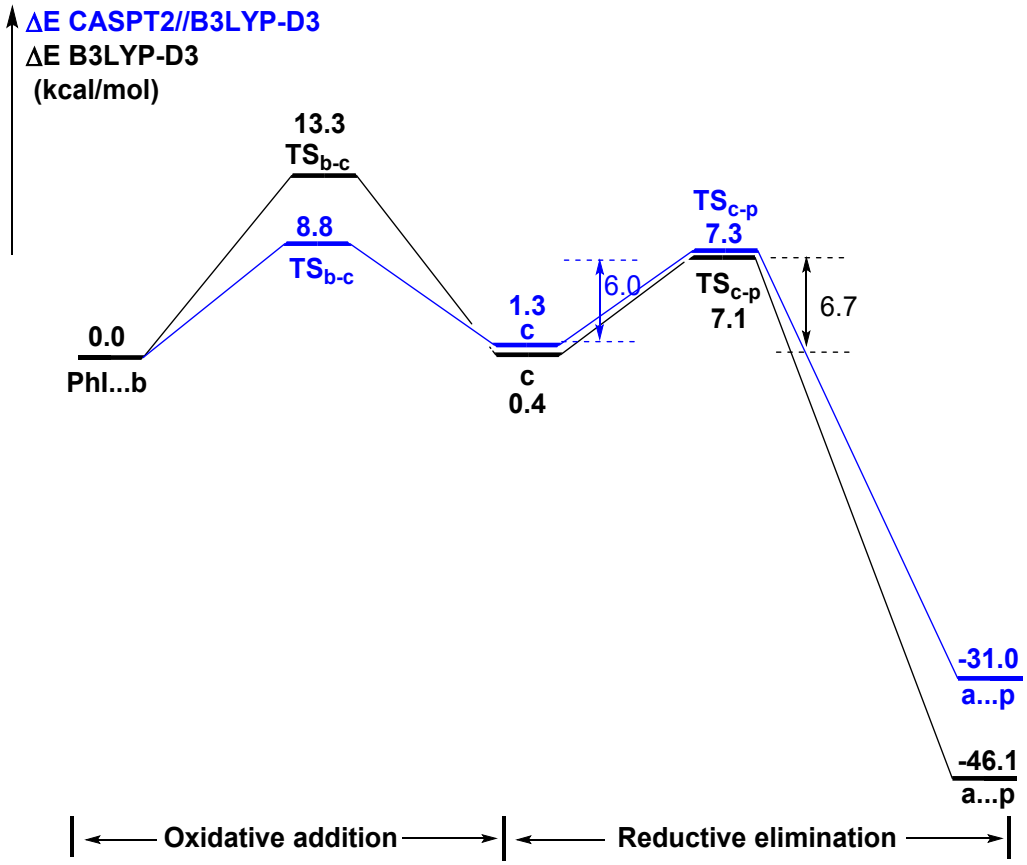


**Figure S20.** Electronic energy profile of OA-RE mechanism calculated by B3LYP-D3 (black) and CASPT2//B3LYP-D3 method (blue).

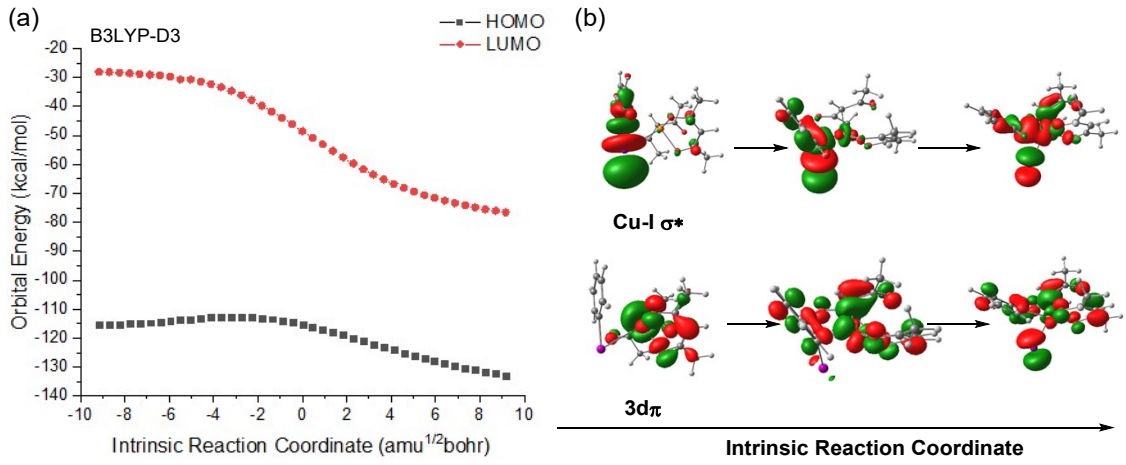


**Figure S21.** Change in the HOMO and LUMO calculated by B3LYP-D3 functional along the IRC of **TS$_{b-c}$** in the OA step.

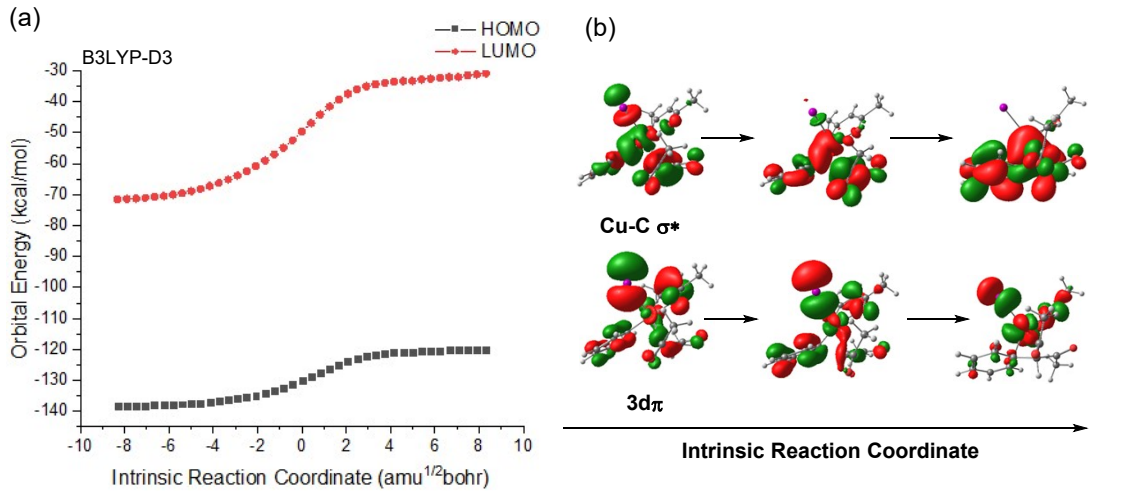


**Figure S22.** Change in the HOMO and LUMO calculated by B3LYP-D3 functional along the IRC of **TS$_{c-p}$** in the RE step.

## 10. ω-B97XD-optimised geometries (singlet spin state)

**Complex a**

| | | | |
|---|---|---|---|
| C | -2.59687500 | -1.25090800 | -0.00037300 |
| C | -3.24516500 | 0.00007500 | -0.00084400 |
| H | -4.33074100 | 0.00016900 | -0.00132300 |
| C | -3.46674800 | -2.50332400 | 0.00008700 |
| H | -3.22812200 | -3.10316800 | 0.88523000 |
| H | -4.53894800 | -2.28376100 | -0.00578000 |
| H | -3.21953700 | -3.10990600 | -0.87803000 |
| C | -2.59667600 | 1.25092000 | -0.00016600 |
| C | -3.46627500 | 2.50351100 | 0.00004000 |
| H | -3.22259500 | 3.10729000 | -0.88101500 |
| H | -4.53853600 | 2.28416300 | -0.00085300 |
| H | -3.22384200 | 3.10607200 | 0.88227700 |
| O | -1.35659600 | -1.45997600 | 0.00028100 |
| O | -1.35633100 | 1.45976400 | 0.00040700 |
| Cu | 0.08314700 | 0.00010400 | 0.00025500 |
| I | 2.60047000 | -0.00007200 | -0.00011100 |

**Complex b**

| | | | |
|---|---|---|---|
| O | 1.54633800 | -1.45129800 | -0.36568200 |
| O | 1.04257300 | 1.36444100 | 0.17360100 |
| C | 2.72716300 | -1.05787600 | -0.14610500 |
| C | 2.28609600 | 1.35831700 | 0.32190700 |
| C | 2.91919700 | 2.69778900 | 0.68310600 |
| H | 2.45407600 | 3.07617900 | 1.59962600 |
| H | 4.00240200 | 2.63776200 | 0.82755500 |
| H | 2.70202300 | 3.42027500 | -0.11113400 |
| C | 3.79026100 | -2.14298300 | -0.25627800 |
| H | 3.72089000 | -2.61322300 | -1.24302700 |
| H | 4.80588900 | -1.76395000 | -0.10778400 |
| H | 3.58682900 | -2.92080800 | 0.48829300 |
| C | 3.14240500 | 0.24107400 | 0.18195100 |
| H | 4.20424200 | 0.40112400 | 0.33993700 |
| Cu | -0.12073900 | -0.36067900 | -0.32240500 |
| C | -2.10917000 | -0.24960800 | -0.52990900 |
| H | -2.27277100 | -0.76807500 | -1.47947700 |
| C | -2.38668400 | 1.19155700 | -0.66800400 |
| C | -2.49675600 | -1.04337100 | 0.63193000 |
| O | -2.61053000 | 1.69676000 | -1.76707500 |
| O | -2.76458000 | -0.63534800 | 1.76625400 |
| C | -2.33588900 | 2.07575500 | 0.56722300 |
| H | -2.78586700 | 1.57273300 | 1.42624100 |
| H | -1.28193600 | 2.26062700 | 0.80829700 |

| | | | |
|---|---|---|---|
| H | -2.82557100 | 3.02828500 | 0.34372000 |
| C | -2.62095500 | -2.55275400 | 0.38027900 |
| H | -2.08604700 | -2.88155900 | -0.51534300 |
| H | -2.24267500 | -3.09331900 | 1.25260400 |
| H | -3.68446600 | -2.80021300 | 0.26685500 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | 1.50512000 | 2.29610300 | -0.67329400 |
| O | 0.77392700 | 0.28799400 | 1.30866300 |
| C | 0.45119000 | 2.81935400 | -0.20530200 |
| C | -0.17516400 | 1.08611800 | 1.48642500 |
| C | -1.20102300 | 0.67256900 | 2.53047800 |
| H | -0.70218000 | 0.56606700 | 3.50007900 |
| H | -2.03022200 | 1.37965100 | 2.62521000 |
| H | -1.60113200 | -0.30902700 | 2.25729300 |
| C | 0.04701600 | 4.12979500 | -0.86658800 |
| H | -0.15489400 | 3.94545800 | -1.92842900 |
| H | -0.83747300 | 4.58523200 | -0.41146800 |
| H | 0.88295200 | 4.83554000 | -0.81570600 |
| C | -0.37014400 | 2.31564700 | 0.81092300 |
| H | -1.24897600 | 2.89428500 | 1.07648500 |
| Cu | 2.27422200 | 0.52916500 | -0.14891500 |
| C | 3.68036700 | -0.87736300 | -0.45953700 |
| H | 3.88978300 | -0.78734100 | -1.52926900 |
| C | 2.97338700 | -2.12725700 | -0.16143500 |
| C | 4.73144600 | -0.31514500 | 0.38534000 |
| O | 2.54755400 | -2.85236900 | -1.06871500 |
| O | 4.95660600 | -0.57230400 | 1.57033200 |
| C | 2.68792100 | -2.49958300 | 1.28055200 |
| H | 3.54012100 | -2.26201400 | 1.92136300 |
| H | 1.84288500 | -1.89085100 | 1.62679400 |
| H | 2.41887700 | -3.55909900 | 1.32931700 |
| C | 5.67251900 | 0.67294500 | -0.31615300 |
| H | 5.23715900 | 1.10523000 | -1.22173900 |
| H | 5.93600900 | 1.47184400 | 0.38259500 |
| H | 6.59651500 | 0.14553700 | -0.58646100 |
| C | -0.49536500 | -2.06187700 | -0.90786300 |
| C | 0.06695500 | -1.10190100 | -1.74525700 |
| C | -0.62759500 | 0.07026300 | -2.02386200 |
| C | -1.88989700 | 0.29110900 | -1.47617800 |
| C | -2.43842700 | -0.68841300 | -0.66024900 |
| C | -1.75991900 | -1.86419900 | -0.35955200 |
| H | 0.08451000 | -2.94801100 | -0.66999000 |
| H | 1.06070600 | -1.27897400 | -2.14389000 |
| H | -0.17021900 | 0.84111800 | -2.63604100 |

| | | | |
|---|---|---|---|
| H | -2.41610000 | 1.21927100 | -1.66679100 |
| H | -2.19719000 | -2.60721700 | 0.29879800 |
| I | -4.38620400 | -0.36038200 | 0.18762300 |

**Complex $TS_{b-c}$**

| | | | |
|---|---|---|---|
| Cu | -0.11385600 | 0.01630400 | 0.12431800 |
| C | -1.99880500 | -0.00599800 | -1.99611600 |
| C | -0.62052900 | 0.44389500 | -1.95773600 |
| C | -0.21967900 | 1.84100800 | -2.04098200 |
| O | -3.00810400 | 0.69217800 | -1.85773400 |
| O | 0.90627600 | 2.17906200 | -2.43740600 |
| H | 0.08269400 | -0.23797100 | -2.43411800 |
| C | 1.87701000 | -0.59379400 | -0.10638800 |
| C | 2.00125800 | -1.87036700 | 0.44422000 |
| C | 2.63497600 | -2.86295000 | -0.29960500 |
| C | 3.17150900 | -2.57458700 | -1.55078600 |
| C | 3.06812800 | -1.28137300 | -2.06550800 |
| C | 2.44289300 | -0.27225800 | -1.34197900 |
| I | 1.81725400 | 1.15923400 | 1.47477300 |
| H | 1.57067800 | -2.09412200 | 1.41166400 |
| H | 2.71026800 | -3.86551100 | 0.11333100 |
| H | 3.67355600 | -3.35129000 | -2.12164900 |
| H | 3.47622800 | -1.04913200 | -3.04565600 |
| H | 2.30861600 | 0.72131800 | -1.76516000 |
| C | -1.19273800 | 2.91623200 | -1.59080700 |
| C | -2.19088700 | -1.50345500 | -2.25677600 |
| H | -0.68135500 | 3.88238900 | -1.62312700 |
| H | -1.55593500 | 2.69919700 | -0.58131100 |
| H | -2.07467100 | 2.92146900 | -2.23831100 |
| H | -1.33074800 | -2.09604200 | -1.93062400 |
| H | -2.34252900 | -1.66610800 | -3.33192500 |
| H | -3.08788400 | -1.83686200 | -1.72793300 |
| O | -1.72428900 | 0.92686700 | 1.03078500 |
| O | -0.85950000 | -1.82266800 | 0.88446400 |
| C | -2.84125200 | 0.37005000 | 1.18711500 |
| C | -2.08538200 | -2.00688900 | 1.12376100 |
| C | -2.51328700 | -3.46506200 | 1.21933400 |
| H | -1.84561300 | -3.99550500 | 1.90629600 |
| H | -3.54873900 | -3.58880000 | 1.55071900 |
| H | -2.39967500 | -3.92726900 | 0.23155100 |
| C | -4.03583400 | 1.30086700 | 1.24578900 |
| H | -4.23374600 | 1.61235100 | 0.21391400 |
| H | -4.93194100 | 0.82577800 | 1.65696900 |
| H | -3.78262500 | 2.19025700 | 1.83068400 |
| C | -3.07088000 | -1.02052000 | 1.27395600 |

| | | | |
|---|---|---|---|
| H | -4.09327400 | -1.34865800 | 1.43064400 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | -0.01526900 | 0.10575900 | -0.13507500 |
| C | 1.26447300 | 2.48079500 | 0.66821600 |
| C | 0.05378100 | 2.16022600 | -0.14177300 |
| C | -0.02427500 | 2.51945400 | -1.59336100 |
| O | 2.38297900 | 2.66887500 | 0.21426000 |
| O | -1.10532400 | 2.84103800 | -2.07297100 |
| H | -0.84520600 | 2.51989800 | 0.35246200 |
| C | -1.82060700 | 0.37672000 | 0.42300200 |
| C | -2.08610700 | 0.14200400 | 1.76727200 |
| C | -3.39118200 | 0.29758000 | 2.23902400 |
| C | -4.41274600 | 0.68653900 | 1.37799200 |
| C | -4.12560300 | 0.92169600 | 0.03445100 |
| C | -2.82785200 | 0.77099200 | -0.44947400 |
| H | -1.29023100 | -0.17926600 | 2.43029700 |
| H | -3.60283200 | 0.10689400 | 3.28884900 |
| H | -5.42703400 | 0.80716600 | 1.75057800 |
| H | -4.91426100 | 1.22839300 | -0.64828800 |
| H | -2.60580500 | 0.97994800 | -1.48976400 |
| C | 1.21390500 | 2.49017500 | -2.45828300 |
| C | 1.01046800 | 2.60086200 | 2.16188400 |
| H | 1.94157000 | 3.21744500 | -2.08688300 |
| H | 0.92594100 | 2.71773900 | -3.48755600 |
| H | 1.69435100 | 1.51091700 | -2.38452800 |
| H | 1.95175000 | 2.81616400 | 2.67273400 |
| H | 0.58918800 | 1.66325200 | 2.53753100 |
| H | 0.28841200 | 3.40207500 | 2.36037600 |
| O | 1.77916700 | -0.05557700 | -0.86515900 |
| O | 0.83165400 | -0.52183200 | 1.83807800 |
| C | 2.83426500 | -0.51165900 | -0.33227600 |
| C | 1.98438000 | -0.99732000 | 1.96055300 |
| C | 2.30917900 | -1.62129500 | 3.30950300 |
| H | 3.37358400 | -1.83929200 | 3.43693600 |
| H | 1.97541100 | -0.94920400 | 4.10637300 |
| H | 1.74376200 | -2.55505400 | 3.40650500 |
| C | 4.03967500 | -0.48487900 | -1.24911900 |
| H | 4.26105200 | 0.56164500 | -1.48612700 |
| H | 4.92414800 | -0.94705300 | -0.80229000 |
| H | 3.79251700 | -0.99527000 | -2.18534900 |
| C | 2.98704500 | -1.00407700 | 0.96706100 |
| H | 3.95929000 | -1.40281300 | 1.23498500 |
| I | -0.70666800 | -2.26712300 | -1.02096900 |

**Complex $TS_{c-p}$**

| | | | |
|---|---|---|---|
| Cu | 0.02601000 | 0.17067200 | 0.05693100 |
| C | -0.03365300 | 2.87113600 | 0.29735000 |
| C | -1.11046600 | 1.89376700 | -0.15948100 |
| C | -1.45497800 | 1.99278400 | -1.64020500 |
| O | 0.46703100 | 3.65851700 | -0.48058100 |
| O | -2.58303900 | 2.32951900 | -1.95157300 |
| H | -2.01000800 | 2.20207700 | 0.37396300 |
| C | -1.80723600 | 0.09085300 | 0.61883400 |
| C | -1.94904200 | 0.04418100 | 2.00768200 |
| C | -3.06229400 | -0.58103400 | 2.56448900 |
| C | -4.04788700 | -1.12791500 | 1.74805400 |
| C | -3.91141700 | -1.05101300 | 0.36329100 |
| C | -2.80344200 | -0.43351300 | -0.20522000 |
| I | 0.32484900 | -2.20955600 | -1.23990300 |
| H | -1.17274200 | 0.44568800 | 2.64864900 |
| H | -3.15425500 | -0.63958100 | 3.64629200 |
| H | -4.91775700 | -1.60954600 | 2.18650600 |
| H | -4.66973800 | -1.47989000 | -0.28611700 |
| H | -2.70488200 | -0.38818500 | -1.28352400 |
| C | -0.42219100 | 1.63013000 | -2.67286700 |
| C | 0.27293800 | 2.90687900 | 1.77712200 |
| H | 0.57562900 | 1.95062300 | -2.36960500 |
| H | -0.71079800 | 2.06474700 | -3.63291100 |
| H | -0.38918800 | 0.53581200 | -2.76809400 |
| H | 0.87001200 | 3.79386200 | 1.99993500 |
| H | 0.81982000 | 1.99975100 | 2.05673400 |
| H | -0.65627200 | 2.92105900 | 2.35899000 |
| O | 1.78480800 | 0.94967200 | -0.53957200 |
| O | 1.01379400 | -0.21760100 | 1.96602100 |
| C | 2.92684300 | 0.60948700 | -0.11946800 |
| C | 2.24689900 | -0.46495300 | 2.02074800 |
| C | 2.70604200 | -1.26835500 | 3.22637800 |
| H | 3.79479800 | -1.31774500 | 3.32240500 |
| H | 2.27598400 | -0.83752400 | 4.13640700 |
| H | 2.31216900 | -2.28589700 | 3.12588200 |
| C | 4.07558800 | 0.97954700 | -1.03798600 |
| H | 3.98984700 | 2.03674200 | -1.30875000 |
| H | 5.05675800 | 0.79301700 | -0.59201400 |
| H | 3.98255500 | 0.39436600 | -1.95957100 |
| C | 3.21235300 | -0.06807200 | 1.07541600 |
| H | 4.24769700 | -0.32672500 | 1.26950500 |

**Complex p**

| | | | |
|---|---|---|---|
| C | 0.86584300 | -0.02724000 | -0.57222900 |

| | | | |
|---|---|---|---|
| H | 1.00095500 | 0.00119200 | -1.65816300 |
| C | 1.54874400 | -1.33333100 | -0.11921900 |
| C | 1.55101800 | 1.21201300 | 0.01681200 |
| O | 2.24481500 | -1.92955500 | -0.91061400 |
| O | 2.04187100 | 1.21863600 | 1.12543100 |
| C | 1.32329200 | -1.80996100 | 1.29140200 |
| H | 1.62766800 | -1.02254700 | 1.98819100 |
| H | 0.25976400 | -2.00796700 | 1.46016100 |
| H | 1.90201300 | -2.71844500 | 1.46352300 |
| C | 1.54509500 | 2.43305300 | -0.87164000 |
| H | 0.54558000 | 2.59655800 | -1.28856500 |
| H | 1.86985600 | 3.30858500 | -0.30766200 |
| H | 2.22806500 | 2.26885000 | -1.71368300 |
| C | -0.62651900 | 0.01246800 | -0.27067100 |
| C | -1.52944800 | -0.42619600 | -1.24204900 |
| C | -1.11989700 | 0.45003000 | 0.96156600 |
| C | -2.89714500 | -0.43104500 | -0.98894000 |
| H | -1.15500400 | -0.77274400 | -2.20200400 |
| C | -2.48840900 | 0.44814500 | 1.21341900 |
| H | -0.43077200 | 0.79226500 | 1.72819600 |
| C | -3.38087200 | 0.00802700 | 0.24037700 |
| H | -3.58588000 | -0.77658100 | -1.75400800 |
| H | -2.85748500 | 0.79447100 | 2.17423600 |
| H | -4.44846200 | 0.00794100 | 0.43826800 |

**Complex d**

| | | | |
|---|---|---|---|
| O | -1.18592200 | -1.74615200 | 0.68226500 |
| O | -1.43976700 | -0.03403300 | -1.61653500 |
| C | -2.44316900 | -1.63914900 | 0.65921400 |
| C | -2.66166700 | -0.10524400 | -1.30124900 |
| C | -3.59630900 | 0.72693000 | -2.15219400 |
| H | -3.37421700 | 0.56032500 | -3.21075000 |
| H | -4.65279300 | 0.51804700 | -1.95944800 |
| H | -3.38393700 | 1.77744800 | -1.92500000 |
| C | -3.18582500 | -2.43774300 | 1.71857800 |
| H | -2.81214500 | -2.14926600 | 2.70693900 |
| H | -4.26924200 | -2.29143500 | 1.68388900 |
| H | -2.96344600 | -3.50202800 | 1.58530800 |
| C | -3.19658300 | -0.85684700 | -0.23647500 |
| H | -4.27260800 | -0.83359600 | -0.10112300 |
| Cu | 0.02160100 | -0.31719100 | -0.25990200 |
| C | -0.42517500 | 1.31552500 | 0.87648400 |
| H | -1.43949000 | 0.99512000 | 1.13517100 |
| C | -0.47793800 | 2.48660700 | -0.03680300 |
| C | 0.48311100 | 1.28820100 | 2.04578700 |
| O | -1.55557300 | 2.91775600 | -0.43110600 |

| | | | |
|---|---|---|---|
| O | 1.43068000 | 2.04215100 | 2.22261600 |
| C | 0.82023800 | 3.09978500 | -0.51043800 |
| H | 1.44565200 | 3.35697200 | 0.34830100 |
| H | 1.37987600 | 2.35718400 | -1.09209700 |
| H | 0.60269100 | 3.97333900 | -1.12995300 |
| C | 0.14188700 | 0.23674700 | 3.09507400 |
| H | -0.00135500 | -0.74576600 | 2.63331900 |
| H | 0.94020700 | 0.19580300 | 3.83893500 |
| H | -0.80101800 | 0.50546300 | 3.58904300 |
| I | 2.49488000 | -0.86124000 | -0.61077700 |

**Complex e**

| | | | |
|---|---|---|---|
| O | 0.65583200 | 2.91348400 | -0.57297300 |
| O | -0.12861400 | 1.01350800 | 1.49851200 |
| C | -0.42236800 | 3.44750700 | -0.18588800 |
| C | -1.11877500 | 1.79218700 | 1.55965300 |
| C | -2.24231800 | 1.36095900 | 2.48232100 |
| H | -1.82345300 | 0.98266100 | 3.41923800 |
| H | -2.95445100 | 2.16512200 | 2.68994300 |
| H | -2.77511300 | 0.52653800 | 2.01107600 |
| C | -0.81151300 | 4.71651000 | -0.93070300 |
| H | -0.96680800 | 4.47731700 | -1.98893800 |
| H | -1.71804900 | 5.18338700 | -0.53459500 |
| H | 0.01525800 | 5.43265600 | -0.87994500 |
| C | -1.28768100 | 2.97998100 | 0.81648300 |
| H | -2.19631000 | 3.54611200 | 0.99249100 |
| Cu | 1.42662800 | 1.19707000 | 0.13301900 |
| C | -0.88973700 | -1.66889200 | 0.08244000 |
| H | -0.02316500 | -1.01206100 | -0.06041900 |
| C | -1.00473900 | -1.95290300 | 1.58608500 |
| C | -0.59508600 | -2.97213100 | -0.66962800 |
| O | -2.06966200 | -2.00706000 | 2.16257300 |
| O | -0.86916300 | -4.05872500 | -0.20199800 |
| C | 0.31274100 | -2.13740800 | 2.29265600 |
| H | 0.99564200 | -2.76206100 | 1.70866600 |
| H | 0.77561400 | -1.14786200 | 2.38401800 |
| H | 0.14895800 | -2.56820000 | 3.28273300 |
| C | 0.04916700 | -2.80238800 | -2.02313100 |
| H | 1.05543400 | -2.38516500 | -1.88560400 |
| H | 0.10737000 | -3.76463800 | -2.53574300 |
| H | -0.51570600 | -2.08169600 | -2.62434300 |
| I | 3.21415400 | -0.49529600 | -0.33392400 |
| C | -3.10906400 | 0.86564800 | -1.68669500 |
| C | -1.99192900 | 0.24206700 | -1.13798300 |
| C | -2.10736600 | -1.00439300 | -0.52056400 |
| C | -3.35796900 | -1.62920300 | -0.47765000 |

| | | | |
|---|---|---|---|
| C | -4.47268600 | -1.00775400 | -1.03121100 |
| C | -4.35229900 | 0.24295100 | -1.63483200 |
| H | -3.00111100 | 1.84549000 | -2.14301000 |
| H | -1.02625700 | 0.74002800 | -1.16796300 |
| H | -3.45083400 | -2.59736100 | 0.00243500 |
| H | -5.44061400 | -1.50010200 | -0.98593300 |
| H | -5.22619700 | 0.72939100 | -2.06068000 |

**Complex e'**

| | | | |
|---|---|---|---|
| O | 0.59837900 | -0.35824400 | 1.61191900 |
| O | 0.54329800 | -0.54260900 | -1.38311100 |
| C | 1.30836800 | -1.32185900 | 1.42545200 |
| C | 1.31986400 | -1.44088300 | -1.13399500 |
| C | 1.59680100 | -2.55972300 | -2.10571000 |
| H | 1.06687300 | -2.37901400 | -3.04251600 |
| H | 2.67449500 | -2.64591900 | -2.29008400 |
| H | 1.23703500 | -3.48684500 | -1.64832800 |
| C | 1.49601100 | -2.40306200 | 2.45944000 |
| H | 1.08217300 | -3.32907600 | 2.05023400 |
| H | 2.56263300 | -2.54690600 | 2.67155900 |
| H | 0.96456200 | -2.13266200 | 3.37379000 |
| C | 2.15700100 | -1.46475900 | 0.15188900 |
| H | 2.67164800 | -2.42961500 | 0.19605700 |
| Cu | -1.27292200 | 0.23507000 | 0.00487200 |
| C | -2.14953900 | -1.55204200 | 0.53521400 |
| H | -1.81799600 | -1.51428700 | 1.57585600 |
| C | -1.43343700 | -2.53433200 | -0.24265000 |
| C | -3.56274200 | -1.21927600 | 0.34367800 |
| O | -0.39233800 | -3.08140300 | 0.18029700 |
| O | -4.25018300 | -1.47963100 | -0.64350700 |
| C | -1.89375300 | -2.87444200 | -1.64747700 |
| H | -2.98142900 | -2.94729200 | -1.70316700 |
| H | -1.59771800 | -2.05707200 | -2.31621700 |
| H | -1.40228900 | -3.79723300 | -1.96941700 |
| C | -4.22268300 | -0.51749200 | 1.53229700 |
| H | -3.55752500 | 0.22251700 | 1.98777000 |
| H | -5.14106400 | -0.03084100 | 1.19669100 |
| H | -4.47697500 | -1.26438200 | 2.29611200 |
| I | -1.25716600 | 2.75523200 | -0.18226900 |
| C | 3.77877000 | 1.98181800 | -0.04244300 |
| C | 2.81137800 | 0.98450800 | 0.01744000 |
| C | 3.19875200 | -0.35805000 | 0.09035500 |
| C | 4.55753900 | -0.67816300 | 0.10143600 |
| C | 5.52347000 | 0.32354600 | 0.04168500 |
| C | 5.13450600 | 1.65797600 | -0.03054000 |
| H | 3.46236600 | 3.01918300 | -0.10061800 |

| | | | |
|---|---|---|---|
| H | 1.75754900 | 1.24659700 | 0.00743500 |
| H | 4.86240400 | -1.72130000 | 0.15855500 |
| H | 6.57788700 | 0.05966200 | 0.05196300 |
| H | 5.88478900 | 2.44268000 | -0.07791500 |

**Complex f**

| | | | |
|---|---|---|---|
| O | -1.69473300 | -1.40746200 | -0.06046200 |
| O | -0.77295400 | 1.27320600 | -0.13429400 |
| C | -2.80853900 | -0.83539400 | 0.15850500 |
| C | -2.00613300 | 1.51191800 | 0.09697400 |
| C | -2.34957600 | 2.97713700 | 0.20376100 |
| H | -2.06317700 | 3.48154100 | -0.72475100 |
| H | -3.41145500 | 3.14690600 | 0.39286500 |
| H | -1.76228300 | 3.42453200 | 1.01214500 |
| C | -3.98231000 | -1.77012100 | 0.31735900 |
| H | -3.75386700 | -2.50372600 | 1.09633000 |
| H | -4.90686800 | -1.24618300 | 0.56861900 |
| H | -4.12470400 | -2.32263200 | -0.61721400 |
| C | -3.01078600 | 0.55149600 | 0.24878000 |
| H | -4.01720800 | 0.90227300 | 0.44143900 |
| Cu | -0.02364300 | -0.48725300 | -0.28394000 |
| C | 1.98586900 | 0.00654600 | -0.56024900 |
| H | 1.73340400 | 0.14659000 | -1.61541100 |
| C | 2.13960400 | -1.37515200 | -0.17207500 |
| C | 2.62415300 | 1.13542100 | 0.12893000 |
| O | 1.17081300 | -2.12302700 | -0.49564300 |
| O | 3.22971000 | 1.01560000 | 1.18530500 |
| C | 3.27038500 | -1.91676400 | 0.64020300 |
| H | 4.21938200 | -1.73372100 | 0.12599600 |
| H | 3.32226700 | -1.36118400 | 1.58086700 |
| H | 3.12532800 | -2.98329200 | 0.81913800 |
| C | 2.42840300 | 2.49089700 | -0.52060200 |
| H | 1.35580500 | 2.70560600 | -0.58716900 |
| H | 2.92814800 | 3.25841300 | 0.07284700 |
| H | 2.83175800 | 2.49278100 | -1.54019600 |

**Complex g**

| | | | |
|---|---|---|---|
| O | 0.19195700 | 0.43948200 | 1.90934500 |
| O | -0.20854900 | -1.97288600 | 0.51327500 |
| C | 1.18588100 | -0.20139300 | 2.37512500 |
| C | 0.83365100 | -2.31940500 | 1.16562400 |
| C | 1.37039000 | -3.68210300 | 0.80894500 |
| H | 1.87853300 | -3.59243000 | -0.15817900 |
| H | 2.08611400 | -4.05428200 | 1.54614000 |
| H | 0.54626200 | -4.39161600 | 0.69167100 |

| | | | |
|---|---|---|---|
| C | 2.10457600 | 0.60997400 | 3.24996700 |
| H | 1.52410700 | 1.31339600 | 3.85250900 |
| H | 2.73018800 | -0.01608300 | 3.89151400 |
| H | 2.75406200 | 1.18220700 | 2.57587800 |
| C | 1.50278700 | -1.54007100 | 2.10510300 |
| H | 2.40372300 | -1.94395400 | 2.55020200 |
| Cu | -0.89751900 | -0.18067400 | 0.45311800 |
| C | -2.22979700 | -0.63611100 | -0.92942600 |
| H | -2.65476200 | 0.26317200 | -1.37411100 |
| C | -3.31202200 | -1.32810800 | -0.13612800 |
| C | -1.46790100 | -1.39375000 | -1.99578300 |
| O | -4.26958900 | -0.67916700 | 0.26167600 |
| O | -1.74261200 | -2.53912200 | -2.30290900 |
| C | -3.20454200 | -2.80204000 | 0.17242300 |
| H | -3.39746000 | -3.36490700 | -0.74511500 |
| H | -2.18984200 | -3.05919900 | 0.48550400 |
| H | -3.94004400 | -3.05518800 | 0.93956300 |
| C | -0.38230300 | -0.62155600 | -2.70090800 |
| H | 0.54227500 | -0.64864200 | -2.10461600 |
| H | -0.17552100 | -1.07716700 | -3.67177400 |
| H | -0.64304200 | 0.43545500 | -2.81800000 |
| C | -1.91905000 | 4.31637700 | -0.01443800 |
| C | -2.90656500 | 3.47934900 | 0.49955500 |
| C | -2.69626300 | 2.10142200 | 0.57121000 |
| C | -1.47857100 | 1.59159300 | 0.14354300 |
| C | -0.47942700 | 2.40429000 | -0.38087800 |
| C | -0.71264800 | 3.77804400 | -0.45643100 |
| H | -2.09173800 | 5.38776300 | -0.07664000 |
| H | -3.85318500 | 3.89340700 | 0.83805800 |
| H | -3.48174800 | 1.43715800 | 0.91824900 |
| H | 0.47939400 | 1.99447300 | -0.69707600 |
| H | 0.06520000 | 4.42324400 | -0.85572900 |
| I | 3.10239100 | 0.48277800 | -0.92159600 |

**Complex $TS_{g\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | -0.73975800 | 0.35276700 | -0.43384000 |
| C | -1.44110600 | 1.36495400 | 1.92864400 |
| C | -2.19736800 | 0.39916600 | 1.00206600 |
| C | -3.39897200 | 1.05318500 | 0.32958400 |
| O | -1.84054100 | 2.50416400 | 2.06159200 |
| O | -4.51819800 | 0.66800600 | 0.60398900 |
| H | -2.60234400 | -0.36042300 | 1.67227200 |
| C | -1.66788400 | -1.25002000 | -0.01780600 |
| C | -0.80212100 | -2.15004600 | 0.61003500 |
| C | -0.94527900 | -3.51190000 | 0.36317600 |
| C | -1.95982100 | -3.97854500 | -0.46955300 |

| | | | |
|---|---|---|---|
| C | -2.83179100 | -3.07409500 | -1.07044100 |
| C | -2.69447900 | -1.70738800 | -0.84430000 |
| I | 2.93130100 | -0.80043700 | 1.00342800 |
| H | 0.01834100 | -1.79955600 | 1.23149700 |
| H | -0.24494400 | -4.20415200 | 0.82119800 |
| H | -2.07108100 | -5.04399300 | -0.65057200 |
| H | -3.62402200 | -3.42906300 | -1.72423700 |
| H | -3.38582500 | -1.01229000 | -1.31019700 |
| C | -3.16437500 | 2.12989600 | -0.70399700 |
| C | -0.29634000 | 0.80034000 | 2.72143500 |
| H | -2.38777700 | 2.82455400 | -0.37676900 |
| H | -4.10490900 | 2.65123200 | -0.89504900 |
| H | -2.82006300 | 1.66710100 | -1.63940400 |
| H | -0.03319300 | 1.49281800 | 3.52329900 |
| H | 0.58560000 | 0.64970100 | 2.08121100 |
| H | -0.55108800 | -0.18146000 | 3.13566800 |
| O | 0.08800400 | 2.11322400 | -0.36080200 |
| O | 0.19389000 | -0.19813500 | -2.07984800 |
| C | 1.14867300 | 2.39402900 | -1.00924100 |
| C | 1.25503300 | 0.37853300 | -2.46168400 |
| C | 2.11986700 | -0.41629400 | -3.41155000 |
| H | 2.76875200 | 0.21928600 | -4.02111100 |
| H | 2.75056900 | -1.06893100 | -2.79517500 |
| H | 1.49438400 | -1.04427400 | -4.05143100 |
| C | 1.85974500 | 3.64414400 | -0.54538200 |
| H | 2.38937100 | 3.39984000 | 0.38293300 |
| H | 2.58669400 | 4.01047100 | -1.27523800 |
| H | 1.12719600 | 4.42452200 | -0.31986700 |
| C | 1.71021600 | 1.64205900 | -2.04292400 |
| H | 2.64917700 | 1.99134400 | -2.45715200 |

**Complex h**

| | | | |
|---|---|---|---|
| Cu | -0.95074400 | 0.81282500 | -0.96829300 |
| C | -2.71081700 | -1.40009600 | 1.54430200 |
| C | -1.85671900 | -2.35367500 | 0.68847600 |
| C | -2.71490700 | -3.13483100 | -0.32240000 |
| O | -3.90277800 | -1.60625300 | 1.65700800 |
| O | -2.52581900 | -4.32340900 | -0.46559900 |
| H | -1.50681800 | -3.11336900 | 1.40151600 |
| C | -0.61596200 | -1.73224800 | 0.06630200 |
| C | 0.55735700 | -1.66278500 | 0.80339500 |
| C | 1.71360400 | -1.04457400 | 0.30427000 |
| C | 1.70733400 | -0.47597700 | -0.95411900 |
| C | 0.54064700 | -0.54837500 | -1.74541100 |
| C | -0.61901900 | -1.19444500 | -1.25125000 |
| I | 5.48604500 | -0.00709600 | 0.23080800 |

| | | | |
|---|---|---|---|
| H | 0.58454400 | -2.10534800 | 1.79666700 |
| H | 2.63295000 | -1.00986200 | 0.88325900 |
| H | 2.61520800 | -0.01022600 | -1.32683100 |
| H | 0.58383000 | -0.25187700 | -2.79121100 |
| H | -1.43912600 | -1.41659800 | -1.92971400 |
| C | -3.76485200 | -2.40045200 | -1.12930700 |
| C | -2.01793800 | -0.31075100 | 2.32541800 |
| H | -4.73668900 | -2.60256600 | -0.66743900 |
| H | -3.77578500 | -2.80673900 | -2.14497000 |
| H | -3.62427000 | -1.31629400 | -1.13223000 |
| H | -2.75868200 | 0.22592500 | 2.92068900 |
| H | -1.50314800 | 0.38894900 | 1.66138200 |
| H | -1.25572900 | -0.74329800 | 2.98399400 |
| O | -2.94628000 | 0.77324300 | -0.58961200 |
| O | -0.74525300 | 2.69045400 | -0.48806900 |
| C | -3.54365200 | 1.72573700 | -0.00230400 |
| C | -1.65536800 | 3.37528800 | 0.06606700 |
| C | -1.23556400 | 4.77304300 | 0.47486000 |
| H | -2.05327700 | 5.35370800 | 0.90934400 |
| H | -0.41855500 | 4.70102100 | 1.20037800 |
| H | -0.84195200 | 5.29774200 | -0.40140600 |
| C | -4.98627100 | 1.44967900 | 0.36546900 |
| H | -5.01605300 | 0.58054100 | 1.03224800 |
| H | -5.47328700 | 2.30023400 | 0.84965800 |
| H | -5.54222200 | 1.18230100 | -0.53958700 |
| C | -2.97748900 | 2.96690200 | 0.33296000 |
| H | -3.62103000 | 3.68302100 | 0.83174000 |

**Complex h'**

| | | | |
|---|---|---|---|
| O | 0.61616600 | 0.76109000 | -1.96544300 |
| O | 0.49176500 | 2.04684300 | 0.58317300 |
| C | -0.51610500 | 0.49292400 | -1.55766400 |
| C | -0.14658000 | 1.06199200 | 0.91140200 |
| C | -0.34040000 | 0.69425800 | 2.35860100 |
| H | -0.34093200 | 1.60680200 | 2.95883400 |
| H | -1.26184000 | 0.12784900 | 2.51682900 |
| H | 0.51703500 | 0.07982400 | 2.66177900 |
| C | -1.65568000 | 0.43265500 | -2.51925100 |
| H | -1.31548700 | 0.63714700 | -3.53548300 |
| H | -2.12799200 | -0.55440700 | -2.45947900 |
| H | -2.43540600 | 1.13801900 | -2.20427900 |
| C | -0.82581300 | 0.15813400 | -0.11016300 |
| H | -1.90929600 | 0.32979100 | 0.04208800 |
| Cu | 2.25990900 | 0.95405000 | -0.95270300 |
| C | 3.95669400 | 0.88892800 | 0.03251100 |
| H | 4.44295600 | 1.84570600 | -0.18054200 |

| | | | |
|---|---|---|---|
| C | 4.72812500 | -0.21669100 | -0.58996200 |
| C | 3.41871000 | 0.81587700 | 1.39885300 |
| O | 5.60483600 | 0.01844300 | -1.41292100 |
| O | 3.05477600 | -0.21185300 | 1.97816800 |
| C | 4.40534400 | -1.65906100 | -0.23200300 |
| H | 4.27244100 | -1.78240400 | 0.84530300 |
| H | 3.45555000 | -1.94556800 | -0.70040100 |
| H | 5.19911200 | -2.30229700 | -0.61935300 |
| C | 3.32219200 | 2.14507500 | 2.13720800 |
| H | 3.06047200 | 2.96675700 | 1.46581500 |
| H | 2.57625800 | 2.06968300 | 2.93097500 |
| H | 4.29798000 | 2.36611600 | 2.58837400 |
| C | 0.90972900 | -3.18330300 | 0.55698500 |
| C | 0.69805700 | -1.81575100 | 0.41174100 |
| C | -0.57598000 | -1.33209100 | 0.10202900 |
| C | -1.63637400 | -2.22949700 | -0.04840000 |
| C | -1.41785400 | -3.59684300 | 0.09367400 |
| C | -0.14464300 | -4.07760000 | 0.38991100 |
| H | 1.90365200 | -3.54096100 | 0.81029300 |
| H | 1.52979900 | -1.13750000 | 0.59330900 |
| H | -2.63594000 | -1.84599400 | -0.24527300 |
| H | -2.25052700 | -4.28544000 | -0.01781000 |
| H | 0.02255800 | -5.14508200 | 0.50521800 |
| I | -4.63688000 | 0.55310000 | 0.11689700 |

**Complex a...p**

| | | | |
|---|---|---|---|
| Cu | -1.81571400 | 0.85948400 | 0.10369900 |
| C | 2.58870900 | 0.15277600 | -1.83597400 |
| C | 3.16228400 | -0.99622900 | -0.99750500 |
| C | 4.29451600 | -0.47644800 | -0.09681400 |
| O | 3.21270500 | 1.19265800 | -1.92912200 |
| O | 5.44232200 | -0.80650100 | -0.30454300 |
| H | 3.65106900 | -1.65683300 | -1.72697000 |
| C | 2.14897800 | -1.80650000 | -0.21380300 |
| C | 1.07499500 | -1.19518500 | 0.43610300 |
| C | 0.17494400 | -1.94718500 | 1.18493700 |
| C | 0.34848600 | -3.32420500 | 1.29788000 |
| C | 1.42192200 | -3.94342700 | 0.66188200 |
| C | 2.31643800 | -3.18797000 | -0.09052700 |
| I | -3.70087900 | -0.68597600 | -0.44020200 |
| H | 0.92569900 | -0.12249700 | 0.35340200 |
| H | -0.66061400 | -1.44491000 | 1.66148700 |
| H | -0.35920300 | -3.91348100 | 1.87360300 |
| H | 1.56150300 | -5.01788500 | 0.74663800 |
| H | 3.15604100 | -3.67160300 | -0.58513300 |
| C | 3.90189500 | 0.39849200 | 1.07017100 |

| | | | |
|---|---|---|---|
| C | 1.29316700 | -0.06763100 | -2.57409500 |
| H | 3.15813800 | 1.14763800 | 0.78062600 |
| H | 4.79349500 | 0.87999400 | 1.47590100 |
| H | 3.44384300 | -0.22588900 | 1.84622200 |
| H | 1.36155000 | 0.41010000 | -3.55505400 |
| H | 0.48149900 | 0.42945100 | -2.02537000 |
| H | 1.03771400 | -1.12535300 | -2.67289100 |
| O | -0.77119000 | 1.08379000 | 1.88655100 |
| O | -0.55275400 | 2.15941900 | -0.81281300 |
| C | 0.26448500 | 1.78320900 | 2.03040800 |
| C | 0.41527900 | 2.76557300 | -0.27361000 |
| C | 1.18944500 | 3.70534400 | -1.18041400 |
| H | 1.83918100 | 4.38613500 | -0.62240600 |
| H | 1.81386600 | 3.10808300 | -1.85446800 |
| H | 0.48501400 | 4.28246900 | -1.78663400 |
| C | 0.94876100 | 1.67196600 | 3.38455700 |
| H | 1.36575300 | 0.66205400 | 3.47990600 |
| H | 1.75485800 | 2.39921100 | 3.51986700 |
| H | 0.20551500 | 1.79427200 | 4.17843300 |
| C | 0.85760300 | 2.61488100 | 1.05666100 |
| H | 1.72726700 | 3.19100000 | 1.35654500 |

**Complex PhI**

| | | | |
|---|---|---|---|
| C | -2.66651500 | 1.20749400 | -0.00000100 |
| C | -3.36684500 | 0.00000500 | 0.00000300 |
| C | -2.66655000 | -1.20747700 | -0.00000100 |
| C | -1.26884500 | -1.21676500 | -0.00000100 |
| C | -0.58793100 | -0.00001900 | -0.00000200 |
| C | -1.26883600 | 1.21676200 | -0.00000200 |
| H | -3.20369900 | 2.15213600 | 0.00000400 |
| H | -4.45306500 | 0.00003300 | 0.00000200 |
| H | -3.20371500 | -2.15213000 | 0.00000400 |
| H | -0.72680400 | -2.15608900 | -0.00000600 |
| H | -0.72675000 | 2.15606000 | -0.00000500 |
| I | 1.57107900 | 0.00000000 | 0.00000000 |

**Complex PhI-radical**

| | | | |
|---|---|---|---|
| C | -3.91980800 | -0.00010600 | -0.00032900 |
| C | -3.22250300 | 1.20859600 | -0.00017800 |
| C | -1.82366500 | 1.21262600 | 0.00012800 |
| C | -1.16064400 | 0.00010800 | 0.00028100 |
| C | -1.82347500 | -1.21251300 | 0.00012900 |
| C | -3.22231300 | -1.20870100 | -0.00017800 |
| H | -5.00765400 | -0.00019200 | -0.00057300 |
| H | -3.76981200 | 2.15012900 | -0.00029800 |
| H | -1.26719600 | 2.14663100 | 0.00024800 |

| | | | |
|---|---|---|---|
| H | -1.26685700 | -2.14642900 | 0.00024900 |
| H | -3.76947700 | -2.15031700 | -0.00029800 |
| I | 2.00217800 | 0.00000200 | 0.00002900 |

**Complex Ph-radical**

| | | | |
|---|---|---|---|
| C | 1.21071300 | 0.63068200 | 0.00000400 |
| C | 1.22337000 | -0.76916800 | -0.00000300 |
| C | 0.00000200 | -1.39771300 | 0.00000000 |
| C | -1.22337200 | -0.76916500 | 0.00000000 |
| C | -1.21071500 | 0.63067700 | -0.00000400 |
| C | 0.00000200 | 1.32124300 | 0.00000100 |
| H | 2.15027900 | 1.17670900 | 0.00000800 |
| H | 2.15932700 | -1.31993700 | 0.00000200 |
| H | -2.15932200 | -1.31994500 | 0.00000000 |
| H | -2.15027600 | 1.17671300 | -0.00000400 |
| H | -0.00000500 | 2.40712200 | 0.00000400 |

## 11. B3LYP-D3-optimised geometries (singlet spin state)

**Complex a**

| | | | |
|---|---|---|---|
| C | -2.61253700 | -1.25377300 | 0.00003500 |
| C | -3.26196600 | -0.00017700 | 0.00021300 |
| H | -4.34771700 | -0.00025500 | 0.00025300 |
| C | -3.47917800 | -2.51256900 | -0.00005300 |
| H | -3.23342800 | -3.11749100 | 0.88108500 |
| H | -4.55404500 | -2.30112800 | 0.00006400 |
| H | -3.23357600 | -3.11726000 | -0.88139000 |
| C | -2.61275100 | 1.25350600 | 0.00033800 |
| C | -3.47958900 | 2.51216500 | 0.00049100 |
| H | -3.23399100 | 3.11712600 | -0.88066300 |
| H | -4.55442400 | 2.30056400 | 0.00045000 |
| H | -3.23401700 | 3.11689500 | 0.88181100 |
| O | -1.36456300 | -1.46178600 | -0.00003100 |
| O | -1.36480000 | 1.46178100 | 0.00031600 |
| Cu | 0.08052100 | 0.00034100 | 0.00001700 |
| I | 2.61447400 | -0.00006100 | -0.00019900 |

**Complex b**

| | | | |
|---|---|---|---|
| O | 1.55895400 | -1.43801000 | -0.41755700 |
| O | 1.01181500 | 1.37258800 | 0.12928000 |
| C | 2.73573000 | -1.03368200 | -0.15317200 |
| C | 2.25569400 | 1.37929000 | 0.32297800 |
| C | 2.85777100 | 2.72576500 | 0.72508600 |
| H | 2.35977900 | 3.08036100 | 1.63522200 |
| H | 3.93872900 | 2.68756400 | 0.89903000 |
| H | 2.64707800 | 3.46030700 | -0.06139000 |
| C | 3.80864200 | -2.11534000 | -0.24063600 |
| H | 3.80431800 | -2.54568900 | -1.24944700 |
| H | 4.81478800 | -1.74758500 | -0.01330200 |
| H | 3.55875700 | -2.92650400 | 0.45399700 |
| C | 3.12791600 | 0.26843000 | 0.20047000 |
| H | 4.18243300 | 0.43551800 | 0.39746600 |
| Cu | -0.12957400 | -0.39508100 | -0.37210300 |
| C | -2.13148900 | -0.26624300 | -0.51757900 |
| H | -2.35071600 | -0.79704600 | -1.44990700 |
| C | -2.40069500 | 1.17908500 | -0.66602300 |
| C | -2.46211400 | -1.03975700 | 0.68059500 |
| O | -2.68207100 | 1.66746400 | -1.76541800 |
| O | -2.68141300 | -0.60489100 | 1.82110800 |
| C | -2.26409400 | 2.08613400 | 0.55045600 |
| H | -2.72409000 | 1.63065400 | 1.43095400 |
| H | -1.19495600 | 2.20490800 | 0.76578600 |
| H | -2.69969300 | 3.06296200 | 0.31655200 |

| | | | |
|---|---|---|---|
| C | -2.58464400 | -2.56010600 | 0.46811100 |
| H | -2.09817600 | -2.90209000 | -0.45062400 |
| H | -2.14534100 | -3.07651700 | 1.32753700 |
| H | -3.64984700 | -2.82816700 | 0.42807700 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | 1.65782600 | -2.30168800 | 0.66765300 |
| O | 0.83268500 | -0.30270100 | -1.29908200 |
| C | 0.63698800 | -2.88228900 | 0.17083200 |
| C | -0.08283400 | -1.14463700 | -1.49031300 |
| C | -1.15647500 | -0.74398000 | -2.49617600 |
| H | -0.67599100 | -0.40457900 | -3.42053500 |
| H | -1.86331800 | -1.54854400 | -2.72403500 |
| H | -1.71525100 | 0.10376000 | -2.08454600 |
| C | 0.32027200 | -4.23739100 | 0.79514700 |
| H | 0.11926300 | -4.10210300 | 1.86560700 |
| H | -0.53775200 | -4.73718700 | 0.33383000 |
| H | 1.20013400 | -4.88677300 | 0.71611000 |
| C | -0.20804000 | -2.40091700 | -0.83951700 |
| H | -1.04993500 | -3.02447200 | -1.12301400 |
| Cu | 2.36678400 | -0.50968300 | 0.18485500 |
| C | 3.68497600 | 0.99831000 | 0.47180600 |
| H | 3.88055400 | 0.96320800 | 1.54825700 |
| C | 2.90752300 | 2.19453400 | 0.11721700 |
| C | 4.77831800 | 0.45596700 | -0.33856100 |
| O | 2.41076700 | 2.91574300 | 0.99861700 |
| O | 5.01151100 | 0.68763400 | -1.53260800 |
| C | 2.63769600 | 2.50909700 | -1.34483600 |
| H | 3.53515000 | 2.36305500 | -1.95061500 |
| H | 1.88454700 | 1.79906000 | -1.70865000 |
| H | 2.24882200 | 3.52936600 | -1.42372200 |
| C | 5.75094900 | -0.47154800 | 0.41113200 |
| H | 5.32217800 | -0.88188800 | 1.33072700 |
| H | 6.04480800 | -1.29063400 | -0.25267000 |
| H | 6.65829000 | 0.09432500 | 0.66461000 |
| C | -0.58792500 | 2.04803100 | 0.91661200 |
| C | 0.01949000 | 1.04287700 | 1.67230500 |
| C | -0.64913100 | -0.15881500 | 1.90159400 |
| C | -1.93218900 | -0.36731900 | 1.38675500 |
| C | -2.52226900 | 0.65707200 | 0.65306000 |
| C | -1.87335700 | 1.86476700 | 0.40071100 |
| H | -0.02612700 | 2.95333700 | 0.70992800 |
| H | 1.02783200 | 1.20488500 | 2.03711900 |
| H | -0.15099500 | -0.96335800 | 2.43392600 |
| H | -2.43818900 | -1.31400900 | 1.53557500 |
| H | -2.34668800 | 2.63881500 | -0.19404200 |

| | | | |
|---|---|---|---|
| I | -4.51698800 | 0.34170000 | -0.16335600 |

**Complex $TS_{b-c}$**

| | | | |
|---|---|---|---|
| Cu | 0.20334100 | -0.03783900 | -0.05362400 |
| C | 1.95724700 | 0.31944600 | 2.03584200 |
| C | 0.56044800 | 0.70821000 | 1.93697800 |
| C | 0.09486600 | 2.08462100 | 1.80415700 |
| O | 2.94485000 | 1.04098400 | 1.82370500 |
| O | -1.05755800 | 2.42269100 | 2.13532100 |
| H | -0.12756200 | 0.07224400 | 2.49253900 |
| C | -1.94926800 | -0.60890600 | 0.10051300 |
| C | -1.96618600 | -1.94587700 | -0.31873000 |
| C | -2.44801300 | -2.91728800 | 0.56071600 |
| C | -2.95142200 | -2.55553100 | 1.81214100 |
| C | -2.96474800 | -1.20743900 | 2.19121200 |
| C | -2.49033300 | -0.21700200 | 1.33322000 |
| I | -1.90005800 | 0.97989100 | -1.55480200 |
| H | -1.54542300 | -2.22075000 | -1.27683800 |
| H | -2.42596500 | -3.96173100 | 0.25781400 |
| H | -3.33507400 | -3.31686500 | 2.48727000 |
| H | -3.34235800 | -0.91790600 | 3.16938900 |
| H | -2.42946100 | 0.82058300 | 1.64958200 |
| C | 1.03030600 | 3.12257900 | 1.20096800 |
| C | 2.21569700 | -1.14155300 | 2.43853700 |
| H | 0.48349700 | 4.06377400 | 1.08826600 |
| H | 1.40639300 | 2.76806300 | 0.23572400 |
| H | 1.91088300 | 3.25354000 | 1.83783100 |
| H | 1.31623700 | -1.76286800 | 2.38491600 |
| H | 2.61899300 | -1.17322800 | 3.45965100 |
| H | 2.97347200 | -1.55000000 | 1.76282300 |
| O | 1.77476100 | 0.84985400 | -1.13462400 |
| O | 0.90557500 | -1.88136700 | -0.78527400 |
| C | 2.90426700 | 0.29016000 | -1.21095600 |
| C | 2.14121000 | -2.08417200 | -1.00515100 |
| C | 2.55620500 | -3.55278700 | -1.02302900 |
| H | 3.60269400 | -3.70529000 | -1.30769800 |
| H | 2.39399200 | -3.97799700 | -0.02448800 |
| H | 1.90931200 | -4.10283000 | -1.71659200 |
| C | 4.10178100 | 1.22358000 | -1.27915000 |
| H | 4.22531300 | 1.63697000 | -0.27134400 |
| H | 5.02827600 | 0.72299000 | -1.58118300 |
| H | 3.88688500 | 2.05143100 | -1.96346000 |
| C | 3.13407900 | -1.10891400 | -1.19783900 |
| H | 4.15823100 | -1.44910000 | -1.31418500 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | -0.01709500 | 0.12954700 | -0.11356500 |
| C | 1.38159200 | 2.46369100 | 0.68121500 |
| C | 0.12407300 | 2.23106200 | -0.07728300 |
| C | -0.02249600 | 2.60799200 | -1.51415300 |
| O | 2.49247600 | 2.61951700 | 0.17997700 |
| O | -1.11699400 | 2.99200500 | -1.93019400 |
| H | -0.74873200 | 2.56409200 | 0.47841500 |
| C | -1.82996600 | 0.38609700 | 0.45635300 |
| C | -2.11758400 | 0.08583300 | 1.78686700 |
| C | -3.42776700 | 0.25047000 | 2.25469000 |
| C | -4.43245600 | 0.71096900 | 1.40159800 |
| C | -4.12349100 | 1.01168100 | 0.07184100 |
| C | -2.81922700 | 0.85269700 | -0.40595200 |
| H | -1.33585000 | -0.28791400 | 2.43825300 |
| H | -3.65754900 | 0.00915600 | 3.29128500 |
| H | -5.44907800 | 0.83555900 | 1.76899800 |
| H | -4.89695000 | 1.37539300 | -0.60176600 |
| H | -2.57565200 | 1.11320800 | -1.42929100 |
| C | 1.16159700 | 2.50754600 | -2.45328800 |
| C | 1.20402100 | 2.51903500 | 2.19488700 |
| H | 1.99043500 | 3.11498400 | -2.07818100 |
| H | 0.84850300 | 2.83171000 | -3.44949400 |
| H | 1.52917000 | 1.47729700 | -2.46875700 |
| H | 2.17923000 | 2.65323100 | 2.67001300 |
| H | 0.74457300 | 1.58765900 | 2.54072800 |
| H | 0.54115800 | 3.34915400 | 2.47156400 |
| O | 1.76268300 | -0.05032400 | -0.86653600 |
| O | 0.81835000 | -0.59631600 | 1.83703200 |
| C | 2.82113500 | -0.53461000 | -0.34938300 |
| C | 1.97370600 | -1.08837500 | 1.93701500 |
| C | 2.29939500 | -1.75113600 | 3.27140200 |
| H | 3.33872000 | -2.08602800 | 3.34910600 |
| H | 2.08271400 | -1.04821200 | 4.08416500 |
| H | 1.63591000 | -2.61411600 | 3.40345000 |
| C | 4.02110200 | -0.48629400 | -1.27683800 |
| H | 4.24353300 | 0.56655600 | -1.48616400 |
| H | 4.90926100 | -0.96611600 | -0.85458100 |
| H | 3.76222600 | -0.96634700 | -2.22711400 |
| C | 2.97282100 | -1.07036700 | 0.93621700 |
| H | 3.94322600 | -1.48445800 | 1.18727600 |
| I | -0.74264100 | -2.25808500 | -1.07637500 |

**Complex $TS_{c\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | 0.06583800 | 0.16361000 | 0.03560000 |
| C | 0.01117100 | 2.87734500 | 0.06099200 |
| C | -1.13819200 | 1.94458400 | -0.30342400 |

| | | | |
|---|---|---|---|
| C | -1.48844800 | 1.88713000 | -1.78606700 |
| O | 0.60919900 | 3.51209100 | -0.79297800 |
| O | -2.61842500 | 2.20624600 | -2.12823500 |
| H | -2.01278500 | 2.35178900 | 0.20188300 |
| C | -1.78529100 | 0.26870400 | 0.62979700 |
| C | -1.87327200 | 0.32571300 | 2.02959300 |
| C | -2.94409500 | -0.28984000 | 2.68103800 |
| C | -3.95243000 | -0.92079900 | 1.94999000 |
| C | -3.87941300 | -0.93942500 | 0.55317100 |
| C | -2.81296300 | -0.33577800 | -0.10838600 |
| I | 0.17734600 | -2.34958500 | -1.04639100 |
| H | -1.08089000 | 0.78756100 | 2.60435500 |
| H | -2.98459000 | -0.27320300 | 3.76834500 |
| H | -4.78836000 | -1.39229200 | 2.46127500 |
| H | -4.65310600 | -1.43447200 | -0.02895100 |
| H | -2.76052200 | -0.36498900 | -1.18960300 |
| C | -0.46698800 | 1.38303800 | -2.77408900 |
| C | 0.29505200 | 3.07109600 | 1.53791000 |
| H | 0.53332000 | 1.73933700 | -2.52616400 |
| H | -0.76767000 | 1.67950100 | -3.78263100 |
| H | -0.43138500 | 0.28540600 | -2.71403300 |
| H | 0.93025300 | 3.95080000 | 1.66831200 |
| H | 0.80500100 | 2.17867800 | 1.91871900 |
| H | -0.63549600 | 3.18651300 | 2.10607800 |
| O | 1.82383900 | 0.78947400 | -0.71504300 |
| O | 1.10048800 | 0.00074900 | 1.96777600 |
| C | 2.97530400 | 0.48465000 | -0.27806000 |
| C | 2.34222500 | -0.24240400 | 2.02678400 |
| C | 2.83319500 | -0.83844300 | 3.34091000 |
| H | 3.92395500 | -0.90983100 | 3.40491200 |
| H | 2.45747900 | -0.23549300 | 4.17577100 |
| H | 2.40495100 | -1.84250600 | 3.44734600 |
| C | 4.10322700 | 0.68221200 | -1.27853500 |
| H | 4.03236600 | 1.68939300 | -1.70405500 |
| H | 5.09741400 | 0.53769700 | -0.84340300 |
| H | 3.96561000 | -0.03025900 | -2.10085500 |
| C | 3.28329200 | -0.01328800 | 1.00176900 |
| H | 4.32075900 | -0.25577600 | 1.20652700 |

**Complex p**

| | | | |
|---|---|---|---|
| C | 0.85240300 | -0.01952300 | -0.55755800 |
| H | 0.99976100 | 0.02356900 | -1.64035400 |
| C | 1.50931000 | -1.35690900 | -0.12766600 |
| C | 1.58218500 | 1.17926200 | 0.07482700 |
| O | 2.18126500 | -1.96309100 | -0.93811300 |
| O | 1.84378900 | 1.22604200 | 1.26269100 |

| | | | |
|---|---|---|---|
| C | 1.29237900 | -1.84048100 | 1.28570800 |
| H | 1.58307300 | -1.05304800 | 1.98870200 |
| H | 0.22930600 | -2.04637000 | 1.45287700 |
| H | 1.87754900 | -2.74667100 | 1.45235400 |
| C | 1.92988500 | 2.30435800 | -0.87460400 |
| H | 1.03239200 | 2.62649100 | -1.41709500 |
| H | 2.35845500 | 3.14313400 | -0.32283200 |
| H | 2.64717700 | 1.94615000 | -1.62407800 |
| C | -0.64560900 | 0.04241300 | -0.27045300 |
| C | -1.54262500 | -0.29507700 | -1.29334100 |
| C | -1.15566100 | 0.39797900 | 0.98619500 |
| C | -2.91913600 | -0.28239300 | -1.06742700 |
| H | -1.15794800 | -0.57509600 | -2.27117000 |
| C | -2.53287400 | 0.41198900 | 1.21048100 |
| H | -0.47328900 | 0.66922900 | 1.78494800 |
| C | -3.41923200 | 0.07178000 | 0.18687400 |
| H | -3.59934400 | -0.54802800 | -1.87221900 |
| H | -2.91266800 | 0.69267900 | 2.18925400 |
| H | -4.49104100 | 0.08396500 | 0.36477200 |

**Complex d**

| | | | |
|---|---|---|---|
| O | -1.18407700 | -1.84747900 | 0.50482600 |
| O | -1.50813200 | 0.12458000 | -1.57105800 |
| C | -2.44300800 | -1.73557300 | 0.54682600 |
| C | -2.72832800 | 0.01716900 | -1.21965200 |
| C | -3.67856900 | 0.95818700 | -1.93304200 |
| H | -3.48966700 | 0.92388200 | -3.01156100 |
| H | -4.73301900 | 0.73879900 | -1.73594500 |
| H | -3.43912900 | 1.96944700 | -1.58387300 |
| C | -3.15191600 | -2.63718100 | 1.55205100 |
| H | -2.79202400 | -2.39554100 | 2.55952400 |
| H | -4.24225200 | -2.54093600 | 1.52912700 |
| H | -2.87703800 | -3.67972900 | 1.35480000 |
| C | -3.22795000 | -0.85253300 | -0.23226700 |
| H | -4.29816400 | -0.84062800 | -0.05412100 |
| Cu | 0.01280500 | -0.28232500 | -0.36497100 |
| C | -0.42238600 | 1.26642000 | 0.96836400 |
| H | -1.42605800 | 0.90326900 | 1.20862800 |
| C | -0.48481800 | 2.49687900 | 0.14471300 |
| C | 0.53200900 | 1.10864400 | 2.08658500 |
| O | -1.57042000 | 2.95761500 | -0.21434900 |
| O | 1.49799100 | 1.83857000 | 2.30353400 |
| C | 0.81591900 | 3.14294400 | -0.29099700 |
| H | 1.41762200 | 3.39683500 | 0.58606200 |
| H | 1.40470400 | 2.41638800 | -0.86503700 |
| H | 0.59807300 | 4.02354300 | -0.90154200 |

| | | | |
|---|---|---|---|
| C | 0.22016300 | -0.04920000 | 3.03567000 |
| H | -0.03947000 | -0.95556300 | 2.47885000 |
| H | 1.08379200 | -0.23024900 | 3.68011500 |
| H | -0.64479600 | 0.21418900 | 3.66093300 |
| I | 2.50257500 | -0.80447400 | -0.65009300 |

**Complex e**

| | | | |
|---|---|---|---|
| O | -0.56949400 | 1.98313400 | 1.25630100 |
| O | -0.51770700 | 1.32173400 | -1.58468700 |
| C | 0.37553600 | 2.74263200 | 0.88157000 |
| C | 0.44779600 | 2.14147600 | -1.55744300 |
| C | 1.23137900 | 2.27545900 | -2.85465700 |
| H | 0.53383900 | 2.39610200 | -3.69036100 |
| H | 1.94144800 | 3.10888600 | -2.84462600 |
| H | 1.78262400 | 1.34128100 | -3.01871000 |
| C | 1.05082600 | 3.53351300 | 1.99720100 |
| H | 1.59670000 | 2.83658800 | 2.64640500 |
| H | 1.75245400 | 4.28855900 | 1.62763200 |
| H | 0.28465600 | 4.01659900 | 2.61294800 |
| C | 0.88111000 | 2.87701300 | -0.42831500 |
| H | 1.71589500 | 3.55570700 | -0.57093400 |
| Cu | -1.73176000 | 0.85383700 | 0.02299400 |
| C | 1.42017000 | -0.99632500 | -0.13483900 |
| H | 0.86548700 | -0.06455400 | 0.02695600 |
| C | 1.20761600 | -1.33979500 | -1.62688300 |
| C | 0.84655500 | -2.06516400 | 0.81133600 |
| O | 2.09255000 | -1.15336300 | -2.44228700 |
| O | 0.99728400 | -3.25317300 | 0.57697600 |
| C | -0.15314300 | -1.86793300 | -2.01093100 |
| H | -0.24854200 | -2.89889600 | -1.65192500 |
| H | -0.95059500 | -1.28138600 | -1.54170400 |
| H | -0.25912100 | -1.84049800 | -3.09744300 |
| C | 0.13442600 | -1.55375100 | 2.03758800 |
| H | -0.84454100 | -1.15432200 | 1.73388400 |
| H | -0.01162100 | -2.36252100 | 2.75740900 |
| H | 0.68417900 | -0.71900000 | 2.48693200 |
| I | -3.68774000 | -0.71073800 | 0.25739200 |
| C | 4.69575500 | 0.66745900 | 0.93102900 |
| C | 3.35133200 | 0.47952200 | 0.60055700 |
| C | 2.88274100 | -0.78143900 | 0.21679200 |
| C | 3.78526900 | -1.85381200 | 0.16731100 |
| C | 5.12666400 | -1.66677200 | 0.49680800 |
| C | 5.58789800 | -0.40454000 | 0.88277300 |
| H | 5.04311400 | 1.65570900 | 1.22411800 |
| H | 2.66395300 | 1.31961000 | 0.60948200 |
| H | 3.41957900 | -2.83429000 | -0.12121300 |

| | | | |
|---|---|---|---|
| H | 5.81444700 | -2.50819300 | 0.45232000 |
| H | 6.63467200 | -0.25943100 | 1.14043400 |

**Complex e'**

| | | | |
|---|---|---|---|
| O | -0.57013100 | 0.48248500 | 1.61805900 |
| O | -0.51797700 | 0.62449600 | -1.39154400 |
| C | -1.28609900 | 1.44420100 | 1.40632600 |
| C | -1.29653600 | 1.53060600 | -1.14146300 |
| C | -1.54365100 | 2.67193400 | -2.09974500 |
| H | -0.96178200 | 2.52161700 | -3.01126200 |
| H | -2.61259900 | 2.73957400 | -2.34149600 |
| H | -1.22780500 | 3.59825100 | -1.61005000 |
| C | -1.45661600 | 2.56777300 | 2.40228500 |
| H | -1.13152300 | 3.50071200 | 1.93410800 |
| H | -2.51286500 | 2.65825400 | 2.69031200 |
| H | -0.84643100 | 2.36703300 | 3.28566500 |
| C | -2.15620100 | 1.52805400 | 0.13557600 |
| H | -2.71692700 | 2.46727800 | 0.16678600 |
| Cu | 1.18381300 | -0.20925500 | -0.00039800 |
| C | 2.16087100 | 1.54613200 | 0.57390600 |
| H | 1.79579000 | 1.53406100 | 1.60198900 |
| C | 1.50033400 | 2.53794200 | -0.24121500 |
| C | 3.55101300 | 1.10487400 | 0.40890900 |
| O | 0.46250100 | 3.12990000 | 0.15042500 |
| O | 4.28882100 | 1.34849500 | -0.55301400 |
| C | 1.99788900 | 2.82866500 | -1.64878400 |
| H | 3.08822100 | 2.83568900 | -1.69463000 |
| H | 1.65460700 | 2.01932600 | -2.30551700 |
| H | 1.56421100 | 3.77320100 | -1.99207800 |
| C | 4.09805900 | 0.23092500 | 1.54536500 |
| H | 3.78110900 | -0.80478800 | 1.37150600 |
| H | 5.19115900 | 0.27356200 | 1.53650700 |
| H | 3.71475200 | 0.53093700 | 2.52764900 |
| I | 1.17341800 | -2.75689400 | -0.19629200 |
| C | -3.60055400 | -2.00988100 | -0.01534700 |
| C | -2.68350000 | -0.96026500 | 0.03000100 |
| C | -3.14030100 | 0.36567700 | 0.08798500 |
| C | -4.51834300 | 0.61577700 | 0.09807100 |
| C | -5.43375800 | -0.43830100 | 0.05277100 |
| C | -4.97530200 | -1.75585200 | -0.00419200 |
| H | -3.22836200 | -3.03001100 | -0.06106700 |
| H | -1.61952700 | -1.16862300 | 0.01948900 |
| H | -4.87742300 | 1.64261000 | 0.14199000 |
| H | -6.50104700 | -0.22803000 | 0.06159500 |
| H | -5.68477400 | -2.57945100 | -0.04056700 |

**Complex f**

| | | | |
|---|---|---|---|
| O | 1.82173500 | -1.38087500 | -0.24057900 |
| O | 0.50376800 | 1.09641900 | 0.25051000 |
| C | 2.87160400 | -0.66041900 | -0.06951700 |
| C | 1.71456900 | 1.50260000 | 0.35763100 |
| C | 1.84051700 | 2.97760600 | 0.66370800 |
| H | 1.29115600 | 3.19885800 | 1.58514100 |
| H | 2.87939100 | 3.29777400 | 0.77061800 |
| H | 1.36414100 | 3.54979400 | -0.14018800 |
| C | 4.17724100 | -1.40639000 | -0.19984900 |
| H | 4.23404500 | -1.85738000 | -1.19698600 |
| H | 5.04681000 | -0.76417100 | -0.04329700 |
| H | 4.19654100 | -2.22696800 | 0.52617700 |
| C | 2.86899000 | 0.71300600 | 0.21650600 |
| H | 3.82737500 | 1.20271700 | 0.33624300 |
| Cu | 0.05181100 | -0.73397000 | -0.15234700 |
| C | -1.92494500 | -0.69600500 | -0.21354600 |
| H | -2.10434800 | -1.75360900 | -0.45633200 |
| C | -2.15010300 | 0.14817200 | -1.42921200 |
| C | -2.39928900 | -0.31536900 | 1.14307700 |
| O | -2.03554100 | -0.36270500 | -2.54165700 |
| O | -2.62740600 | 0.83534500 | 1.49526000 |
| C | -2.44179300 | 1.62512800 | -1.27272200 |
| H | -3.36154100 | 1.77962800 | -0.70084600 |
| H | -1.64355200 | 2.09598800 | -0.69093600 |
| H | -2.51983500 | 2.07370400 | -2.26579500 |
| C | -2.57774800 | -1.47428800 | 2.12232900 |
| H | -1.69812800 | -2.13055600 | 2.13015200 |
| H | -2.75433700 | -1.08074100 | 3.12550400 |
| H | -3.43493600 | -2.08963000 | 1.81991900 |

**Complex g**

| | | | |
|---|---|---|---|
| O | -0.27259100 | 0.38130500 | -1.87214300 |
| O | 0.41436600 | -2.00269000 | -0.54247000 |
| C | -1.24402200 | -0.33748700 | -2.28821100 |
| C | -0.62157900 | -2.44359000 | -1.16078400 |
| C | -0.95894900 | -3.88392400 | -0.85074500 |
| H | -1.31988200 | -3.93321000 | 0.18373100 |
| H | -1.72912100 | -4.28806900 | -1.51339600 |
| H | -0.05380200 | -4.49748400 | -0.91165400 |
| C | -2.27986700 | 0.40973400 | -3.09049900 |
| H | -1.80267900 | 1.19453800 | -3.68437200 |
| H | -2.86985800 | -0.25107800 | -3.73259800 |
| H | -2.95005100 | 0.88164000 | -2.35928900 |
| C | -1.42991600 | -1.70510500 | -2.02278400 |
| H | -2.31068600 | -2.18375800 | -2.43247900 |

| | | | |
|---|---|---|---|
| Cu | 0.92997000 | -0.14440000 | -0.45570900 |
| C | 2.28993900 | -0.52551400 | 0.96837000 |
| H | 2.59143100 | 0.41573200 | 1.42626200 |
| C | 3.45583200 | -1.08900500 | 0.19827900 |
| C | 1.54050600 | -1.36988200 | 1.97539400 |
| O | 4.38623900 | -0.34918400 | -0.11562600 |
| O | 1.85470400 | -2.52315400 | 2.23411100 |
| C | 3.46727800 | -2.54920000 | -0.19886600 |
| H | 3.57809200 | -3.16023800 | 0.70179700 |
| H | 2.50697900 | -2.82981300 | -0.63918400 |
| H | 4.29484100 | -2.72128300 | -0.89210200 |
| C | 0.38816100 | -0.68333800 | 2.67370000 |
| H | -0.50479400 | -0.70680600 | 2.02995100 |
| H | 0.15242300 | -1.20476300 | 3.60477000 |
| H | 0.59729200 | 0.37474400 | 2.86432800 |
| C | 1.62776500 | 4.45315000 | -0.06708000 |
| C | 2.70171700 | 3.66718000 | -0.49103600 |
| C | 2.58017700 | 2.27227300 | -0.54141600 |
| C | 1.36388300 | 1.69704800 | -0.18907400 |
| C | 0.27963600 | 2.45701700 | 0.24535500 |
| C | 0.42407800 | 3.84830800 | 0.30452800 |
| H | 1.73068500 | 5.53519400 | -0.01993200 |
| H | 3.64508100 | 4.13152100 | -0.77138700 |
| H | 3.42693900 | 1.64984500 | -0.81176000 |
| H | -0.67015600 | 1.99289500 | 0.50683000 |
| H | -0.41814300 | 4.45152300 | 0.63576600 |
| I | -3.15911800 | 0.37698600 | 0.91714200 |

**Complex $TS_{g\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | 1.35736300 | 0.12422400 | 0.56127700 |
| C | 1.34607400 | 0.32020000 | -2.04023400 |
| C | 1.85988200 | -0.88886100 | -1.24157700 |
| C | 3.36657600 | -1.07436300 | -1.13465600 |
| O | 2.12912100 | 1.07395700 | -2.59739700 |
| O | 3.81364400 | -2.21413300 | -1.13244400 |
| H | 1.45949100 | -1.77722900 | -1.72976300 |
| C | 0.92604500 | -1.72747700 | 0.33089800 |
| C | -0.45762900 | -1.93973400 | 0.24554800 |
| C | -1.02155700 | -3.00150000 | 0.94905200 |
| C | -0.21667300 | -3.85947600 | 1.70644300 |
| C | 1.16231900 | -3.65129000 | 1.76570600 |
| C | 1.74762700 | -2.59350900 | 1.06218100 |
| I | -3.79313400 | -0.03484900 | -0.77235200 |
| H | -1.11834800 | -1.26907700 | -0.29482700 |
| H | -2.09959300 | -3.13075800 | 0.90524000 |
| H | -0.66440700 | -4.68964200 | 2.24738400 |

| | | | |
|---|---|---|---|
| H | 1.79464600 | -4.31615100 | 2.34953900 |
| H | 2.82243000 | -2.45933200 | 1.07576300 |
| C | 4.29425000 | 0.11840400 | -1.01899500 |
| C | -0.14918500 | 0.47775300 | -2.18678700 |
| H | 4.49882400 | 0.48866200 | -2.02886100 |
| H | 5.22732900 | -0.21881000 | -0.55823000 |
| H | 3.85071800 | 0.95091100 | -0.46854100 |
| H | -0.35877900 | 1.21671800 | -2.96263600 |
| H | -0.61655700 | 0.81855600 | -1.25376700 |
| H | -0.64295700 | -0.46801800 | -2.43028400 |
| O | 2.13434900 | 1.90633800 | 0.55239800 |
| O | -0.13650100 | 0.66800600 | 1.78600700 |
| C | 1.43601100 | 2.95962100 | 0.79348100 |
| C | -0.56068100 | 1.86442700 | 1.82658900 |
| C | -1.95290400 | 2.04446300 | 2.38250700 |
| H | -2.20266700 | 3.09122000 | 2.58097200 |
| H | -2.66020400 | 1.63398100 | 1.64645800 |
| H | -2.06009300 | 1.45277100 | 3.29756700 |
| C | 2.11154600 | 4.25340900 | 0.38304700 |
| H | 2.31011300 | 4.21951100 | -0.69467500 |
| H | 1.51332400 | 5.13958900 | 0.61345800 |
| H | 3.08216000 | 4.33100700 | 0.88746200 |
| C | 0.16252400 | 2.99656900 | 1.36653600 |
| H | -0.31308400 | 3.96544000 | 1.46844500 |

**Complex h**

| | | | |
|---|---|---|---|
| Cu | -0.97576800 | 0.83951200 | -0.92512500 |
| C | -2.68121000 | -1.48362600 | 1.52601600 |
| C | -1.80766400 | -2.40920300 | 0.64700400 |
| C | -2.64014600 | -3.18000200 | -0.40090000 |
| O | -3.87930600 | -1.68911100 | 1.61682800 |
| O | -2.40450400 | -4.35716700 | -0.59570900 |
| H | -1.45413300 | -3.18228700 | 1.34460300 |
| C | -0.56761800 | -1.75293900 | 0.05135800 |
| C | 0.60544600 | -1.68797100 | 0.79831100 |
| C | 1.75445400 | -1.02833200 | 0.32641600 |
| C | 1.74533900 | -0.41304300 | -0.91542600 |
| C | 0.58173600 | -0.47948800 | -1.71760500 |
| C | -0.57476000 | -1.16360100 | -1.24955900 |
| I | 5.49250600 | 0.02865200 | 0.22959200 |
| H | 0.63522200 | -2.16346800 | 1.77650100 |
| H | 2.67070100 | -0.99743300 | 0.91040700 |
| H | 2.64893700 | 0.07985100 | -1.26356300 |
| H | 0.62863200 | -0.15623100 | -2.75604100 |
| H | -1.37731000 | -1.39790200 | -1.94494100 |
| C | -3.71997200 | -2.44915300 | -1.17750100 |

| | | | |
|---|---|---|---|
| C | -1.99261600 | -0.41928500 | 2.35167800 |
| H | -4.67438800 | -2.64681100 | -0.67709800 |
| H | -3.76566600 | -2.85919700 | -2.19096400 |
| H | -3.58312000 | -1.36528000 | -1.18349600 |
| H | -2.72821900 | 0.05772900 | 3.00245700 |
| H | -1.53178800 | 0.33213800 | 1.70431900 |
| H | -1.18745000 | -0.85731500 | 2.95259400 |
| O | -2.95534800 | 0.72934200 | -0.49208100 |
| O | -0.82879800 | 2.73652000 | -0.49635100 |
| C | -3.59196700 | 1.68722500 | 0.05965100 |
| C | -1.76668000 | 3.41478100 | 0.03740700 |
| C | -1.39203800 | 4.84724600 | 0.37570500 |
| H | -2.20920400 | 5.40851500 | 0.83805000 |
| H | -0.52905500 | 4.84033000 | 1.05106400 |
| H | -1.07535000 | 5.35967100 | -0.54004900 |
| C | -5.02235700 | 1.36372700 | 0.44978000 |
| H | -5.01573500 | 0.48716700 | 1.10766800 |
| H | -5.53154000 | 2.19529100 | 0.94585600 |
| H | -5.58515300 | 1.08364200 | -0.44886200 |
| C | -3.07270500 | 2.96719700 | 0.33203500 |
| H | -3.74072100 | 3.67931900 | 0.80400400 |

**Complex h'**

| | | | |
|---|---|---|---|
| O | -0.60659600 | -0.81382400 | -1.89261500 |
| O | -0.39837600 | -2.12502100 | 0.67406200 |
| C | 0.53096000 | -0.53605900 | -1.48377500 |
| C | 0.15085800 | -1.07966200 | 0.99412200 |
| C | 0.22028300 | -0.64026600 | 2.43808700 |
| H | 0.30149200 | -1.52675000 | 3.07245200 |
| H | 1.05114500 | 0.04516900 | 2.62390700 |
| H | -0.72388500 | -0.13163200 | 2.67501400 |
| C | 1.66634100 | -0.47241200 | -2.45307600 |
| H | 1.32976600 | -0.73079100 | -3.45915800 |
| H | 2.09425600 | 0.53721500 | -2.43855600 |
| H | 2.48304900 | -1.12401400 | -2.11324800 |
| C | 0.83725400 | -0.18325800 | -0.03499300 |
| H | 1.92054600 | -0.35949800 | 0.12536900 |
| Cu | -2.28845900 | -0.95688200 | -0.95598000 |
| C | -4.01143300 | -0.87741200 | -0.00424400 |
| H | -4.51945000 | -1.82022600 | -0.22732900 |
| C | -4.73953700 | 0.24606600 | -0.65885700 |
| C | -3.50438800 | -0.80367500 | 1.37967600 |
| O | -5.59975900 | 0.02281800 | -1.50912200 |
| O | -3.14024000 | 0.23279300 | 1.95627800 |
| C | -4.39581600 | 1.68558500 | -0.29467000 |

| | | | |
|---|---|---|---|
| H | -4.38676700 | 1.82842800 | 0.78894400 |
| H | -3.38348100 | 1.92137000 | -0.64408400 |
| H | -5.11242100 | 2.35084500 | -0.78352400 |
| C | -3.36404700 | -2.13163500 | 2.12340800 |
| H | -2.37200200 | -2.54410300 | 1.90535300 |
| H | -3.43067000 | -1.94280500 | 3.19870400 |
| H | -4.11571200 | -2.86839700 | 1.82215500 |
| C | -0.88880400 | 3.19056800 | 0.55134300 |
| C | -0.68232400 | 1.81520500 | 0.43680400 |
| C | 0.59482500 | 1.31638600 | 0.14350100 |
| C | 1.66315300 | 2.20830700 | -0.02570200 |
| C | 1.44941300 | 3.58346500 | 0.08571000 |
| C | 0.17390900 | 4.07855000 | 0.36817600 |
| H | -1.88281700 | 3.55839300 | 0.79125900 |
| H | -1.51594300 | 1.14375000 | 0.62250800 |
| H | 2.66078000 | 1.81694700 | -0.21528400 |
| H | 2.28628400 | 4.26564500 | -0.04088300 |
| H | 0.01082600 | 5.15015600 | 0.45607300 |
| I | 4.66841900 | -0.54250500 | 0.08192200 |

**Complex a...p**

| | | | |
|---|---|---|---|
| Cu | -1.60374300 | -0.82893200 | -0.25128100 |
| C | 3.26312400 | 0.12889700 | -1.12652800 |
| C | 2.83295000 | 1.48213200 | -0.54050200 |
| C | 1.93079000 | 2.25025200 | -1.54483000 |
| O | 3.20254600 | -0.06807100 | -2.32795600 |
| O | 2.33941400 | 3.29231200 | -2.02262100 |
| H | 3.76285100 | 2.06757500 | -0.50111200 |
| C | 2.23845800 | 1.43080800 | 0.85453100 |
| C | 1.21788400 | 0.52624400 | 1.17574100 |
| C | 0.63658400 | 0.52285100 | 2.44381600 |
| C | 1.08250600 | 1.42149600 | 3.41596600 |
| C | 2.10498000 | 2.32345600 | 3.11133900 |
| C | 2.67631300 | 2.32908500 | 1.83766500 |
| I | -3.33531000 | 0.98992200 | -0.24503100 |
| H | 0.85902600 | -0.17519000 | 0.43012700 |
| H | -0.16504000 | -0.18118900 | 2.64198700 |
| H | 0.62864900 | 1.42450600 | 4.40400800 |
| H | 2.45443600 | 3.02892800 | 3.86193700 |
| H | 3.46230600 | 3.04247300 | 1.59834600 |
| C | 0.56801100 | 1.68035700 | -1.84829500 |
| C | 3.81161200 | -0.91890600 | -0.17921600 |
| H | 0.60760000 | 0.60691500 | -2.05764600 |
| H | 0.13378300 | 2.21485500 | -2.69565500 |
| H | -0.10057500 | 1.79830800 | -0.98573900 |
| H | 4.49172100 | -1.57517000 | -0.72845200 |

| | | | |
|---|---|---|---|
| H | 2.97609100 | -1.52421600 | 0.19712600 |
| H | 4.31029500 | -0.47066500 | 0.68597600 |
| O | -0.17614200 | -1.63705000 | -1.46814400 |
| O | -0.89542700 | -2.01749200 | 1.32697500 |
| C | 0.64791700 | -2.55694100 | -1.17458200 |
| C | 0.07790000 | -2.82192300 | 1.25860100 |
| C | 0.47742700 | -3.47882400 | 2.57631200 |
| H | 1.22581600 | -4.26967600 | 2.45944000 |
| H | 0.88403800 | -2.70590300 | 3.24126000 |
| H | -0.41445400 | -3.88824600 | 3.06292000 |
| C | 1.53275800 | -3.03147900 | -2.31918800 |
| H | 2.19517000 | -2.21381200 | -2.62443800 |
| H | 2.14021900 | -3.90406700 | -2.05597000 |
| H | 0.89914900 | -3.27801300 | -3.17845400 |
| C | 0.82836000 | -3.13569600 | 0.10145500 |
| H | 1.60032900 | -3.89269200 | 0.19839000 |

**Complex PhI**

| | | | |
|---|---|---|---|
| C | -2.66651500 | 1.20749400 | -0.00000100 |
| C | -3.36684500 | 0.00000500 | 0.00000300 |
| C | -2.66655000 | -1.20747700 | -0.00000100 |
| C | -1.26884500 | -1.21676500 | -0.00000100 |
| C | -0.58793100 | -0.00001900 | -0.00000200 |
| C | -1.26883600 | 1.21676200 | -0.00000200 |
| H | -3.20369900 | 2.15213600 | 0.00000400 |
| H | -4.45306500 | 0.00003300 | 0.00000200 |
| H | -3.20371500 | -2.15213000 | 0.00000400 |
| H | -0.72680400 | -2.15608900 | -0.00000600 |
| H | -0.72675000 | 2.15606000 | -0.00000500 |
| I | 1.57107900 | 0.00000000 | 0.00000000 |

**Complex PhI-radical**

| | | | |
|---|---|---|---|
| C | 3.91413400 | -0.00012200 | 0.00028400 |
| C | 3.21409900 | 1.21165200 | 0.00010600 |
| C | 1.81054600 | 1.21355600 | -0.00027300 |
| C | 1.14041900 | 0.00012400 | -0.00045300 |
| C | 1.81033000 | -1.21342700 | -0.00026400 |
| C | 3.21388300 | -1.21177200 | 0.00009800 |
| H | 5.00290500 | -0.00021900 | 0.00057500 |
| H | 3.76241400 | 2.15423200 | 0.00025800 |
| H | 1.25810400 | 2.15135400 | -0.00040600 |
| H | 1.25771500 | -2.15112100 | -0.00039900 |
| H | 3.76202900 | -2.15444900 | 0.00024900 |
| I | -1.99365300 | 0.00000300 | 0.00005200 |

**Complex Ph-radical**

| | | | |
|---|---|---|---|
| C | -1.21437700 | 0.63277300 | -0.00000600 |
| C | -1.22652500 | -0.77200200 | 0.00002200 |
| C | -0.00001200 | -1.40049900 | -0.00001000 |
| C | 1.22652700 | -0.77199300 | -0.00000800 |
| C | 1.21439000 | 0.63274600 | 0.00001800 |
| C | -0.00000300 | 1.32510100 | -0.00000500 |
| H | -2.15492700 | 1.17909500 | -0.00002700 |
| H | -2.16321900 | -1.32327800 | -0.00000900 |
| H | 2.16319100 | -1.32332300 | -0.00002600 |
| H | 2.15492100 | 1.17910400 | 0.00001100 |
| H | 0.00002600 | 2.41165600 | -0.00002200 |

## 12. TPSS-optimised geometries (singlet spin state)

**Complex b**

| | | | |
|---|---|---|---|
| O | 1.39164000 | -1.40174100 | -0.19066100 |
| O | 1.08985400 | 1.50484600 | -0.05368500 |
| C | 2.61755400 | -1.07367200 | -0.02082400 |
| C | 2.35535300 | 1.42503500 | 0.10312900 |
| C | 3.07608500 | 2.76256400 | 0.29095400 |
| H | 2.67963500 | 3.26838000 | 1.18317000 |
| H | 4.16367300 | 2.65067900 | 0.39831400 |
| H | 2.86500500 | 3.41461500 | -0.56850000 |
| C | 3.59988600 | -2.24608900 | 0.03195200 |
| H | 3.52912100 | -2.82558400 | -0.89991200 |
| H | 4.64045200 | -1.92434400 | 0.17414200 |
| H | 3.31900800 | -2.92132600 | 0.85300000 |
| C | 3.12684400 | 0.23747500 | 0.11992700 |
| H | 4.20255100 | 0.34241200 | 0.26262200 |
| Cu | -0.14388500 | -0.10224100 | -0.28641300 |
| C | -2.11752100 | -0.16120000 | -0.58309100 |
| H | -2.21561700 | -0.42380100 | -1.64367500 |
| C | -2.63077500 | 1.19390800 | -0.30806200 |
| C | -2.19423200 | -1.30818600 | 0.33369500 |
| O | -2.99722700 | 1.95198000 | -1.22785100 |
| O | -2.41648500 | -1.27987300 | 1.57047700 |
| C | -2.68744600 | 1.68586600 | 1.14236400 |
| H | -2.91404200 | 0.85671700 | 1.82441000 |
| H | -1.69912600 | 2.08191000 | 1.42273100 |
| H | -3.42148900 | 2.49977300 | 1.21414900 |
| C | -2.05203800 | -2.69842300 | -0.32563300 |
| H | -1.73811600 | -2.64717100 | -1.37688000 |
| H | -1.32094200 | -3.29364100 | 0.23625200 |
| H | -3.02195800 | -3.21900700 | -0.26655700 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | 4.96557600 | 0.90092300 | -0.37691000 |
| O | 2.09820300 | 1.30259800 | 0.10731100 |
| C | 4.96095800 | 2.16710900 | -0.18832700 |
| C | 2.50134900 | 2.51261400 | 0.22801700 |
| C | 1.41122500 | 3.54105800 | 0.53490400 |
| H | 0.86480500 | 3.23657600 | 1.43883300 |
| H | 1.81136400 | 4.55299000 | 0.68190900 |
| H | 0.68623800 | 3.56371200 | -0.29191000 |
| C | 6.32904300 | 2.84248100 | -0.29245500 |
| H | 6.75387800 | 2.65716200 | -1.28949400 |
| H | 6.28276800 | 3.92590500 | -0.11985200 |
| H | 7.01492600 | 2.39187800 | 0.43895900 |

| | | | |
|---|---|---|---|
| C | 3.83314400 | 2.97054000 | 0.09938000 |
| H | 4.00563900 | 4.03800600 | 0.23512800 |
| Cu | 3.34762000 | -0.27557500 | -0.26767100 |
| C | 2.93406800 | -2.21640900 | -0.50231600 |
| H | 3.00931300 | -2.36724500 | -1.58579000 |
| C | 1.55040900 | -2.31715200 | -0.02572700 |
| C | 4.14157800 | -2.58785900 | 0.25242900 |
| O | 0.59335900 | -2.41301700 | -0.83156500 |
| O | 4.23308300 | -2.78530500 | 1.48775800 |
| C | 1.26190000 | -2.28165400 | 1.47743000 |
| H | 2.13628400 | -2.61346200 | 2.04969000 |
| H | 1.02797600 | -1.24759500 | 1.77344000 |
| H | 0.37755000 | -2.89998000 | 1.68409900 |
| C | 5.40808300 | -2.81846000 | -0.59954300 |
| H | 5.30955200 | -2.44696500 | -1.62806100 |
| H | 6.26309400 | -2.32685300 | -0.11883600 |
| H | 5.62005600 | -3.89954200 | -0.63163900 |
| C | -1.93641100 | -0.60808900 | -0.23644100 |
| C | -1.43589200 | 0.67545600 | 0.03168500 |
| C | -2.32060800 | 1.73556600 | 0.27089600 |
| C | -3.71072300 | 1.53299300 | 0.24417800 |
| C | -4.17911300 | 0.24540700 | -0.02659600 |
| C | -3.32354400 | -0.83239700 | -0.26703400 |
| H | -1.23571800 | -1.42984800 | -0.42042100 |
| H | -0.35822200 | 0.84059100 | 0.05102900 |
| H | -1.93684100 | 2.73451200 | 0.48097600 |
| H | -4.39865600 | 2.35464900 | 0.42858300 |
| H | -3.71732400 | -1.82450900 | -0.47457000 |
| I | -6.34475900 | -0.08787000 | -0.07613700 |

**Complex $TS_{b-c}$**

| | | | |
|---|---|---|---|
| Cu | -0.39517400 | -0.24676700 | 0.24040900 |
| C | -1.10301000 | -2.61636300 | 1.28538300 |
| C | 0.00895300 | -2.27426300 | 0.39115100 |
| C | 0.10189700 | -2.70206100 | -1.01283200 |
| O | -2.22185900 | -3.05965600 | 0.95097400 |
| O | 1.20838800 | -2.79049000 | -1.59844200 |
| H | 0.98306800 | -2.24593000 | 0.88664400 |
| C | 1.99634100 | 0.47577300 | 0.15199800 |
| C | 2.14322900 | 1.40341100 | 1.19731800 |
| C | 3.07607600 | 1.13396100 | 2.20831900 |
| C | 3.88058300 | -0.01379400 | 2.15219400 |
| C | 3.73865100 | -0.90635800 | 1.07646900 |
| C | 2.81458700 | -0.66312000 | 0.05126300 |
| I | 1.07317500 | 1.25336300 | -1.76915900 |
| H | 1.50525600 | 2.27989600 | 1.24683600 |

| | | | |
|---|---|---|---|
| H | 3.17144800 | 1.83266900 | 3.04074600 |
| H | 4.61466800 | -0.20845300 | 2.93453500 |
| H | 4.34929000 | -1.80909400 | 1.02878800 |
| H | 2.65246300 | -1.38988400 | -0.74682300 |
| C | -1.17477400 | -3.03353900 | -1.78101600 |
| C | -0.83904500 | -2.40392300 | 2.79329800 |
| H | -0.89978600 | -3.36026700 | -2.79210100 |
| H | -1.82496300 | -2.14943600 | -1.82623200 |
| H | -1.74881000 | -3.80533700 | -1.25172100 |
| H | 0.18167000 | -2.06335400 | 3.01192500 |
| H | -1.03265600 | -3.34727200 | 3.32614500 |
| H | -1.54661900 | -1.65690300 | 3.17866800 |
| O | -2.22851300 | -0.02150400 | -0.74867000 |
| O | -0.82581000 | 1.29829200 | 1.48126100 |
| C | -3.11892100 | 0.82649300 | -0.42357700 |
| C | -1.93441700 | 1.94435600 | 1.49916500 |
| C | -2.02960800 | 3.01925900 | 2.58421300 |
| H | -2.98654500 | 3.55739200 | 2.56577600 |
| H | -1.90094200 | 2.55366900 | 3.57203900 |
| H | -1.21087200 | 3.74284900 | 2.45943300 |
| C | -4.38931100 | 0.81067600 | -1.27768500 |
| H | -4.83763500 | -0.19162700 | -1.23614000 |
| H | -5.13220100 | 1.55176200 | -0.95303900 |
| H | -4.12472600 | 1.00479300 | -2.32695700 |
| C | -3.03642600 | 1.76653800 | 0.63780400 |
| H | -3.89680100 | 2.41711900 | 0.79324000 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | 0.02087100 | 0.16885000 | -0.06370200 |
| C | 1.19109300 | 2.61754300 | 0.78997600 |
| C | 0.05265900 | 2.29321900 | -0.11056700 |
| C | 0.05359000 | 2.61676400 | -1.56974100 |
| O | 2.35383800 | 2.83969300 | 0.41813200 |
| O | -1.02199500 | 2.88333600 | -2.13640000 |
| H | -0.91120300 | 2.55389100 | 0.32781200 |
| C | -1.84661100 | 0.31155600 | 0.43661100 |
| C | -2.18820400 | -0.12457700 | 1.72348100 |
| C | -3.52651200 | -0.03454700 | 2.14821700 |
| C | -4.51136500 | 0.48191100 | 1.29636100 |
| C | -4.15257000 | 0.91754400 | 0.01222300 |
| C | -2.81956100 | 0.83717400 | -0.42363900 |
| H | -1.42608100 | -0.54222700 | 2.37763000 |
| H | -3.79165200 | -0.38102500 | 3.14920100 |
| H | -5.54853000 | 0.54602600 | 1.62905900 |
| H | -4.90795100 | 1.32845900 | -0.65987100 |
| H | -2.54459800 | 1.21181300 | -1.40754500 |

| | | | |
|---|---|---|---|
| C | 1.35454500 | 2.63937600 | -2.35524600 |
| C | 0.84012700 | 2.68141200 | 2.28047700 |
| H | 2.08884900 | 3.28515400 | -1.85736400 |
| H | 1.14137800 | 2.98046300 | -3.37530000 |
| H | 1.79168200 | 1.63239600 | -2.36396200 |
| H | 1.71381200 | 3.03189800 | 2.84217800 |
| H | 0.55573000 | 1.67745400 | 2.62601600 |
| H | -0.01261700 | 3.35274100 | 2.45961900 |
| O | 1.84332600 | 0.04297500 | -0.75056400 |
| O | 0.74074100 | -0.56609600 | 1.88050300 |
| C | 2.83876000 | -0.58031500 | -0.22991200 |
| C | 1.86898200 | -1.14002100 | 2.01277700 |
| C | 2.10786700 | -1.84055800 | 3.35131300 |
| H | 3.12553700 | -2.24067400 | 3.44723300 |
| H | 1.91683500 | -1.13595200 | 4.17262400 |
| H | 1.38952200 | -2.66624000 | 3.45539800 |
| C | 4.06276300 | -0.64451000 | -1.13478400 |
| H | 4.37745800 | 0.37744300 | -1.38652100 |
| H | 4.90067800 | -1.17547300 | -0.66607800 |
| H | 3.79255900 | -1.14954500 | -2.07244200 |
| C | 2.89862700 | -1.17847100 | 1.04117800 |
| H | 3.82314700 | -1.68882600 | 1.30556500 |
| I | -0.61796700 | -2.20027700 | -1.18984200 |

**Complex $TS_{c\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | 0.11558400 | 0.17128600 | 0.02840700 |
| C | 0.04922800 | 2.78618600 | -0.40478300 |
| C | -1.16245300 | 1.86934400 | -0.58851500 |
| C | -1.55832800 | 1.57770200 | -2.03481100 |
| O | 0.72105000 | 3.18126200 | -1.36086300 |
| O | -2.69620100 | 1.88886500 | -2.39819300 |
| H | -2.00853800 | 2.39759400 | -0.13893100 |
| C | -1.75090500 | 0.40938300 | 0.60031800 |
| C | -1.84615600 | 0.73478500 | 1.97316600 |
| C | -2.90690900 | 0.23829200 | 2.74171200 |
| C | -3.91379200 | -0.53838100 | 2.15192400 |
| C | -3.84403600 | -0.82355400 | 0.77892000 |
| C | -2.78643700 | -0.34215500 | 0.00194000 |
| I | 0.11101200 | -2.49171300 | -0.72243500 |
| H | -1.06413900 | 1.31895300 | 2.44986600 |
| H | -2.94229000 | 0.46561300 | 3.80845500 |
| H | -4.74387800 | -0.91358500 | 2.75099300 |
| H | -4.61435800 | -1.43313100 | 0.30562700 |
| H | -2.74501400 | -0.58451000 | -1.05644900 |
| C | -0.57667500 | 0.89272300 | -2.95774500 |
| C | 0.30636600 | 3.31679000 | 1.00248200 |

| | | | |
|---|---|---|---|
| H | 0.41373000 | 1.35256200 | -2.86965600 |
| H | -0.95457100 | 0.94192000 | -3.98590800 |
| H | -0.46500800 | -0.16341100 | -2.65497400 |
| H | 0.99306400 | 4.16856200 | 0.93812400 |
| H | 0.76006200 | 2.52120300 | 1.61246100 |
| H | -0.63011700 | 3.62398500 | 1.49013400 |
| O | 1.86990400 | 0.53316300 | -0.87230100 |
| O | 1.09748400 | 0.31056300 | 1.92105500 |
| C | 3.02528500 | 0.34968600 | -0.35693400 |
| C | 2.35571800 | 0.11056300 | 2.04907400 |
| C | 2.83582600 | -0.14858400 | 3.47730700 |
| H | 3.92764500 | -0.23937800 | 3.54968000 |
| H | 2.49698000 | 0.66554700 | 4.13401500 |
| H | 2.37533400 | -1.07607100 | 3.84601800 |
| C | 4.18122500 | 0.38135200 | -1.35245900 |
| H | 4.12435900 | 1.30378600 | -1.94614400 |
| H | 5.16235300 | 0.32240600 | -0.86334800 |
| H | 4.07629800 | -0.46335000 | -2.04788600 |
| C | 3.31077600 | 0.12257100 | 1.00933100 |
| H | 4.35222600 | -0.04626500 | 1.28000900 |

**Complex a...p**

| | | | |
|---|---|---|---|
| Cu | -0.98026800 | -0.07034100 | 0.38038400 |
| C | 3.19295900 | 0.89801800 | -1.34034900 |
| C | 2.96761000 | -0.30654700 | -0.39251600 |
| C | 4.31295500 | -0.90192100 | 0.09030500 |
| O | 4.01415900 | 1.78207700 | -1.09460700 |
| O | 4.68825800 | -1.98397100 | -0.35153600 |
| H | 2.48287700 | -1.10629600 | -0.96442900 |
| C | 2.02306400 | 0.09895400 | 0.74539000 |
| C | 0.98420000 | -0.80791900 | 1.09851000 |
| C | 0.10769100 | -0.50266000 | 2.18245100 |
| C | 0.27184300 | 0.72220400 | 2.87940000 |
| C | 1.28099200 | 1.61302100 | 2.50802400 |
| C | 2.15417900 | 1.30642700 | 1.44471300 |
| I | -1.85231300 | -2.51121100 | -0.52369400 |
| H | 0.94766400 | -1.79577400 | 0.64252000 |
| H | -0.57596700 | -1.26637500 | 2.55188000 |
| H | -0.40089500 | 0.96284000 | 3.70133800 |
| H | 1.39251400 | 2.56037800 | 3.03609000 |
| H | 2.92740000 | 2.01656400 | 1.15453900 |
| C | 5.13823700 | -0.10401300 | 1.08237100 |
| C | 2.29233000 | 0.93492600 | -2.55502000 |
| H | 5.31444300 | 0.89887100 | 0.66843300 |
| H | 6.08308100 | -0.62359100 | 1.27350000 |
| H | 4.58145700 | 0.02636900 | 2.02029900 |

| | | | |
|---|---|---|---|
| H | 2.54602500 | 1.79841000 | -3.18011200 |
| H | 1.24138800 | 1.00107400 | -2.21782800 |
| H | 2.38965900 | 0.00454500 | -3.13331500 |
| O | -2.56262700 | 0.97893000 | 1.11611200 |
| O | -0.66317500 | 1.24588900 | -1.16983800 |
| C | -3.05265400 | 2.00320000 | 0.53431900 |
| C | -1.44276200 | 2.23635400 | -1.40286600 |
| C | -1.08476100 | 3.07471800 | -2.63147200 |
| H | -1.79365600 | 3.89496600 | -2.80389700 |
| H | -0.07674100 | 3.49740900 | -2.51047200 |
| H | -1.06250600 | 2.42879500 | -3.52051000 |
| C | -4.28839700 | 2.60420200 | 1.20823000 |
| H | -4.05135300 | 2.85664600 | 2.25162300 |
| H | -4.65737100 | 3.50284100 | 0.69646200 |
| H | -5.08900200 | 1.85139200 | 1.23107900 |
| C | -2.57239700 | 2.62231100 | -0.64689700 |
| H | -3.12211900 | 3.49396200 | -1.00115600 |

**Complex PhI**

| | | | |
|---|---|---|---|
| C | 2.67465200 | 1.21205800 | -0.00000300 |
| C | 3.37727200 | 0.00000200 | -0.00000400 |
| C | 2.67466200 | -1.21205300 | -0.00000300 |
| C | 1.27145000 | -1.22246800 | -0.00000100 |
| C | 0.59126900 | -0.00000600 | -0.00000100 |
| C | 1.27144600 | 1.22246600 | -0.00000100 |
| H | 3.21272000 | 2.15923100 | -0.00000400 |
| H | 4.46611400 | 0.00001000 | -0.00000500 |
| H | 3.21272700 | -2.15922800 | -0.00000400 |
| H | 0.72693900 | -2.16343500 | 0.00000000 |
| H | 0.72692100 | 2.16342500 | -0.00000100 |
| I | -1.57565900 | 0.00000000 | 0.00000200 |

## 13. PBE0-optimised geometries (singlet spin state)

**Complex b**

| | | | |
|---|---|---|---|
| O | 1.48652900 | -1.43130700 | -0.33934900 |
| O | 1.07820100 | 1.41584900 | 0.09561000 |
| C | 2.67927700 | -1.07756400 | -0.12247900 |
| C | 2.32403200 | 1.36864900 | 0.25095000 |
| C | 2.99911800 | 2.69282700 | 0.56923800 |
| H | 2.56234800 | 3.10738100 | 1.48506100 |
| H | 4.08289600 | 2.60624300 | 0.69649400 |
| H | 2.78766200 | 3.40586500 | -0.23582400 |
| C | 3.70242100 | -2.19905900 | -0.17701500 |
| H | 3.65777800 | -2.68087500 | -1.16063700 |
| H | 4.72561500 | -1.85780600 | 0.00849300 |
| H | 3.43949500 | -2.96235900 | 0.56458700 |
| C | 3.13886600 | 0.21990600 | 0.15810400 |
| H | 4.20495500 | 0.34793800 | 0.32040000 |
| Cu | -0.13000500 | -0.23451600 | -0.31862700 |
| C | -2.11665800 | -0.22575900 | -0.54424700 |
| H | -2.23945600 | -0.66127300 | -1.54045100 |
| C | -2.47376600 | 1.19895300 | -0.53976800 |
| C | -2.39964700 | -1.15295700 | 0.54278800 |
| O | -2.73873400 | 1.79925400 | -1.58217000 |
| O | -2.66701400 | -0.87563500 | 1.71902300 |
| C | -2.47024000 | 1.95156900 | 0.77745400 |
| H | -2.86063900 | 1.32599400 | 1.58494200 |
| H | -1.43169000 | 2.20055900 | 1.03068300 |
| H | -3.03775200 | 2.87982600 | 0.65818000 |
| C | -2.40480800 | -2.63460900 | 0.15681500 |
| H | -1.99798100 | -2.82528800 | -0.84079100 |
| H | -1.82769700 | -3.19988400 | 0.89547500 |
| H | -3.43881100 | -3.00238500 | 0.19760100 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | 4.86947200 | 1.02235600 | -0.42339800 |
| O | 2.02499900 | 1.30524900 | 0.15199300 |
| C | 4.81945600 | 2.26703300 | -0.22724400 |
| C | 2.37844600 | 2.51113000 | 0.26351800 |
| C | 1.26936400 | 3.49173000 | 0.60230700 |
| H | 0.76596600 | 3.16348000 | 1.51906600 |
| H | 1.62754700 | 4.51676500 | 0.73727000 |
| H | 0.52155300 | 3.47957700 | -0.19973000 |
| C | 6.14248300 | 2.99838000 | -0.36626800 |
| H | 6.54418500 | 2.82859100 | -1.37185400 |
| H | 6.05948300 | 4.07526900 | -0.19101700 |
| H | 6.86354000 | 2.57412300 | 0.34180000 |

| | | | |
|---|---|---|---|
| C | 3.67887900 | 3.02360600 | 0.10013500 |
| H | 3.81288100 | 4.09245400 | 0.23538200 |
| Cu | 3.31690200 | -0.25643400 | -0.27993500 |
| C | 2.96240200 | -2.21636200 | -0.48052900 |
| H | 3.09664900 | -2.35021500 | -1.55797100 |
| C | 1.55883100 | -2.32778200 | -0.09489100 |
| C | 4.09370900 | -2.66747000 | 0.32255200 |
| O | 0.66212000 | -2.40607600 | -0.94509700 |
| O | 4.10036200 | -2.92500800 | 1.53171200 |
| C | 1.18634700 | -2.30650200 | 1.37518100 |
| H | 1.98528200 | -2.73243300 | 1.98735100 |
| H | 1.04648500 | -1.26312200 | 1.68644300 |
| H | 0.23667800 | -2.83343400 | 1.51150300 |
| C | 5.39601500 | -2.87925800 | -0.45063700 |
| H | 5.39325700 | -2.40616000 | -1.43701800 |
| H | 6.23039400 | -2.48625800 | 0.13793500 |
| H | 5.55821800 | -3.95826000 | -0.57525200 |
| C | -1.86806200 | -0.59994600 | -0.29339200 |
| C | -1.36777500 | 0.65015400 | 0.07092800 |
| C | -2.24694000 | 1.68184400 | 0.39045900 |
| C | -3.62739300 | 1.48377600 | 0.34963500 |
| C | -4.09973100 | 0.23063900 | -0.01688900 |
| C | -3.24588400 | -0.81671000 | -0.33872800 |
| H | -1.17126900 | -1.40391800 | -0.53958200 |
| H | -0.29129100 | 0.81339600 | 0.10164500 |
| H | -1.86106800 | 2.65769900 | 0.67680600 |
| H | -4.31200400 | 2.28833400 | 0.59774800 |
| H | -3.63889300 | -1.78790800 | -0.62159800 |
| I | -6.22819300 | -0.09338000 | -0.08828900 |

**Complex $TS_{b-c}$**

| | | | |
|---|---|---|---|
| Cu | -0.21876800 | -0.16460200 | 0.02659900 |
| C | -1.31270400 | -2.54245000 | 0.87935500 |
| C | -0.10971700 | -2.27628100 | 0.10448300 |
| C | 0.04588700 | -2.60948100 | -1.30734800 |
| O | -2.42916900 | -2.81913600 | 0.43193800 |
| O | 1.16412000 | -2.75636000 | -1.82362600 |
| H | 0.81808300 | -2.38454000 | 0.66565700 |
| C | 1.92536900 | 0.29618400 | 0.29217400 |
| C | 2.03159600 | 0.86677200 | 1.56525200 |
| C | 2.92164900 | 0.30835600 | 2.47867100 |
| C | 3.72721600 | -0.77003000 | 2.11811000 |
| C | 3.62954600 | -1.30174700 | 0.83136700 |
| C | 2.75014500 | -0.76291900 | -0.10116200 |
| I | 1.22695400 | 1.68527000 | -1.37526700 |
| H | 1.38412700 | 1.68819900 | 1.84730200 |

| | | | |
|---|---|---|---|
| H | 2.98343800 | 0.72880300 | 3.48013900 |
| H | 4.42945000 | -1.19180000 | 2.83311900 |
| H | 4.23858000 | -2.15553000 | 0.54334500 |
| H | 2.62803500 | -1.22637900 | -1.07573900 |
| C | -1.18882200 | -2.76156700 | -2.17084800 |
| C | -1.14885400 | -2.41891900 | 2.39466200 |
| H | -0.87133000 | -2.99838200 | -3.19089700 |
| H | -1.77547500 | -1.83700000 | -2.15105200 |
| H | -1.84296300 | -3.54109000 | -1.76843100 |
| H | -1.96871300 | -2.94972800 | 2.88750900 |
| H | -1.19507900 | -1.35839900 | 2.67176900 |
| H | -0.18570700 | -2.80849700 | 2.74398400 |
| O | -2.00152300 | 0.21125800 | -0.98038400 |
| O | -0.92533200 | 1.03672300 | 1.61257700 |
| C | -3.00152000 | 0.82067000 | -0.52818800 |
| C | -2.07530600 | 1.55610500 | 1.67760800 |
| C | -2.36554800 | 2.32460800 | 2.95606900 |
| H | -3.36331600 | 2.77368300 | 2.97113100 |
| H | -2.26565800 | 1.64797900 | 3.81292700 |
| H | -1.61552800 | 3.11436800 | 3.08159300 |
| C | -4.22887200 | 0.81450200 | -1.42107500 |
| H | -4.57523900 | -0.22006200 | -1.52643300 |
| H | -5.04839600 | 1.42756500 | -1.03342600 |
| H | -3.95197400 | 1.16691100 | -2.42075600 |
| C | -3.09026400 | 1.49200800 | 0.71078100 |
| H | -4.03020800 | 1.98330800 | 0.94254600 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | 0.00333300 | 0.16266900 | -0.10139700 |
| C | 1.13383000 | 2.59259900 | 0.80537900 |
| C | -0.01953600 | 2.24119000 | -0.06033100 |
| C | -0.06518200 | 2.62010700 | -1.50108500 |
| O | 2.25839000 | 2.86041400 | 0.40251600 |
| O | -1.14634400 | 2.88104200 | -2.02233400 |
| H | -0.96646900 | 2.49998000 | 0.40792600 |
| C | -1.83761500 | 0.27813500 | 0.40861600 |
| C | -2.13698300 | -0.11830300 | 1.70827300 |
| C | -3.46157000 | -0.06358200 | 2.14954500 |
| C | -4.47225400 | 0.38216300 | 1.30274000 |
| C | -4.15297700 | 0.78041000 | 0.00576100 |
| C | -2.83477500 | 0.73342300 | -0.44725500 |
| H | -1.34900900 | -0.48427200 | 2.35874800 |
| H | -3.69731500 | -0.38159600 | 3.16375700 |
| H | -5.50256800 | 0.42034300 | 1.65005100 |
| H | -4.93241700 | 1.13613200 | -0.66524100 |
| H | -2.58981400 | 1.07768500 | -1.44691800 |

| | | | |
|---|---|---|---|
| C | 1.20306000 | 2.69010600 | -2.31126300 |
| C | 0.83029300 | 2.62350400 | 2.29154400 |
| H | 1.90882600 | 3.38476200 | -1.84621400 |
| H | 0.95029100 | 2.99869100 | -3.32904000 |
| H | 1.69638900 | 1.71298300 | -2.30453000 |
| H | 1.69918900 | 3.01234900 | 2.82878100 |
| H | 0.61354000 | 1.60346800 | 2.63009300 |
| H | -0.04924200 | 3.24231800 | 2.50439200 |
| O | 1.81600600 | 0.09172000 | -0.79420100 |
| O | 0.81840500 | -0.53827000 | 1.85422600 |
| C | 2.82884200 | -0.49779100 | -0.30855800 |
| C | 1.94268400 | -1.08870100 | 1.94491700 |
| C | 2.23639700 | -1.79935500 | 3.25313400 |
| H | 3.26136500 | -2.17635500 | 3.31788500 |
| H | 2.04798000 | -1.11519000 | 4.08794400 |
| H | 1.54101500 | -2.64011300 | 3.35976600 |
| C | 4.02329900 | -0.52588300 | -1.23442000 |
| H | 4.29931700 | 0.50405100 | -1.48672300 |
| H | 4.88700400 | -1.03381300 | -0.79637100 |
| H | 3.74053900 | -1.02858900 | -2.16611600 |
| C | 2.94157200 | -1.09807700 | 0.94881500 |
| H | 3.88135000 | -1.58738700 | 1.18188600 |
| I | -0.57477000 | -2.20229800 | -1.12766200 |

**Complex $TS_{c\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | 0.06067900 | 0.17604700 | 0.04513700 |
| C | 0.00347600 | 2.86225000 | 0.13860300 |
| C | -1.11183900 | 1.90590300 | -0.24812400 |
| C | -1.47931200 | 1.92169800 | -1.72142900 |
| O | 0.58293100 | 3.53451800 | -0.69387600 |
| O | -2.60290400 | 2.27657200 | -2.03446100 |
| H | -1.99453000 | 2.26380400 | 0.28469000 |
| C | -1.77871500 | 0.17668900 | 0.62228800 |
| C | -1.89613900 | 0.19226800 | 2.01703700 |
| C | -2.99697600 | -0.40784400 | 2.62506900 |
| C | -4.00281500 | -0.98760400 | 1.85730100 |
| C | -3.89521300 | -0.97116900 | 0.46716500 |
| C | -2.79920300 | -0.38256700 | -0.15273000 |
| I | 0.22399500 | -2.29395900 | -1.09892400 |
| H | -1.10577100 | 0.61665700 | 2.62622300 |
| H | -3.06178400 | -0.41919300 | 3.71127100 |
| H | -4.86381600 | -1.44813600 | 2.33569800 |
| H | -4.66752700 | -1.42853500 | -0.14684800 |
| H | -2.72724800 | -0.38949500 | -1.23464900 |
| C | -0.47512900 | 1.46836300 | -2.73904600 |

| | | | |
|---|---|---|---|
| C | 0.26737100 | 3.03205200 | 1.61474300 |
| H | 0.51187200 | 1.88151400 | -2.52067300 |
| H | -0.82083300 | 1.75427100 | -3.73592300 |
| H | -0.37492800 | 0.37366100 | -2.68651900 |
| H | 0.91629900 | 3.89825400 | 1.76536500 |
| H | 0.75250500 | 2.12631100 | 1.99981300 |
| H | -0.67099300 | 3.16437900 | 2.16639300 |
| O | 1.81544500 | 0.82116400 | -0.67778700 |
| O | 1.07427800 | -0.04857400 | 1.96093100 |
| C | 2.95826600 | 0.49972900 | -0.24525500 |
| C | 2.30845500 | -0.30156600 | 2.02133000 |
| C | 2.79181400 | -0.93186200 | 3.31328600 |
| H | 3.88119800 | -1.01880400 | 3.36809300 |
| H | 2.42956500 | -0.34477000 | 4.16467100 |
| H | 2.35104800 | -1.93198000 | 3.39894100 |
| C | 4.09605300 | 0.73893500 | -1.21422100 |
| H | 4.03992000 | 1.76642300 | -1.58949600 |
| H | 5.08028800 | 0.56529000 | -0.76916200 |
| H | 3.96921600 | 0.07059200 | -2.07388600 |
| C | 3.25571800 | -0.04773000 | 1.01311200 |
| H | 4.29123800 | -0.30048600 | 1.21677600 |

**Complex a...p**

| | | | |
|---|---|---|---|
| Cu | -1.84991600 | 0.71151100 | 0.02516900 |
| C | 2.77244100 | 0.04720200 | -1.81291200 |
| C | 3.35982000 | -0.99257500 | -0.85462600 |
| C | 4.45947000 | -0.35545400 | 0.00750400 |
| O | 3.32731300 | 1.12132900 | -1.95150600 |
| O | 5.61927200 | -0.66895700 | -0.16002500 |
| H | 3.89059000 | -1.70142500 | -1.50738400 |
| C | 2.35340200 | -1.76919200 | -0.03364500 |
| C | 1.24676200 | -1.14934000 | 0.55532600 |
| C | 0.34836200 | -1.88276900 | 1.32615600 |
| C | 0.55272500 | -3.24591500 | 1.52607000 |
| C | 1.65683300 | -3.87213500 | 0.95233500 |
| C | 2.54952300 | -3.13810600 | 0.17713400 |
| I | -3.77962400 | -0.80935400 | -0.44834200 |
| H | 1.06015100 | -0.08848300 | 0.40594200 |
| H | -0.51404400 | -1.37603200 | 1.74943300 |
| H | -0.15569800 | -3.81927900 | 2.11812500 |
| H | 1.82067500 | -4.93699400 | 1.10068100 |
| H | 3.41084300 | -3.62915800 | -0.27191800 |
| C | 4.03495200 | 0.61654200 | 1.07675800 |
| C | 1.54738200 | -0.32117100 | -2.60401100 |
| H | 3.32662700 | 1.35632600 | 0.69004200 |
| H | 4.91981200 | 1.11276000 | 1.48083600 |

| | | | |
|---|---|---|---|
| H | 3.52462400 | 0.07363200 | 1.88124600 |
| H | 1.65624600 | 0.06333300 | -3.62245300 |
| H | 0.67735200 | 0.18214300 | -2.15773500 |
| H | 1.35271700 | -1.39657600 | -2.61397600 |
| O | -0.91694800 | 1.22024800 | 1.80749000 |
| O | -0.52183800 | 1.86563800 | -1.00099600 |
| C | -0.03788900 | 2.11444200 | 1.92746700 |
| C | 0.28063700 | 2.69869600 | -0.48981800 |
| C | 1.01109200 | 3.59501500 | -1.46933100 |
| H | 1.53205700 | 4.42228500 | -0.97747800 |
| H | 1.74805000 | 2.99963700 | -2.02177100 |
| H | 0.29308900 | 3.99437400 | -2.19328200 |
| C | 0.39839700 | 2.41996500 | 3.34961800 |
| H | 0.78794200 | 1.50462700 | 3.81015800 |
| H | 1.16160200 | 3.20194400 | 3.40792100 |
| H | -0.47563900 | 2.72535200 | 3.93595300 |
| C | 0.56617900 | 2.84479100 | 0.88240900 |
| H | 1.28773300 | 3.60746500 | 1.15957400 |

**Complex PhI**

| | | | |
|---|---|---|---|
| C | 2.64994800 | 1.20412800 | -0.00000300 |
| C | 3.34793300 | 0.00000200 | -0.00000400 |
| C | 2.64995700 | -1.20412300 | -0.00000300 |
| C | 1.25627900 | -1.21330900 | -0.00000100 |
| C | 0.57778800 | -0.00000500 | -0.00000100 |
| C | 1.25627500 | 1.21330700 | -0.00000200 |
| H | 3.18763400 | 2.14844200 | -0.00000400 |
| H | 4.43415300 | 0.00001000 | -0.00000500 |
| H | 3.18763900 | -2.14843900 | -0.00000400 |
| H | 0.71293900 | -2.15220700 | -0.00000100 |
| H | 0.71292200 | 2.15219800 | -0.00000100 |
| I | -1.55970500 | 0.00000000 | 0.00000200 |

## 14. MN15-optimised geometries (singlet spin state)

**Complex b**

| | | | |
|---|---|---|---|
| O | 1.34912600 | -1.33630600 | -0.26027700 |
| O | 1.24694100 | 1.56626400 | -0.04496600 |
| C | 2.56828400 | -1.10913800 | -0.03670900 |
| C | 2.48387600 | 1.38472500 | 0.14223400 |
| C | 3.29513600 | 2.65169000 | 0.37328100 |
| H | 2.89891700 | 3.17442400 | 1.25158900 |
| H | 4.36192400 | 2.45377900 | 0.52092000 |
| H | 3.16529300 | 3.32045200 | -0.48545400 |
| C | 3.46775000 | -2.33702200 | 0.02465100 |
| H | 3.39513400 | -2.88177800 | -0.92395500 |
| H | 4.51643700 | -2.08947000 | 0.21995000 |
| H | 3.10153000 | -3.00722300 | 0.81097100 |
| C | 3.16889500 | 0.15414100 | 0.15822300 |
| H | 4.24101700 | 0.17892300 | 0.33923300 |
| Cu | -0.17344300 | 0.14246000 | -0.33189100 |
| C | -2.18213300 | -0.23542800 | -0.59779400 |
| H | -2.22666400 | -0.48474300 | -1.66192500 |
| C | -2.78252700 | 1.06043900 | -0.28917800 |
| C | -2.15761000 | -1.36506300 | 0.31565400 |
| O | -3.14736900 | 1.84829100 | -1.16989200 |
| O | -2.42283500 | -1.34041400 | 1.52853800 |
| C | -2.95626600 | 1.45533100 | 1.17234100 |
| H | -3.67495600 | 0.79010000 | 1.66239800 |
| H | -2.01634800 | 1.33967800 | 1.72482800 |
| H | -3.29894900 | 2.49460600 | 1.20477100 |
| C | -1.71530600 | -2.69959400 | -0.29313600 |
| H | -1.87854400 | -2.74155800 | -1.37645200 |
| H | -0.64227600 | -2.83045800 | -0.10831200 |
| H | -2.26017500 | -3.51122800 | 0.20164800 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | 1.06773800 | 2.12750200 | -0.71420500 |
| O | 0.45388400 | 0.19224600 | 1.43408300 |
| C | 0.03761200 | 2.66455600 | -0.21323200 |
| C | -0.47403800 | 1.02481900 | 1.62241300 |
| C | -1.40773900 | 0.70176500 | 2.77821300 |
| H | -0.83473600 | 0.70756800 | 3.71323900 |
| H | -2.24715000 | 1.39993200 | 2.85923900 |
| H | -1.79591800 | -0.31429300 | 2.63645800 |
| C | -0.42718600 | 3.94152000 | -0.90086600 |
| H | -0.73189500 | 3.70133100 | -1.92772300 |
| H | -1.26399300 | 4.42408900 | -0.38569800 |
| H | 0.41386000 | 4.64068200 | -0.96898400 |

| | | | |
|---|---|---|---|
| C | -0.72490300 | 2.20068000 | 0.87711900 |
| H | -1.58667100 | 2.79586800 | 1.17042500 |
| Cu | 1.80012400 | 0.26572900 | -0.11599600 |
| C | 3.61577200 | -0.70283100 | -0.52943000 |
| H | 3.62275300 | -0.77744700 | -1.62040000 |
| C | 3.33689100 | -1.95697300 | 0.14664200 |
| C | 4.34677100 | 0.41330600 | 0.04084500 |
| O | 2.97887300 | -2.97539000 | -0.47443800 |
| O | 4.72943400 | 0.52292600 | 1.21654200 |
| C | 3.44021900 | -2.01779800 | 1.66267800 |
| H | 4.45741600 | -1.78391200 | 1.99192200 |
| H | 2.78808400 | -1.26192300 | 2.11841300 |
| H | 3.14098900 | -3.02115600 | 1.98301500 |
| C | 4.61574300 | 1.58146700 | -0.91436900 |
| H | 4.61711700 | 1.27313700 | -1.96646400 |
| H | 3.82212300 | 2.32873900 | -0.78495600 |
| H | 5.57495800 | 2.04226200 | -0.65463800 |
| C | -0.19517700 | -2.40209700 | -0.56093200 |
| C | 0.45353600 | -1.63887000 | -1.53447400 |
| C | -0.15763200 | -0.48601000 | -2.03750600 |
| C | -1.42415900 | -0.10295100 | -1.58905400 |
| C | -2.06077300 | -0.90080600 | -0.64418900 |
| C | -1.46605500 | -2.04037900 | -0.10920100 |
| H | 0.32222800 | -3.26199400 | -0.14336100 |
| H | 1.44433700 | -1.94923000 | -1.85758400 |
| H | 0.36082400 | 0.13681900 | -2.76313000 |
| H | -1.89083800 | 0.80758600 | -1.95467800 |
| H | -1.97588400 | -2.62692100 | 0.65061100 |
| I | -4.02516900 | -0.33173400 | 0.01895100 |

**Complex $TS_{b-c}$**

| | | | |
|---|---|---|---|
| Cu | -0.07851500 | 0.06804200 | -0.18280100 |
| C | -1.79531200 | -2.03602400 | 0.50408900 |
| C | -0.47742000 | -2.08318800 | -0.10961700 |
| C | -0.23335800 | -2.44204500 | -1.50459200 |
| O | -2.87997800 | -2.06428400 | -0.09159000 |
| O | 0.87501200 | -2.85433700 | -1.87973300 |
| H | 0.33193700 | -2.37295000 | 0.56346200 |
| C | 1.83463400 | -0.23893000 | 0.45074500 |
| C | 1.88011500 | -0.05339200 | 1.83121300 |
| C | 2.74019000 | -0.87101400 | 2.57117200 |
| C | 3.55060100 | -1.81284300 | 1.93389900 |
| C | 3.50441800 | -1.94328400 | 0.54343500 |
| C | 2.65540300 | -1.14000400 | -0.21981600 |
| I | 1.59717200 | 1.93429400 | -0.95141000 |
| H | 1.22500200 | 0.67013500 | 2.30803100 |

| | | | |
|---|---|---|---|
| H | 2.77284100 | -0.76323800 | 3.65424500 |
| H | 4.22126900 | -2.43969000 | 2.51826100 |
| H | 4.12700200 | -2.68003900 | 0.03993200 |
| H | 2.58953000 | -1.26377800 | -1.29593600 |
| C | -1.35345500 | -2.28921000 | -2.51649700 |
| C | -1.79269500 | -1.97121500 | 2.03108700 |
| H | -0.94389200 | -2.49082900 | -3.51146900 |
| H | -1.78535600 | -1.28395100 | -2.46018200 |
| H | -2.16484000 | -2.98728000 | -2.28252500 |
| H | -1.78427900 | -2.99155700 | 2.43877200 |
| H | -2.70781200 | -1.46898500 | 2.36172800 |
| H | -0.91381600 | -1.43560900 | 2.41032800 |
| O | -1.77716200 | 0.62987300 | -1.12958100 |
| O | -0.86373400 | 1.10730300 | 1.57676600 |
| C | -2.89365900 | 0.86285600 | -0.57937600 |
| C | -2.09441900 | 1.34221300 | 1.73764100 |
| C | -2.50849800 | 1.73231400 | 3.14914000 |
| H | -1.86262600 | 2.54339500 | 3.50360000 |
| H | -3.55700100 | 2.03995700 | 3.21770200 |
| H | -2.34520800 | 0.87056100 | 3.80967600 |
| C | -4.10119500 | 0.66886300 | -1.47223100 |
| H | -4.20668400 | -0.41404600 | -1.61488400 |
| H | -5.02359800 | 1.06847500 | -1.03808700 |
| H | -3.91534000 | 1.12799000 | -2.44918900 |
| C | -3.10443800 | 1.24190300 | 0.76176200 |
| H | -4.12886600 | 1.43017100 | 1.07328200 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | 0.00140700 | 0.08737500 | -0.18678300 |
| C | 1.32645500 | 2.33498500 | 0.63149000 |
| C | 0.17968300 | 2.17881800 | -0.29401400 |
| C | 0.27268800 | 2.40418500 | -1.76191800 |
| O | 2.50867100 | 2.29676600 | 0.30172200 |
| O | -0.75634000 | 2.62880000 | -2.40168400 |
| H | -0.73777100 | 2.61622400 | 0.09645200 |
| C | -1.81308400 | 0.54209800 | 0.34211400 |
| C | -2.08948800 | 0.36324500 | 1.69262000 |
| C | -3.39133400 | 0.61935200 | 2.14207500 |
| C | -4.37799100 | 1.04478400 | 1.25301400 |
| C | -4.06543300 | 1.22032300 | -0.09776500 |
| C | -2.77222700 | 0.97368200 | -0.56623800 |
| H | -1.31378500 | 0.00836300 | 2.36665100 |
| H | -3.62901700 | 0.47333200 | 3.19490900 |
| H | -5.38795400 | 1.23935200 | 1.60931500 |
| H | -4.82966500 | 1.55606100 | -0.79684100 |
| H | -2.51246600 | 1.14004600 | -1.60830900 |

| | | | |
|---|---|---|---|
| C | 1.61270600 | 2.39249000 | -2.45842700 |
| C | 0.93546000 | 2.61647800 | 2.07378400 |
| H | 2.28098100 | 3.13396900 | -2.00822800 |
| H | 1.44605200 | 2.60511000 | -3.51842800 |
| H | 2.08782600 | 1.41650900 | -2.31805700 |
| H | 1.75215100 | 2.31583400 | 2.73584500 |
| H | 0.01834200 | 2.08341100 | 2.34486500 |
| H | 0.75883300 | 3.69556100 | 2.18753500 |
| O | 1.78365700 | -0.28372400 | -0.95712200 |
| O | 0.85375200 | -0.35382200 | 1.80527400 |
| C | 2.82836600 | -0.71325400 | -0.37860000 |
| C | 2.00049200 | -0.84564400 | 1.97334400 |
| C | 2.35350300 | -1.22843000 | 3.40261300 |
| H | 3.36711300 | -1.63011300 | 3.49984600 |
| H | 2.25111200 | -0.34282500 | 4.04169600 |
| H | 1.63250200 | -1.97339800 | 3.75813900 |
| C | 4.03319300 | -0.83842100 | -1.28967100 |
| H | 4.31893300 | 0.17143500 | -1.61112300 |
| H | 4.88854500 | -1.31313700 | -0.79885700 |
| H | 3.75443500 | -1.40729700 | -2.18316100 |
| C | 2.97815700 | -1.04866900 | 0.97512400 |
| H | 3.94397700 | -1.43707600 | 1.28731600 |
| I | -0.93048600 | -2.32614200 | -0.80539000 |

**Complex a...p**

| | | | |
|---|---|---|---|
| Cu | 1.56885200 | -0.99715200 | 0.01217600 |
| C | -1.96273300 | 0.65813700 | -1.96518000 |
| C | -2.64651000 | 1.50564200 | -0.88388400 |
| C | -3.96253200 | 0.85439100 | -0.43673600 |
| O | -2.58207600 | -0.24494400 | -2.50441800 |
| O | -5.02203700 | 1.41107100 | -0.66039300 |
| H | -2.94820600 | 2.43227000 | -1.39645900 |
| C | -1.75443800 | 1.87689500 | 0.28370300 |
| C | -0.90840100 | 0.93238500 | 0.87871800 |
| C | -0.09620600 | 1.28677300 | 1.95725400 |
| C | -0.13409100 | 2.58974600 | 2.45751000 |
| C | -0.98106000 | 3.53471100 | 1.87749400 |
| C | -1.78523800 | 3.17901600 | 0.79493500 |
| I | 3.38500000 | 0.70464400 | -0.54350700 |
| H | -0.87214600 | -0.08679800 | 0.48804400 |
| H | 0.56904700 | 0.53849500 | 2.38100600 |
| H | 0.50745300 | 2.86953300 | 3.28998800 |
| H | -1.00965400 | 4.55297600 | 2.26035400 |
| H | -2.44415600 | 3.91515700 | 0.33559600 |
| C | -3.88045500 | -0.45862300 | 0.30145800 |
| C | -0.56337600 | 1.03910700 | -2.36751200 |

| | | | |
|---|---|---|---|
| H | -3.35608700 | -1.19742700 | -0.31477400 |
| H | -4.89111600 | -0.80447600 | 0.53139000 |
| H | -3.30033400 | -0.34649500 | 1.22526500 |
| H | -0.41161700 | 0.79233900 | -3.42155400 |
| H | 0.15650500 | 0.44794700 | -1.78284300 |
| H | -0.35015200 | 2.09502500 | -2.16995200 |
| O | 0.75748500 | -1.75882200 | 1.77582900 |
| O | 0.11397300 | -2.02233100 | -1.05836100 |
| C | -0.34507200 | -2.37107600 | 1.86719800 |
| C | -0.84162000 | -2.69205400 | -0.57202600 |
| C | -1.76189600 | -3.35742400 | -1.58068600 |
| H | -2.59559000 | -3.88676500 | -1.10672500 |
| H | -2.14787200 | -2.59340700 | -2.26400500 |
| H | -1.17692400 | -4.06847900 | -2.17637000 |
| C | -0.87455300 | -2.55367800 | 3.28075100 |
| H | -1.13843700 | -1.56428300 | 3.67801800 |
| H | -1.75635500 | -3.20079300 | 3.32721500 |
| H | -0.08204800 | -2.96017900 | 3.91824500 |
| C | -1.12887400 | -2.86209600 | 0.80219100 |
| H | -2.03041200 | -3.41423300 | 1.05795800 |

**Complex PhI**

| | | | |
|---|---|---|---|
| C | -2.65269300 | 1.20710900 | 0.00000300 |
| C | -3.35185300 | 0.00000000 | 0.00000400 |
| C | -2.65269500 | -1.20710700 | 0.00000300 |
| C | -1.25652000 | -1.21542000 | 0.00000100 |
| C | -0.57569600 | -0.00000100 | 0.00000100 |
| C | -1.25651900 | 1.21542000 | 0.00000200 |
| H | -3.19128500 | 2.15161700 | 0.00000400 |
| H | -4.43878100 | 0.00000300 | 0.00000500 |
| H | -3.19128700 | -2.15161600 | 0.00000400 |
| H | -0.71046100 | -2.15440900 | 0.00000100 |
| H | -0.71045700 | 2.15440700 | 0.00000100 |
| I | 1.56071900 | 0.00000000 | -0.00000200 |

## 15. ω-B97XD-optimised geometries (triplet spin state)

**Complex a**

| | | | |
|---|---|---|---|
| C | -2.51635600 | -1.24699300 | -0.00000300 |
| C | -3.13920100 | 0.00007600 | 0.00016900 |
| H | -4.22789500 | 0.00013000 | 0.00024300 |
| C | -3.29531200 | -2.53134700 | -0.00010200 |
| H | -3.05072800 | -3.14389400 | 0.88134400 |
| H | -4.37547700 | -2.34653700 | 0.00006200 |
| H | -3.05095100 | -3.14363200 | -0.88179200 |
| C | -2.51623200 | 1.24708400 | 0.00025200 |
| C | -3.29507200 | 2.53150900 | 0.00045400 |
| H | -3.05056800 | 3.14402500 | -0.88103600 |
| H | -4.37525200 | 2.34679500 | 0.00046000 |
| H | -3.05052100 | 3.14378200 | 0.88210200 |
| O | -1.18781500 | -1.43261400 | -0.00010700 |
| O | -1.18767500 | 1.43258400 | 0.00018100 |
| Cu | -0.03464500 | -0.00007800 | -0.00002900 |
| I | 2.52383100 | -0.00000300 | -0.00010900 |

**Complex b**

| | | | |
|---|---|---|---|
| O | -1.62836100 | -1.36449500 | 0.51904200 |
| O | -0.67968000 | 1.21011600 | -0.31710900 |
| C | -2.82253400 | -0.82964600 | 0.21728000 |
| C | -1.99284700 | 1.41256000 | -0.50060800 |
| C | -2.30254300 | 2.79197500 | -1.01088000 |
| H | -1.79671500 | 2.98031400 | -1.96985800 |
| H | -3.37891500 | 2.93776500 | -1.15558000 |
| H | -1.94141200 | 3.56092400 | -0.31128600 |
| C | -3.97806800 | -1.75933700 | 0.44669400 |
| H | -4.03369100 | -2.07498000 | 1.50047300 |
| H | -4.93145600 | -1.28827700 | 0.18198700 |
| H | -3.87373500 | -2.68062300 | -0.14753000 |
| C | -2.99072400 | 0.47098100 | -0.25831100 |
| H | -4.01334900 | 0.78546200 | -0.45983100 |
| Cu | -0.06831800 | -0.43660500 | 0.30317600 |
| C | 1.96253100 | -0.48258600 | 0.44185700 |
| H | 2.07012600 | -1.27929800 | 1.18968500 |
| C | 2.36020200 | 0.81871200 | 1.03419600 |
| C | 2.41195500 | -0.91590200 | -0.88865400 |
| O | 2.55741400 | 0.92301200 | 2.24046500 |
| O | 2.80103100 | -0.19593800 | -1.80259300 |
| C | 2.44540500 | 2.02984500 | 0.13092600 |
| H | 3.08941900 | 1.82483800 | -0.72784200 |
| H | 1.44274400 | 2.23160700 | -0.26474900 |
| H | 2.80425500 | 2.88332900 | 0.71226500 |

| | | | |
|---|---|---|---|
| C | 2.39390000 | -2.43305700 | -1.10876700 |
| H | 1.50412200 | -2.90306000 | -0.67600300 |
| H | 2.44026500 | -2.64160600 | -2.18015900 |
| H | 3.27267100 | -2.87767000 | -0.62452100 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | -0.34071200 | -0.53515300 | 1.63096200 |
| O | -1.25462100 | 1.67446900 | 0.11453100 |
| C | 0.65029200 | 0.23530300 | 1.85371400 |
| C | -0.13299800 | 2.15600800 | 0.50105500 |
| C | 0.16088900 | 3.53841600 | -0.02931000 |
| H | -0.69881700 | 4.19104100 | 0.15185600 |
| H | 1.05909000 | 3.97152500 | 0.41496500 |
| H | 0.30300300 | 3.46938700 | -1.11325900 |
| C | 1.74037000 | -0.32120200 | 2.72380700 |
| H | 2.59485800 | -0.55832900 | 2.07400900 |
| H | 2.08308100 | 0.41799500 | 3.45361900 |
| H | 1.39578200 | -1.22613100 | 3.22803100 |
| C | 0.79806900 | 1.52651800 | 1.32370900 |
| H | 1.73066300 | 2.03777800 | 1.52679600 |
| Cu | -1.66097300 | -0.20867900 | 0.32722900 |
| C | -3.50734500 | -0.39110800 | -0.46116100 |
| H | -3.44255100 | -1.38304100 | -0.91748000 |
| C | -3.65014200 | 0.63261700 | -1.53113800 |
| C | -4.35001200 | -0.39220800 | 0.75232100 |
| O | -3.33353600 | 0.35449100 | -2.68223300 |
| O | -4.86694100 | 0.59278600 | 1.26414800 |
| C | -4.14297500 | 2.01826500 | -1.18539400 |
| H | -5.10666200 | 1.97522300 | -0.67226900 |
| H | -3.43396600 | 2.48101300 | -0.49250200 |
| H | -4.20844500 | 2.60351900 | -2.10553400 |
| C | -4.54510900 | -1.76551000 | 1.39577000 |
| H | -3.59471900 | -2.30423400 | 1.49106900 |
| H | -5.00024700 | -1.64491100 | 2.38092600 |
| H | -5.20305600 | -2.37658600 | 0.76575900 |
| C | -0.50166700 | -1.24954400 | -1.69686900 |
| C | -0.74558700 | -2.46138100 | -1.02837800 |
| C | 0.26658000 | -3.06863700 | -0.27992200 |
| C | 1.52140400 | -2.46525200 | -0.18710000 |
| C | 1.74029300 | -1.26161400 | -0.83868300 |
| C | 0.75930100 | -0.64132200 | -1.58969600 |
| H | -1.28018800 | -0.80902800 | -2.31954800 |
| H | -1.71059200 | -2.95057300 | -1.13667800 |
| H | 0.07262500 | -4.01127200 | 0.22727800 |
| H | 2.31661700 | -2.92774300 | 0.39284100 |
| H | 0.95513200 | 0.30420600 | -2.08846900 |

| | | | |
|---|---|---|---|
| I | 4.36481000 | 0.21817000 | -0.29635200 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | 0.10061400 | 0.06786900 | -0.80046300 |
| C | -1.63013700 | 0.69156100 | 2.34156500 |
| C | -0.23913000 | 0.28896900 | 2.52813000 |
| C | 0.24698000 | -1.03948400 | 2.93556400 |
| O | -2.57231700 | 0.00652700 | 2.73521800 |
| O | 1.35651200 | -1.09804300 | 3.45466000 |
| H | 0.53546200 | 1.04229400 | 2.41308600 |
| C | 1.36633400 | 1.46914800 | -0.29168800 |
| C | 1.12883800 | 2.80596400 | -0.64386000 |
| C | 1.93859700 | 3.84230000 | -0.17536500 |
| C | 3.01089300 | 3.56553500 | 0.66899600 |
| C | 3.26908100 | 2.24446900 | 1.02989300 |
| C | 2.46214000 | 1.21356500 | 0.54777600 |
| H | 0.28818600 | 3.03908200 | -1.29321900 |
| H | 1.72890400 | 4.87001800 | -0.46802600 |
| H | 3.64235400 | 4.37032400 | 1.03966900 |
| H | 4.10341500 | 2.01176900 | 1.68846300 |
| H | 2.68544300 | 0.19008100 | 0.83862300 |
| C | -0.59643300 | -2.26058700 | 2.68833800 |
| C | -1.85386900 | 2.03627100 | 1.68447000 |
| H | -1.56596600 | -2.15647600 | 3.18303000 |
| H | -0.06163900 | -3.14189800 | 3.04719500 |
| H | -0.78824100 | -2.34090100 | 1.61149700 |
| H | -2.92087000 | 2.17728200 | 1.50285400 |
| H | -1.30037200 | 2.10382400 | 0.74204600 |
| H | -1.47777400 | 2.83496200 | 2.33590900 |
| O | -1.49409400 | -1.05267500 | -0.23224100 |
| O | -1.21859500 | 1.30128900 | -1.75991400 |
| C | -2.72251000 | -0.84635700 | -0.43396000 |
| C | -2.48013700 | 1.21821400 | -1.78277300 |
| C | -3.18291300 | 2.34121800 | -2.52412500 |
| H | -4.26153000 | 2.18381700 | -2.61168400 |
| H | -3.00157600 | 3.28354700 | -1.99459900 |
| H | -2.74660700 | 2.44112600 | -3.52291800 |
| C | -3.66588600 | -1.83131700 | 0.22160100 |
| H | -3.65115700 | -1.64261800 | 1.30085600 |
| H | -4.69280200 | -1.73983500 | -0.14359900 |
| H | -3.29918900 | -2.84766700 | 0.05098000 |
| C | -3.25769800 | 0.22164500 | -1.17767500 |
| H | -4.33564400 | 0.28383400 | -1.27733200 |
| I | 1.63895900 | -2.03687300 | -1.21721700 |

**Complex $TS_{c\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | 0.03276800 | -0.59099800 | -0.15619200 |
| C | -1.92863800 | 2.26560100 | 0.23099700 |
| C | -0.60150600 | 2.36132400 | 0.86411400 |
| C | -0.42306700 | 1.97815800 | 2.29232200 |
| O | -2.85401300 | 1.56736000 | 0.63874200 |
| O | 0.21924500 | 2.70764000 | 3.03560300 |
| H | -0.11813800 | 3.31917800 | 0.67861500 |
| C | 0.74853900 | 1.26640200 | -0.17868000 |
| C | 0.71621800 | 1.85719700 | -1.49810500 |
| C | 1.65018400 | 2.78140000 | -1.92016200 |
| C | 2.71909500 | 3.14036400 | -1.08606600 |
| C | 2.86648000 | 2.50653800 | 0.15699300 |
| C | 1.94266700 | 1.57513300 | 0.57945000 |
| I | 2.31670500 | -1.94203000 | -0.17702600 |
| H | -0.08792700 | 1.56397200 | -2.16578400 |
| H | 1.57206300 | 3.21658300 | -2.91456900 |
| H | 3.45123300 | 3.87239300 | -1.41716100 |
| H | 3.72757900 | 2.73369000 | 0.78056100 |
| H | 2.09018200 | 1.08655500 | 1.53807400 |
| C | -0.95641200 | 0.65261000 | 2.78307500 |
| C | -2.15687500 | 3.10846000 | -1.01604200 |
| H | -1.93536500 | 0.43577800 | 2.35232500 |
| H | -0.98602800 | 0.65806000 | 3.87574300 |
| H | -0.27073400 | -0.14352900 | 2.46122900 |
| H | -3.12311100 | 3.61525400 | -0.92803300 |
| H | -2.20780600 | 2.42681200 | -1.87140300 |
| H | -1.36473800 | 3.83781400 | -1.20081700 |
| O | -0.99879200 | -2.07122200 | 0.65194600 |
| O | -1.49968500 | -0.21057900 | -1.43817100 |
| C | -2.20560800 | -2.37250700 | 0.42393800 |
| C | -2.65705300 | -0.71367900 | -1.36016400 |
| C | -3.71704700 | -0.05467900 | -2.21741600 |
| H | -4.55967800 | -0.71924700 | -2.42956700 |
| H | -4.08572300 | 0.81385200 | -1.65879800 |
| H | -3.27482600 | 0.29633100 | -3.15410400 |
| C | -2.75652500 | -3.48794700 | 1.28977400 |
| H | -2.62676200 | -3.21775800 | 2.34267800 |
| H | -3.81303100 | -3.69250100 | 1.09559800 |
| H | -2.17243900 | -4.39706400 | 1.11278400 |
| C | -3.04267500 | -1.77609700 | -0.52814100 |
| H | -4.07107400 | -2.11494200 | -0.58568600 |

## 16. B3LYP-D3-optimised geometries (triplet spin state)

**Complex a**

| | | | |
|---|---|---|---|
| C | -2.53861300 | -1.24983300 | 0.00003800 |
| C | -3.16360400 | 0.00013500 | 0.00018800 |
| H | -4.25222700 | 0.00022400 | 0.00024700 |
| C | -3.31369400 | -2.53881100 | -0.00008700 |
| H | -3.06707000 | -3.15447900 | 0.88085100 |
| H | -4.39565700 | -2.36011500 | 0.00001800 |
| H | -3.06720400 | -3.15423400 | -0.88123700 |
| C | -2.53839300 | 1.24997100 | 0.00026500 |
| C | -3.31327700 | 2.53910400 | 0.00047500 |
| H | -3.06659600 | 3.15470400 | -0.88048600 |
| H | -4.39526800 | 2.36059500 | 0.00047500 |
| H | -3.06655800 | 3.15444500 | 0.88160800 |
| O | -1.20418000 | -1.43860100 | -0.00004400 |
| O | -1.20397600 | 1.43852600 | 0.00019400 |
| Cu | -0.03320900 | -0.00012500 | 0.00000700 |
| I | 2.54234700 | -0.00000600 | -0.00015400 |

**Complex b**

| | | | |
|---|---|---|---|
| O | 1.66502100 | -1.35539700 | -0.53205400 |
| O | 0.64346800 | 1.19620300 | 0.32340900 |
| C | 2.84949400 | -0.78728600 | -0.22577500 |
| C | 1.95758100 | 1.43189300 | 0.50681600 |
| C | 2.22427200 | 2.81735600 | 1.03143700 |
| H | 1.71518500 | 2.98237400 | 1.99500700 |
| H | 3.29641400 | 2.99824100 | 1.17369400 |
| H | 1.83353900 | 3.58476000 | 0.34351300 |
| C | 4.02663000 | -1.69130800 | -0.45857900 |
| H | 4.08528000 | -2.01191100 | -1.51255300 |
| H | 4.97232900 | -1.20062600 | -0.19883900 |
| H | 3.94648900 | -2.61662800 | 0.13690600 |
| C | 2.98365900 | 0.51794800 | 0.25791200 |
| H | 3.99716000 | 0.85912300 | 0.46207200 |
| Cu | 0.06316100 | -0.47721200 | -0.31361000 |
| C | -1.98411700 | -0.52125100 | -0.42600000 |
| H | -2.10751300 | -1.35944900 | -1.12521300 |
| C | -2.37730700 | 0.75003100 | -1.08464200 |
| C | -2.38873900 | -0.87404900 | 0.94418700 |
| O | -2.58520300 | 0.79168600 | -2.29877600 |
| O | -2.75835600 | -0.09771400 | 1.82675000 |
| C | -2.44649900 | 2.01157900 | -0.24415000 |
| H | -3.09963100 | 1.86466900 | 0.62019600 |
| H | -1.44352700 | 2.21454800 | 0.14993000 |
| H | -2.78631600 | 2.83994600 | -0.87288600 |

| | | | |
|---|---|---|---|
| C | -2.33716700 | -2.37888900 | 1.25988100 |
| H | -1.42140300 | -2.84221400 | 0.87388600 |
| H | -2.39729600 | -2.52219200 | 2.34187700 |
| H | -3.18867100 | -2.88586500 | 0.78592800 |

**Complex PhI...b**

| | | | |
|---|---|---|---|
| O | 0.28068200 | 0.38205500 | 1.65107500 |
| O | 1.35802900 | -1.67663900 | 0.01376700 |
| C | -0.64564300 | -0.47877300 | 1.84064300 |
| C | 0.28361900 | -2.27055200 | 0.39415300 |
| C | 0.11778200 | -3.66350200 | -0.17718000 |
| H | 1.01686900 | -4.25298500 | 0.03480500 |
| H | -0.76234500 | -4.17654100 | 0.21790900 |
| H | 0.02628600 | -3.58706800 | -1.26691300 |
| C | -1.77450400 | -0.04536700 | 2.73853400 |
| H | -2.60859500 | 0.26825900 | 2.09464200 |
| H | -2.13557800 | -0.86845400 | 3.36303500 |
| H | -1.45820300 | 0.79586100 | 3.36016800 |
| C | -0.69316900 | -1.75491600 | 1.24801500 |
| H | -1.56943700 | -2.35947100 | 1.44537700 |
| Cu | 1.62950600 | 0.23678100 | 0.30766100 |
| C | 3.51444100 | 0.51415800 | -0.44403400 |
| H | 3.44803100 | 1.55633800 | -0.76757400 |
| C | 3.66122700 | -0.37154600 | -1.62809300 |
| C | 4.30054700 | 0.34764800 | 0.79380600 |
| O | 3.34452100 | 0.04415800 | -2.74428100 |
| O | 4.81998100 | -0.69937600 | 1.17984300 |
| C | 4.16006000 | -1.79074200 | -1.45046700 |
| H | 5.13048300 | -1.80510100 | -0.94657700 |
| H | 3.46267200 | -2.33068100 | -0.80347000 |
| H | 4.21598800 | -2.26678400 | -2.43312300 |
| C | 4.43216000 | 1.61610300 | 1.64750700 |
| H | 3.46340800 | 2.11731100 | 1.76832300 |
| H | 4.83628100 | 1.35464200 | 2.62829900 |
| H | 5.10825500 | 2.32843100 | 1.15649700 |
| C | 0.47170200 | 1.40122300 | -1.59002000 |
| C | 0.72121400 | 2.50728500 | -0.74769700 |
| C | -0.30100900 | 3.01899600 | 0.06656100 |
| C | -1.56289700 | 2.41768500 | 0.05751800 |
| C | -1.79107600 | 1.31145500 | -0.75678800 |
| C | -0.80067800 | 0.79608100 | -1.57966200 |
| H | 1.25303100 | 1.05025500 | -2.26323700 |
| H | 1.68948700 | 2.99939100 | -0.78141700 |
| H | -0.10247700 | 3.87724900 | 0.70658800 |
| H | -2.35916200 | 2.80456700 | 0.69062200 |
| H | -0.99289700 | -0.06978300 | -2.20919100 |

| | | | |
|---|---|---|---|
| I | -4.37558700 | -0.18934100 | -0.34333800 |

**Complex c**

| | | | |
|---|---|---|---|
| Cu | -0.03131700 | 0.24968800 | 0.68866400 |
| C | 1.48555200 | 0.26742600 | -2.50160000 |
| C | 0.10439300 | -0.20289400 | -2.48457200 |
| C | -0.36270500 | -1.59412000 | -2.56903100 |
| O | 2.43745400 | -0.45877500 | -2.80920000 |
| O | -1.52139100 | -1.77939700 | -2.95051800 |
| H | -0.68863700 | 0.53766000 | -2.46304100 |
| C | -1.47867600 | 1.42602900 | 0.10337500 |
| C | -1.40426400 | 2.81008800 | 0.33777400 |
| C | -2.36752700 | 3.69042500 | -0.16943700 |
| C | -3.43067300 | 3.20318200 | -0.93395500 |
| C | -3.52446900 | 1.83004800 | -1.17789400 |
| C | -2.56573700 | 0.95452100 | -0.65638400 |
| H | -0.57209500 | 3.19964100 | 0.91776700 |
| H | -2.28538600 | 4.75885400 | 0.02982800 |
| H | -4.17891600 | 3.88554000 | -1.33418400 |
| H | -4.34696900 | 1.43640300 | -1.77330600 |
| H | -2.65543100 | -0.10963800 | -0.85586200 |
| C | 0.55063300 | -2.72861200 | -2.17859600 |
| C | 1.69343800 | 1.73090100 | -2.14984300 |
| H | 1.48275900 | -2.68222900 | -2.74849700 |
| H | 0.03121100 | -3.67631300 | -2.33702700 |
| H | 0.81140100 | -2.60945600 | -1.12022200 |
| H | 2.76248900 | 1.95338200 | -2.14103200 |
| H | 1.25778400 | 1.95265000 | -1.16916600 |
| H | 1.18434700 | 2.37260500 | -2.88077900 |
| O | 1.62436400 | -0.84514600 | 0.31598300 |
| O | 1.22181800 | 1.75245600 | 1.36865200 |
| C | 2.84585800 | -0.53560300 | 0.46405100 |
| C | 2.49129700 | 1.73214300 | 1.41879800 |
| C | 3.12976200 | 2.99900500 | 1.96972300 |
| H | 4.22297800 | 2.95369800 | 1.99585300 |
| H | 2.81843100 | 3.85122200 | 1.35402700 |
| H | 2.75225400 | 3.17975400 | 2.98278200 |
| C | 3.83822100 | -1.57229100 | -0.02598400 |
| H | 3.76839500 | -1.61146100 | -1.11895000 |
| H | 4.86997100 | -1.34634500 | 0.26157400 |
| H | 3.55284400 | -2.55546200 | 0.36258500 |
| C | 3.32161000 | 0.67744400 | 1.00245000 |
| H | 4.39487200 | 0.80941300 | 1.08568800 |
| I | -1.40249700 | -1.90604000 | 1.52619100 |

**Complex $TS_{c\text{-}p}$**

| | | | |
|---|---|---|---|
| Cu | -0.09317700 | -0.56469900 | 0.14059600 |
| C | 2.21010500 | 2.09377600 | -0.11305500 |
| C | 0.92839800 | 2.27643500 | -0.83184700 |
| C | 0.83048500 | 1.90141500 | -2.27736600 |
| O | 3.09801100 | 1.29985400 | -0.43586900 |
| O | 0.21194000 | 2.63605500 | -3.04487800 |
| H | 0.54656700 | 3.28972300 | -0.71107100 |
| C | -0.53347400 | 1.40336700 | 0.08296000 |
| C | -0.54727100 | 1.90790400 | 1.44836100 |
| C | -1.52948200 | 2.75750700 | 1.91670900 |
| C | -2.58982900 | 3.15890400 | 1.07951500 |
| C | -2.66599100 | 2.64437800 | -0.22908900 |
| C | -1.70033200 | 1.78110600 | -0.70397000 |
| I | -2.56441700 | -1.60586400 | 0.12929200 |
| H | 0.24666500 | 1.58075100 | 2.11088100 |
| H | -1.50017600 | 3.10026100 | 2.95033200 |
| H | -3.35957500 | 3.83092500 | 1.45134900 |
| H | -3.51190700 | 2.90502000 | -0.86223400 |
| H | -1.79201400 | 1.38450500 | -1.70924000 |
| C | 1.42346600 | 0.59709500 | -2.76562300 |
| C | 2.44342400 | 2.97128200 | 1.11601000 |
| H | 2.47545000 | 0.52142500 | -2.48052700 |
| H | 1.28896000 | 0.52961200 | -3.84861400 |
| H | 0.91781500 | -0.24992300 | -2.28346300 |
| H | 3.38201100 | 3.52247300 | 0.98380800 |
| H | 2.56258900 | 2.31256800 | 1.98268700 |
| H | 1.62965200 | 3.67222700 | 1.31708900 |
| O | 0.74642900 | -2.17684300 | -0.65413900 |
| O | 1.45971100 | -0.36654200 | 1.44255600 |
| C | 1.89875100 | -2.64430500 | -0.38540600 |
| C | 2.54223700 | -1.02987700 | 1.39372000 |
| C | 3.66728500 | -0.49727200 | 2.26061000 |
| H | 4.45089100 | -1.23861600 | 2.44758400 |
| H | 4.10180200 | 0.35306700 | 1.72125800 |
| H | 3.26534700 | -0.13466100 | 3.21212700 |
| C | 2.30944500 | -3.83578300 | -1.23400300 |
| H | 2.34207000 | -3.52811000 | -2.28594900 |
| H | 3.28280500 | -4.24817100 | -0.95099900 |
| H | 1.54344400 | -4.61454000 | -1.14986600 |
| C | 2.78909800 | -2.15375700 | 0.58304400 |
| H | 3.75721600 | -2.63470500 | 0.67028900 |