Supporting Information

Why Is Copper(I) Complex More Competent Than Dirhodium(II) Complex in Catalytic Asymmetric O–H Insertion Reactions? A Computational Study of the Metal Carbenoid O–H Insertion into Water

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Content

1. Computational Details

All of the DFT calculations were performed with the Gaussian 03 program package.[1] The geometry optimization of all the minima and transition states involved were performed at the B3LYP levels of theory[2] with a basis set consisting of the LANL2DZ basis set[3] for copper and rhodium and the 6-31G(d) basis set[4] for the other atoms.[5] This basis set was denoted as 631LAN.[6] The vibrational frequencies were computed at the same level of theory to check whether every optimized geometrical structure is an energy minimum or a transition state, and to evaluate its zero-point vibration energy (ZPVE). Solvent effects were computed by the CPCM model[7] in CH_2Cl_2 or $CHCl_3$ using the gas phase optimized structures. All of the energies discussed in the paper and the Supporting Information are Gibbs free energies in CH_2Cl_2 (ΔG_{sol}), unless otherwise specified. The relative enthalpies in CH_2Cl_2 (ΔH_{sol}) and Gibbs free energies in gas phase (ΔG_{gas}) are also given in Figures S1, S2, and S3 and Tables S1 and S2.

Diffuse function is believed to be important for describing reactions involving zwitterionic intermediates and transition states. Here we tested two basis sets with diffuse functions. Since copper has 6-31+G(d) basis set, we computed energies at the CPCM-B3LYP/6-31+G(d)//B3LYP/6-31LAN level. It is found that at this level, the free energy difference between **TS-3-F** and **TS-3-O** is 11.2 kcal/mol in solution, close to that obtained at the CPCM-B3LYP/6-31LAN level (9.6 kcal/mol). Besides, all key energies in the paper were computed at the CPCM-B3LYP/6-31+LAN// B3LYP/6-31LAN level (Schemes S1 and S2). The 6-31+LAN basis set is defined as follows: the LANL2DZ basis set for Cu and Rh; the 6-31+G(d) basis set for the other atoms. At this level, the trends for the reaction mechanisms are the same as those obtained at the CPCM-B3LYP/6-31LAN level. In addition, the predicted enantioselectivity is almost the same at both calculation levels (6-31LAN basis set: 88% ee; 6-31+LAN basis set: 86% ee). Finally, previous DFT studies[6,8] of

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[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

[2] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[3] Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.

[4] Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

[5] Each d orbital (for all elements) includes 5d functions.

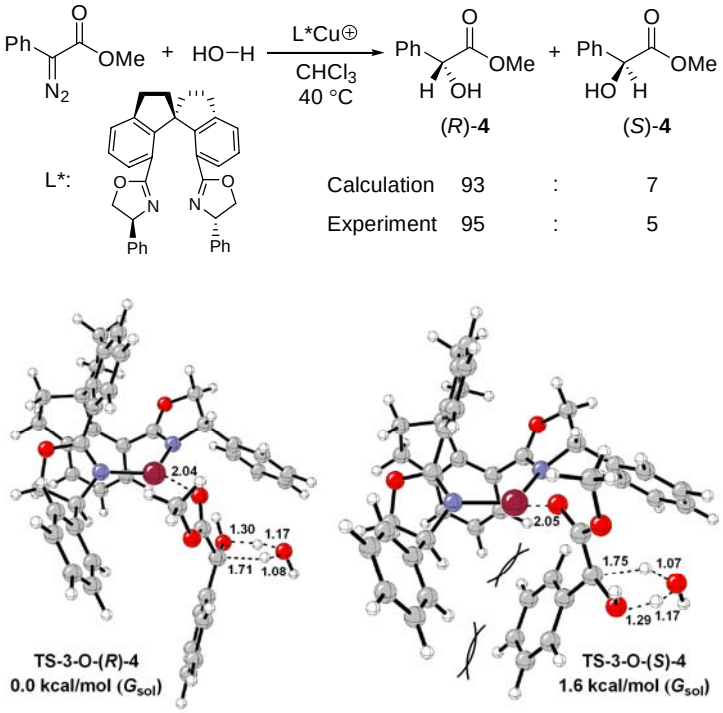
[6] Nakamura, E.; Yoshikai, N.; Yamanaka, M. *J. Am. Chem. Soc.* **2002**, *124*, 7181.

[7] (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669. (c) Takano, Y.; Houk, K. N. *J. Chem. Theory Comput.* **2005**, *1*, 70.

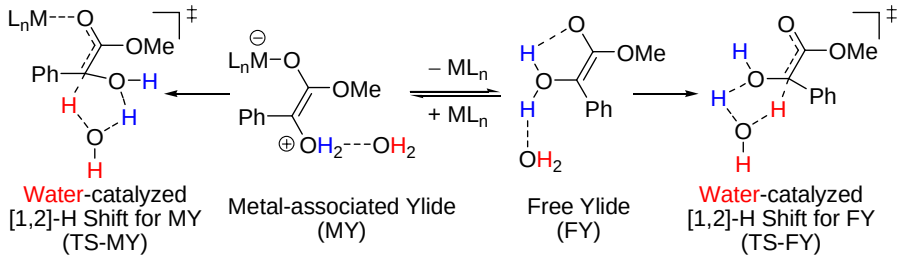
[8] Nowlan, D. T.; Gregg, T. M.; Davies, H. M. L.; Singleton, D. A. *J. Am. Chem. Soc.* **2003**, *125*, 15902.

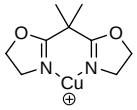
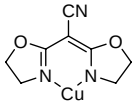
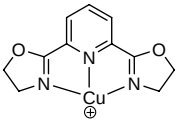
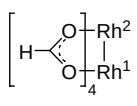
metal carbenoid mediated reactions have also supported the applicability of the 6-31LAN basis set. Therefore, the 6-31LAN basis set is suitable for investigating the present reactions.

Scheme S1. Computed Free Energy Difference and Enantioselectivity for the Reaction Shown in Scheme 3 at the CPCM-B3LYP/6-31+LAN//B3LYP/6-31LAN Level



Scheme S2. Computed Free Energy Differences of the Two Competing Pathways for Various Catalyst Systems Shown in Scheme 4 at the CPCM-B3LYP/6-31+LAN// B3LYP/6-31LAN Level



entry	ML_n	$\Delta\Delta G_{sol}$(FY-MY) [$\Delta\Delta G^{\neq}_{sol}$TS-(FY-MY)] (kcal/mol)	entry	ML_n	$\Delta\Delta G_{sol}$(FY-MY) [$\Delta\Delta G^{\neq}_{sol}$TS-(FY-MY)] (kcal/mol)
1		7.7 [5.1]	2		2.8 [–2.6]
3		–1.7 [–4.6]	4		–10.9 [–10.2]

2. Formations of Cu(I) Carbenoid 1 and Rh(II) Carbenoid 5

The formation of Cu(I) carbenoid **1** requires an activation free energy of 12.5 kcal/mol, and it is exergonic by 20.0 kcal/mol in CH_2Cl_2 (Figure S1). In Figure 1 of the paper, the regenerated Cu(I) catalyst **S1** is coordinatively unsaturated, and it can be coordinated by unreacted α-diazoester **S2** to start another catalytic cycle or stabilized by solvent CH_2Cl_2 to form complex **S4**. These two processes are slightly endergonic by 3.4 kcal/mol and 2.0 kcal/mol, respectively (Figure S1). This indicates that the catalyst resting state shown in Figure 1 of the paper is reasonable.

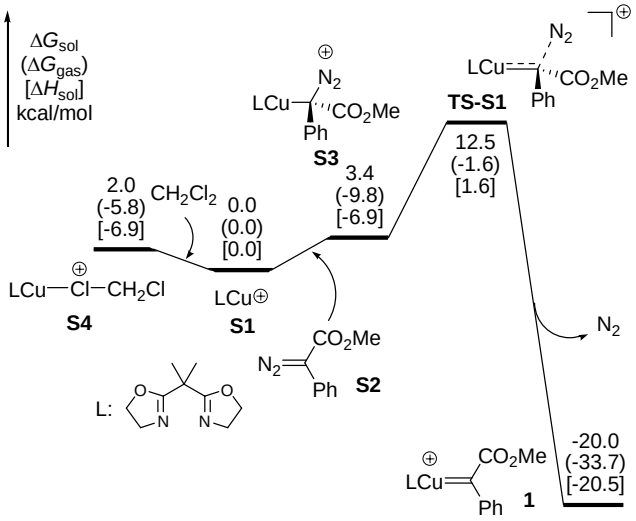


Figure S1. DFT-computed free energy surface for the formation of Cu(I) carbenoid **1**.

The formation of Rh(II) carbenoid **5** requires an activation free energy of 26.2 kcal/mol, and it is exergonic by 4.2 kcal/mol in CH_2Cl_2 (Figure S2). In Figure 2 of the paper, the regenerated Rh(II) catalyst **S5** is coordinatively unsaturated, and it can be coordinated by unreacted α-diazoester **S2** to start another catalytic cycle or stabilized by solvent CH_2Cl_2 to form complex **S7**. These two processes are endergonic by 15.2 kcal/mol and 10.3 kcal/mol, respectively (Figure S2). This indicates that the catalyst resting state shown in Figure 2 of the paper is reasonable.

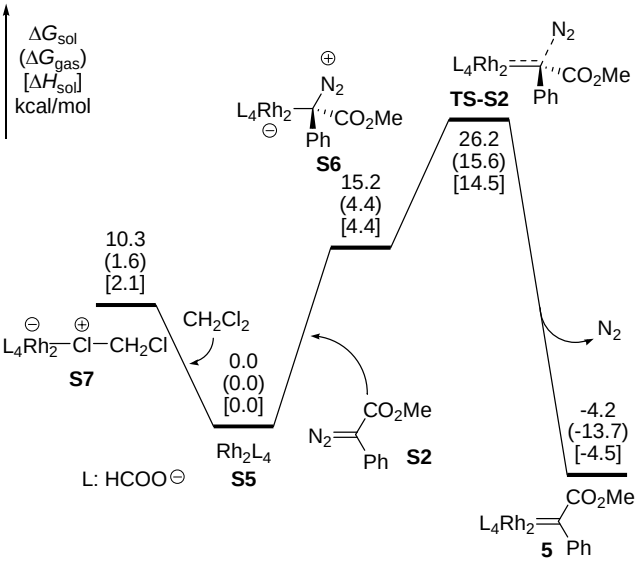
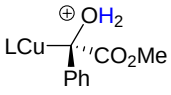
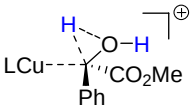
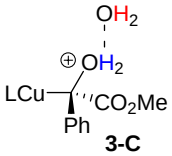
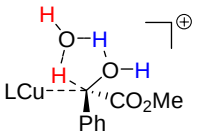
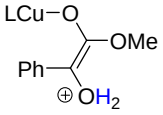
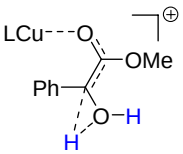
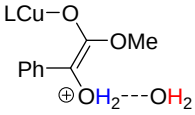
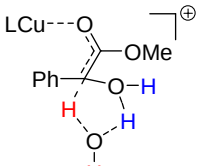
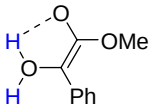
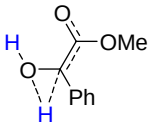
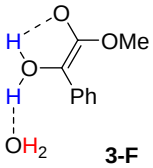
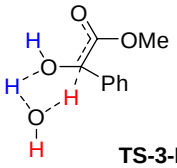


Figure S2. DFT-computed free energy surface for the formation of Rh(II) carbenoid **5**.

3. Detailed Discussions on [1,2]-H Shifts

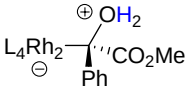
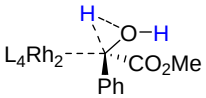
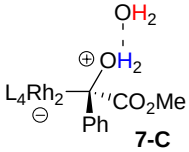
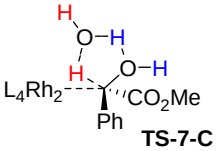
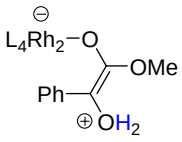
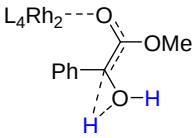
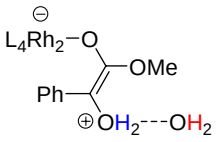
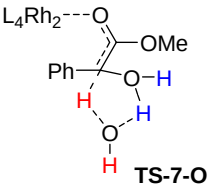
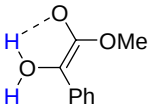
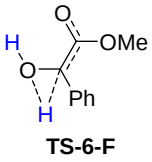
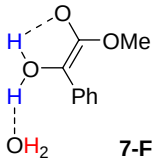
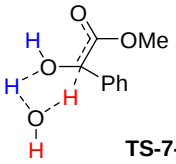
Table S1. The Comparison between Direct [1,2]-H Shift and Water-catalyzed [1,2]-H Shift in the Cu(I)-catalyzed O–H Insertion Reaction

	oxonium ylide intermediate [a]	direct [1,2]-H shift transition state [a]	complex of oxonium ylide with water [b]	water-catalyzed [1,2]-H shift transition state [b]
structrue	 **2-C**	 **TS-2-C**	 **3-C**	 **TS-3-C**
ΔG_{sol} (ΔG_{gas}) [ΔH_{sol}] kcal/mol	8.6 (6.1) [-2.0]	32.7 (29.3) [19.9]	9.6 (-0.3) [-11.4]	27.1 (21.5) [3.3]
structrue	 **2-O**	 **TS-2-O**	 **3-O**	 **TS-3-O**
ΔG_{sol} (ΔG_{gas}) [ΔH_{sol}] kcal/mol	16.4 (17.1) [6.2]	39.2 (33.1) [28.6]	13.2 (5.7) [-7.2]	19.8 (13.1) [-2.7]
structrue	 **2-F**	 **TS-2-F**	 **3-F**	 **TS-3-F**
ΔG_{sol} (ΔG_{gas}) [ΔH_{sol}] kcal/mol	23.8 (39.0) [22.0]	45.4 (53.8) [44.2]	24.7 (31.6) [13.4]	29.4 (36.2) [16.6]

[a] Energies are all calculated relative to Cu(I) carbenoid **1** and one H_2O molecule.

[b] Energies are all calculated relative to Cu(I) carbenoid **1** and two H_2O molecules.

Table S2. The Comparison between Direct [1,2]-H Shift and Water-catalyzed [1,2]-H Shift in the Rh(II)-catalyzed O–H Insertion Reaction

	oxonium ylide intermediate [a]	direct [1,2]-H shift transition state [a]	complex of oxonium ylide with water [b]	water-catalyzed [1,2]-H shift transition state [b]
structrue	 **6-C**	 **TS-6-C**	 **7-C**	 **TS-7-C**
ΔG_{sol} (ΔG_{gas}) [ΔH_{sol}] kcal/mol	0.6 (-7.5) [-12.9]	32.6 (25.8) [19.8]	1.6 (-9.2) [-22.2]	28.9 (20.3) [4.4]
structrue	 **6-O**	 **TS-6-O**	 **7-O**	 **TS-7-O**
ΔG_{sol} (ΔG_{gas}) [ΔH_{sol}] kcal/mol	16.1 (19.2) [5.1]	38.6 (32.7) [28.9]	15.4 (10.0) [-6.5]	19.3 (14.6) [-4.3]
structrue	 **6-F**	 **TS-6-F**	 **7-F**	 **TS-7-F**
ΔG_{sol} (ΔG_{gas}) [ΔH_{sol}] kcal/mol	8.0 (19.0) [6.0]	29.6 (33.8) [28.3]	8.9 (11.6) [-2.5]	13.6 (16.3) [0.6]

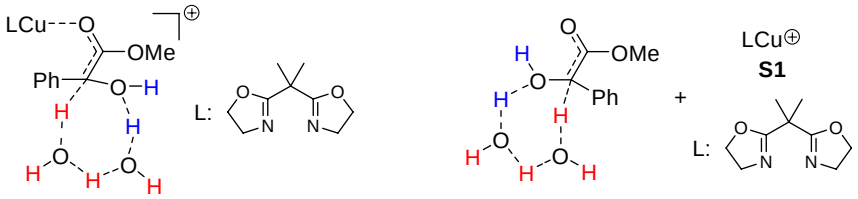
[a] Energies are all calculated relative to Rh(II) carbenoid **5** and one H_2O molecule.

[b] Energies are all calculated relative to Rh(II) carbenoid **5** and two H_2O molecules.

4. [1,2]-H Shifts Catalyzed by Two H_2O Molecules

With the use of two H_2O molecules as the catalyst for the [1,2]-H shift, the activation free energy required in the copper-associated ylide pathway (**TS-3-O-2H$_2$O**, Scheme S3) is 10.3 kcal/mol lower than that in the free-ylide pathway (**TS-3-F-2H$_2$O**, Scheme S3). This is close to the free energy difference (9.6 kcal/mol) between the copper-associated ylide pathway (**TS-3-O**) and the free-ylide pathway (**TS-3-F**) shown in Figure 1 of the paper. This suggests that using one H_2O molecule to simulate water-catalyzed [1,n]-H shift is reasonable.[9]

Scheme S3.



TS-3-O-2H$_2$O **0.0 kcal/mol (G_{sol})** **TS-3-F-2H$_2$O** **10.3 kcal/mol (G_{sol})**

[9] Shi, F.-Q.; Li, X.; Xia, Y.; Zhang, L.; Yu, Z.-X. *J. Am. Chem. Soc.* **2007**, *129*, 15503.

5. Another Free-ylide Pathway via an Enol Intermediate

Another free-ylide pathway via an enol intermediate was proposed in a Rh(II) carbenoid-initiated Claisen rearrangement by Wood and co-workers.[10] In this pathway, generation of enol intermediate **S8** is easy with an energy barrier of 12.5 kcal/mol (Figure S3). Formation of **S8** is exergonic by 15.8 kcal/mol in CH_2Cl_2, but the direct intramolecular [1,3]-H shift requires an activation free energy as high as 48.6 kcal/mol (Figure S3). When the [1,3]-H shift is catalyzed by one molecule of water via **TS-S5**, the energy barrier for the subsequent tautomerization to O–H insertion product **4** decreases to 27.4 kcal/mol (Figure S3). However, this pathway is still less favorable than the water-catalyzed [1,2]-H shift pathway shown in Figure 2 of the paper.

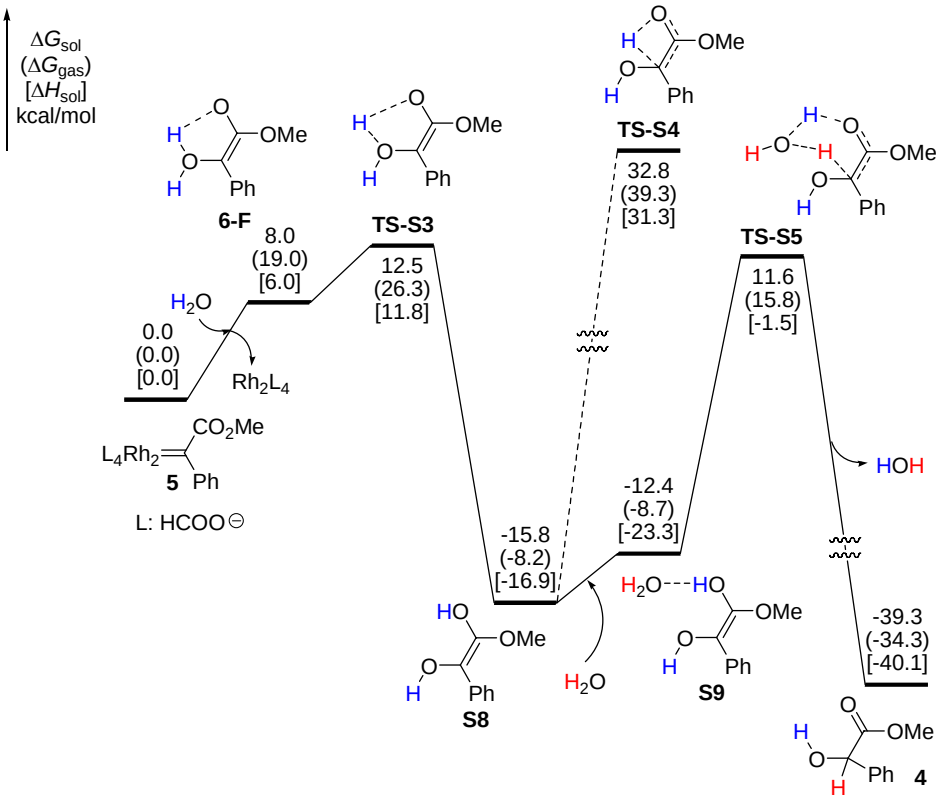
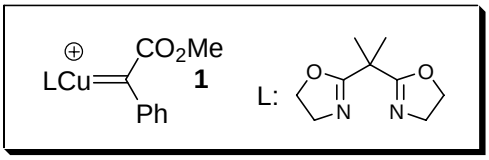


Figure S3. DFT-computed free energy surface for another free-ylide pathway via an enol intermediate.

[10] (a) Wood, J. L.; Moniz, G. A.; Pflum, D. A.; Stoltz, B. M.; Holubec, A. A.; Dietrich, H.-J. *J. Am. Chem. Soc.* **1999**, *121*, 1748. (b) Wood, J. L.; Moniz, G. A. *Org. Lett.* **1999**, *1*, 371.

6. Coordinates of All Stationary Points



Standard orientation:

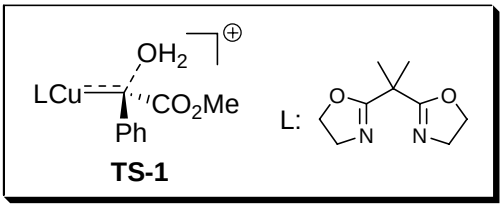
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.926864	0.039863	0.316370
2	6	0	-3.019989	-0.395801	-0.490186
3	6	0	-2.191711	1.053735	1.366867
4	8	0	-1.858466	2.215863	1.200674
5	8	0	-2.751626	0.563689	2.477886
6	6	0	-2.906220	1.495196	3.577220
7	6	0	-4.359233	0.046773	-0.282558
8	6	0	-5.388632	-0.404751	-1.093059
9	6	0	-5.114510	-1.308343	-2.129463
10	6	0	-3.808692	-1.765254	-2.358232
11	6	0	-2.777121	-1.315574	-1.550387
12	1	0	-3.318920	0.905642	4.394413
13	1	0	-3.588194	2.300902	3.297307
14	1	0	-1.937138	1.917539	3.852411
15	1	0	-4.573838	0.740886	0.523222
16	1	0	-6.405057	-0.061971	-0.927256
17	1	0	-5.924807	-1.660987	-2.761445
18	1	0	-3.611765	-2.467545	-3.162078
19	1	0	-1.760006	-1.662983	-1.708444
20	1	0	2.235474	3.569935	-2.502497
21	6	0	2.062733	3.242287	-1.476278
22	6	0	0.744809	2.463514	-1.270236
23	8	0	3.095389	2.261980	-1.149342
24	1	0	2.188168	4.086773	-0.795015
25	7	0	1.192059	1.158892	-0.735395
26	1	0	0.199579	2.299043	-2.205187
27	1	0	0.062365	2.932102	-0.557035
28	6	0	2.475804	1.152941	-0.716078
29	29	0	-0.064024	-0.220495	0.090999
30	6	0	3.431609	0.055999	-0.287828
31	7	0	1.507830	-1.410202	0.513854
32	6	0	2.754108	-1.170108	0.297566
33	6	0	4.394189	0.632068	0.792127

34	6	0	4.248725	-0.383018	-1.538932
35	6	0	1.400548	-2.749050	1.134528
36	8	0	3.623208	-2.129574	0.648896
37	1	0	5.117995	-0.130937	1.084741
38	1	0	4.928401	1.492223	0.384581
39	1	0	3.842805	0.953273	1.682187
40	1	0	4.772530	0.480726	-1.953761
41	1	0	4.982222	-1.139815	-1.253812
42	1	0	3.594863	-0.800623	-2.311807
43	6	0	2.862722	-3.242693	1.202978
44	1	0	0.763287	-3.390087	0.518795
45	1	0	0.934507	-2.656570	2.119906
46	1	0	3.065741	-4.119110	0.584451
47	1	0	3.227575	-3.417259	2.216722

H_2O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.119433	0.000000
2	1	0	0.762822	-0.477734	0.000000
3	1	0	-0.762822	-0.477733	0.000000

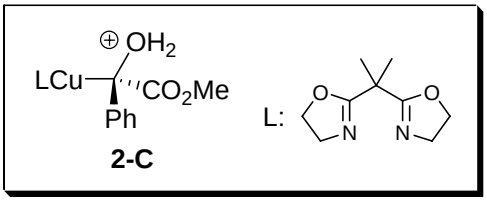


TS-1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.211070	0.084973	-1.397656
2	6	0	4.280325	-0.080455	-0.376229
3	6	0	2.906384	-0.241260	-0.667599
4	6	0	2.506921	-0.244647	-2.020546
5	6	0	3.438159	-0.084998	-3.042409
6	6	0	4.791275	0.082093	-2.731605

7	6	0	1.896617	-0.417752	0.390355
8	29	0	-0.012938	-0.165844	0.111802
9	7	0	-1.271136	1.419679	-0.181187
10	6	0	-2.550763	1.401473	-0.297281
11	8	0	-3.164188	2.586671	-0.463854
12	6	0	-2.139762	3.621934	-0.450516
13	6	0	-0.826242	2.826635	-0.278113
14	6	0	-3.520525	0.234391	-0.278329
15	6	0	2.285797	-0.041251	1.785548
16	8	0	2.425180	1.278589	1.916245
17	6	0	2.710708	1.761710	3.251868
18	8	0	2.020591	-2.305841	0.722136
19	1	0	2.866242	-2.592711	0.325905
20	8	0	2.398919	-0.830835	2.723295
21	7	0	-1.633355	-1.439451	0.044954
22	6	0	-2.870354	-1.125049	-0.098504
23	8	0	-3.762014	-2.132306	-0.091721
24	6	0	-3.022940	-3.374481	0.090530
25	6	0	-1.552265	-2.909284	0.183850
26	1	0	1.886930	1.513890	3.924979
27	1	0	2.816260	2.840397	3.146179
28	1	0	3.634455	1.316393	3.626415
29	1	0	-1.084698	-3.160418	1.139889
30	1	0	-0.923068	-3.316610	-0.612486
31	1	0	-3.234728	-4.012795	-0.769595
32	1	0	-3.397625	-3.849976	0.999181
33	1	0	-2.210272	4.167651	-1.393364
34	1	0	-2.363629	4.295908	0.379007
35	1	0	-0.275733	3.098371	0.626921
36	1	0	-0.147065	2.935129	-1.128990
37	1	0	2.191561	-2.189718	1.703458
38	1	0	4.617269	-0.073901	0.657294
39	1	0	1.453485	-0.373081	-2.255370
40	1	0	3.113820	-0.087381	-4.078708
41	1	0	5.518378	0.211244	-3.528067
42	1	0	6.261836	0.216491	-1.157575
43	6	0	-4.519007	0.452931	0.896881
44	6	0	-4.295113	0.227177	-1.629394
45	1	0	-5.258811	-0.349830	0.903819
46	1	0	-3.998708	0.458267	1.860594
47	1	0	-5.032064	1.408350	0.770913
48	1	0	-5.031238	-0.578979	-1.626094
49	1	0	-4.811238	1.179867	-1.762856
50	1	0	-3.614324	0.076250	-2.473996

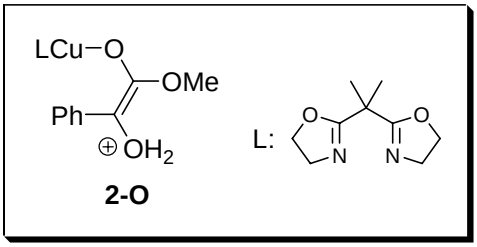


2-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.924149	-0.712716	0.263522
2	6	0	2.266377	-0.623926	1.710764
3	8	0	2.392974	-1.635518	2.416546
4	1	0	1.769481	0.313465	4.166638
5	8	0	2.356819	0.613623	2.180680
6	6	0	2.600280	0.744400	3.603603
7	1	0	2.675774	1.816216	3.780106
8	1	0	3.528900	0.239761	3.876737
9	8	0	2.110170	-2.383985	0.116905
10	1	0	2.257238	-2.564202	1.122482
11	6	0	4.239763	0.091889	-0.387157
12	1	0	4.596289	-0.119005	0.618113
13	6	0	2.887851	-0.134401	-0.718450
14	6	0	2.464010	0.157471	-2.028738
15	1	0	1.424965	-0.016498	-2.297357
16	6	0	3.354736	0.662036	-2.973879
17	1	0	3.010064	0.881080	-3.980198
18	1	0	5.381669	1.291685	-3.357691
19	6	0	4.688220	0.891451	-2.623862
20	1	0	6.163800	0.786533	-1.053418
21	6	0	5.128680	0.607640	-1.328886
22	1	0	2.965350	-2.543179	-0.337288
23	1	0	-3.692970	-3.827308	0.189856
24	6	0	-3.269443	-3.200477	-0.597398
25	6	0	-1.767821	-2.885707	-0.412657
26	8	0	-3.903443	-1.893033	-0.507763
27	1	0	-3.518919	-3.621647	-1.573422
28	7	0	-1.726973	-1.417129	-0.244514
29	1	0	-1.162546	-3.171463	-1.277812
30	1	0	-1.338323	-3.366172	0.471358
31	6	0	-2.933417	-0.980834	-0.311547
32	29	0	-0.010942	-0.319043	0.069658

33	6	0	-3.474264	0.432731	-0.197472
34	7	0	-1.142031	1.399252	0.115658
35	6	0	-2.416827	1.503379	-0.000795
36	6	0	-4.440906	0.480960	1.023381
37	6	0	-4.261321	0.758898	-1.500873
38	6	0	-0.591022	2.759168	0.296186
39	8	0	-2.937214	2.743001	0.064609
40	1	0	-4.879622	1.477387	1.105813
41	1	0	-5.240971	-0.249493	0.887867
42	1	0	-3.911383	0.252512	1.954441
43	1	0	-5.061059	0.029069	-1.640063
44	1	0	-4.698912	1.756208	-1.426711
45	1	0	-3.604270	0.729444	-2.376684
46	6	0	-1.836006	3.674414	0.265925
47	1	0	0.117383	2.974742	-0.509128
48	1	0	-0.045965	2.807949	1.243264
49	1	0	-1.847566	4.383244	-0.564474
50	1	0	-2.020743	4.206088	1.201655

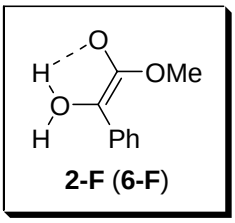


2-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.771819	3.259293	1.667074
2	6	0	-3.772533	3.067773	0.711374
3	6	0	-3.982778	1.811106	0.145702
4	6	0	-3.201463	0.705302	0.542314
5	6	0	-2.210160	0.903679	1.529470
6	6	0	-1.992851	2.170005	2.068768
7	6	0	-3.401005	-0.607120	-0.026728
8	6	0	-2.617039	-1.720659	-0.231535
9	8	0	-3.369940	-2.776729	-0.771704
10	6	0	-2.645752	-3.861944	-1.383080
11	8	0	-4.787360	-0.849601	-0.591176
12	8	0	-1.390770	-1.898768	-0.006946

13	29	0	0.160019	-0.710635	-0.142208
14	7	0	0.948228	1.003226	-0.823999
15	6	0	2.181022	1.361317	-0.753195
16	8	0	2.486058	2.580030	-1.237598
17	6	0	1.255592	3.186657	-1.724385
18	6	0	0.185886	2.107471	-1.446798
19	6	0	3.400513	0.627266	-0.219689
20	6	0	4.083842	1.532888	0.847101
21	7	0	2.012871	-1.350434	0.580072
22	6	0	3.118897	-0.720230	0.422828
23	8	0	4.235893	-1.314514	0.890019
24	6	0	3.842676	-2.588370	1.474620
25	6	0	2.309918	-2.619767	1.274749
26	6	0	4.375427	0.397959	-1.413344
27	1	0	4.376915	-3.376479	0.939719
28	1	0	4.154914	-2.582086	2.520962
29	1	0	1.757244	-2.656545	2.218405
30	1	0	1.977557	-3.460233	0.658277
31	1	0	-0.593851	2.442529	-0.757464
32	1	0	-0.297989	1.744784	-2.358587
33	1	0	1.104208	4.114828	-1.169372
34	1	0	1.396146	3.413456	-2.783200
35	1	0	4.987766	1.045679	1.217114
36	1	0	4.352991	2.491749	0.400679
37	1	0	3.414231	1.716698	1.694120
38	1	0	4.637232	1.357061	-1.864958
39	1	0	5.286031	-0.086660	-1.055512
40	1	0	3.917753	-0.237759	-2.178753
41	1	0	-4.660170	-1.791399	-0.961691
42	1	0	-4.747296	1.689888	-0.616504
43	1	0	-1.636172	0.054788	1.887028
44	1	0	-1.946603	-4.289802	-0.664101
45	1	0	-2.105406	-3.511242	-2.267082
46	1	0	-3.401566	-4.594793	-1.665062
47	1	0	-4.391060	3.903330	0.395761
48	1	0	-1.229244	2.299100	2.831207
49	1	0	-2.612238	4.239952	2.105051
50	1	0	-5.450922	-0.887077	0.133232

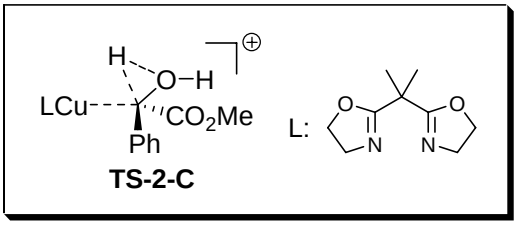


2-F (6-F)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.930386	1.100427	-0.114162
2	6	0	0.837724	0.207846	-0.019324
3	6	0	1.125121	-1.176089	0.085826
4	6	0	2.439414	-1.627109	0.093962
5	6	0	3.513058	-0.733109	0.008884
6	6	0	3.243096	0.631221	-0.095784
7	6	0	-0.515365	0.673856	-0.009117
8	8	0	-0.716646	2.171353	0.015219
9	1	0	-0.435724	2.530361	0.883997
10	6	0	-1.819405	0.187255	0.003486
11	8	0	-2.784247	1.022163	0.037929
12	8	0	-2.017485	-1.145939	-0.035878
13	6	0	-3.387874	-1.565162	-0.074208
14	1	0	-3.892425	-1.169840	-0.960235
15	1	0	-3.924153	-1.231823	0.818675
16	1	0	-3.353843	-2.654903	-0.111500
17	1	0	0.305098	-1.881419	0.159536
18	1	0	2.628587	-2.695052	0.173229
19	1	0	4.536867	-1.095464	0.020147
20	1	0	4.060262	1.344577	-0.172778
21	1	0	1.751269	2.165939	-0.230949
22	1	0	-1.725855	2.112194	0.004355

* This structure was optimized as the distance between atom 8 and atom 22 was frozen at 1.011 Å.

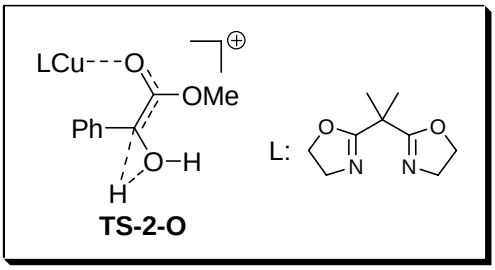


TS-2-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.909563	3.496203	0.997862
2	6	0	0.112349	2.376377	0.702668
3	7	0	-0.731601	1.215015	0.347755
4	6	0	-1.958328	1.597183	0.357272
5	8	0	-2.193641	2.876686	0.688807
6	7	0	-1.930053	-1.298886	-0.532655
7	6	0	-2.302606	-2.655681	-0.995632
8	6	0	-3.843449	-2.606034	-1.085554
9	8	0	-4.162536	-1.244548	-0.673754
10	6	0	-3.013271	-0.615331	-0.391440
11	6	0	-3.227339	0.820862	0.055500
12	6	0	-3.995452	1.567053	-1.075923
13	6	0	-4.094138	0.796591	1.350549
14	1	0	-4.351758	-3.284525	-0.398079
15	1	0	-4.235690	-2.744081	-2.094686
16	1	0	-1.826747	-2.856572	-1.959884
17	1	0	-1.943466	-3.399125	-0.278113
18	1	0	-4.301516	1.819806	1.670183
19	1	0	-5.039744	0.288413	1.152059
20	1	0	-3.577157	0.273319	2.161914
21	1	0	-4.938518	1.056707	-1.279481
22	1	0	-4.205346	2.591087	-0.762198
23	1	0	-3.407301	1.598170	-1.999297
24	1	0	0.773405	2.609346	-0.137514
25	1	0	0.738984	2.122522	1.560994
26	1	0	-0.807584	4.375549	0.359877
27	1	0	-0.939476	3.805390	2.044974
28	29	0	-0.068429	-0.655419	-0.134288
29	6	0	1.939472	-1.107239	-0.012609
30	6	0	2.188006	-1.328012	1.454692
31	6	0	2.740260	-0.104352	-0.768258
32	8	0	2.141469	-0.208104	2.179734
33	8	0	2.371853	-2.443329	1.918225
34	6	0	3.976971	0.355859	-0.285386
35	6	0	2.291503	0.354266	-2.018923
36	6	0	2.347086	-0.376571	3.605813
37	6	0	4.734864	1.259062	-1.029008
38	1	0	4.352302	0.012091	0.673391
39	6	0	3.052658	1.251638	-2.765338
40	1	0	1.345157	-0.008238	-2.415496
41	1	0	1.556304	-1.000790	4.027462

42	1	0	3.317272	-0.840324	3.792888
43	1	0	2.312191	0.630039	4.019628
44	6	0	4.275851	1.709012	-2.268926
45	1	0	5.688803	1.605417	-0.642600
46	1	0	2.694040	1.590595	-3.732737
47	1	0	4.870360	2.409676	-2.847736
48	1	0	1.113156	-2.026350	-0.558265
49	8	0	2.237047	-2.564813	-0.650841
50	1	0	2.385580	-3.106322	0.169830

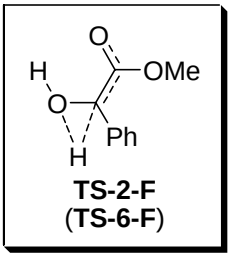


TS-2-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.617744	-2.721102	1.359739
2	7	0	-1.596257	-1.476322	0.563454
3	6	0	-2.791958	-1.009164	0.530878
4	8	0	-3.738211	-1.706146	1.189216
5	6	0	-3.095174	-2.865291	1.790396
6	6	0	-3.349770	0.232256	-0.144812
7	6	0	-2.338521	1.071690	-0.907856
8	7	0	-1.086116	0.883002	-1.128206
9	6	0	-0.591744	2.010067	-1.947611
10	6	0	-1.838627	2.900144	-2.147320
11	8	0	-2.886678	2.180541	-1.438151
12	29	0	0.010833	-0.661866	-0.443905
13	8	0	1.741972	-1.574922	-0.697908
14	6	0	2.922596	-1.171586	-0.671289
15	8	0	3.935728	-2.001169	-0.992689
16	6	0	3.592291	-3.334467	-1.436008
17	6	0	3.309420	0.179922	-0.413572
18	6	0	2.743056	1.035786	0.631839
19	6	0	2.716051	2.431944	0.454573
20	6	0	2.218599	3.267129	1.453256
21	6	0	1.722963	2.717745	2.639307

22	6	0	1.735647	1.332653	2.828897
23	6	0	2.251137	0.498133	1.838780
24	8	0	5.013110	0.257453	-0.338772
25	1	0	5.283472	-0.657658	-0.583025
26	1	0	2.966206	-3.281589	-2.329016
27	1	0	3.066855	-3.871049	-0.643883
28	1	0	4.544527	-3.813492	-1.659282
29	1	0	3.098079	2.854085	-0.471103
30	1	0	2.218464	4.343674	1.309801
31	1	0	1.335674	3.368195	3.418346
32	1	0	1.365516	0.906875	3.757138
33	1	0	2.285658	-0.575820	2.000331
34	1	0	4.371220	0.616843	-1.183894
35	1	0	-0.188157	1.625021	-2.888883
36	1	0	0.216334	2.517529	-1.413222
37	1	0	-1.755145	3.890453	-1.694811
38	1	0	-2.152864	2.999783	-3.188141
39	1	0	-3.251587	-2.807255	2.869539
40	1	0	-3.588026	-3.757094	1.398050
41	1	0	-1.271311	-3.554734	0.741495
42	1	0	-0.934651	-2.624465	2.208956
43	6	0	-3.992407	1.128751	0.954646
44	6	0	-4.444222	-0.223863	-1.156591
45	1	0	-4.757847	0.563281	1.489398
46	1	0	-3.240179	1.467258	1.675159
47	1	0	-4.453933	2.004242	0.494313
48	1	0	-5.217135	-0.789306	-0.632572
49	1	0	-4.899692	0.650581	-1.625515
50	1	0	-4.015954	-0.858551	-1.939739

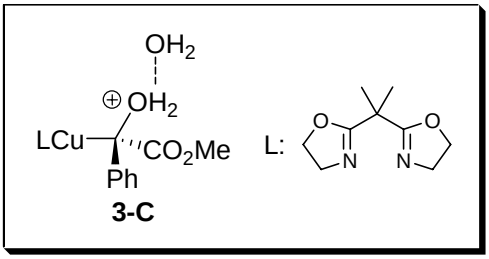


TS-2-F
(TS-6-F)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.116233	0.613263	0.438827

2	6	0	-1.829535	1.100359	0.210061
3	6	0	-0.804801	0.239370	-0.222990
4	6	0	-1.115640	-1.119762	-0.434658
5	6	0	-2.404259	-1.594008	-0.201328
6	6	0	-3.414679	-0.734507	0.236761
7	6	0	0.548711	0.725954	-0.499552
8	6	0	1.806481	0.195018	-0.026309
9	8	0	1.914468	-1.141693	-0.070642
10	6	0	3.190404	-1.675739	0.322956
11	8	0	2.731999	0.939491	0.338843
12	8	0	0.702671	2.315415	-0.210180
13	1	0	1.643997	2.277234	0.157717
14	1	0	3.412471	-1.415498	1.360860
15	1	0	3.983990	-1.289164	-0.321649
16	1	0	3.096098	-2.756006	0.210544
17	1	0	-0.343148	-1.798359	-0.777807
18	1	0	-2.619023	-2.646663	-0.368109
19	1	0	-4.419032	-1.109572	0.412524
20	1	0	-3.889255	1.297838	0.779101
21	1	0	-1.611512	2.149750	0.373210
22	1	0	0.789612	1.885044	-1.233161

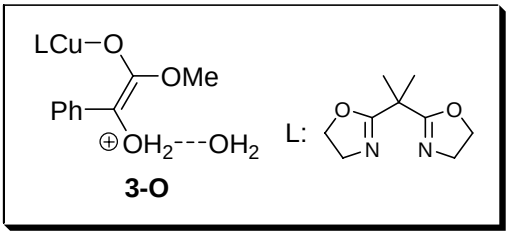


3-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.995406	3.616661	0.482177
2	6	0	-0.756303	2.692497	0.491736
3	7	0	-1.307147	1.352090	0.203766
4	6	0	-2.577190	1.470147	0.066710
5	8	0	-3.096981	2.706066	0.203405
6	29	0	-0.173555	-0.381186	0.060273
7	7	0	-1.888188	-1.436466	-0.344982
8	6	0	-1.935044	-2.893960	-0.591074
9	6	0	-3.435542	-3.189792	-0.811793

10	8	0	-4.063181	-1.885214	-0.664022
11	6	0	-3.091412	-0.989580	-0.405202
12	6	0	-3.630656	0.418635	-0.227670
13	6	0	-4.368807	0.823364	-1.537706
14	6	0	1.802203	-0.660005	0.271187
15	6	0	2.633383	0.268844	-0.564706
16	6	0	3.771650	0.933541	-0.066581
17	6	0	4.544429	1.749865	-0.897611
18	6	0	4.210150	1.902261	-2.245767
19	6	0	3.088953	1.242752	-2.756725
20	6	0	2.306841	0.444115	-1.922964
21	6	0	2.017267	-0.745329	1.736046
22	8	0	1.955552	0.413892	2.395509
23	6	0	2.037438	0.325978	3.837911
24	8	0	2.190006	-2.135579	-0.151056
25	8	0	2.167882	-1.838928	2.295886
26	6	0	-4.639861	0.402746	0.958701
27	1	0	1.184686	-0.233429	4.229635
28	1	0	2.016987	1.357421	4.187504
29	1	0	2.964224	-0.166881	4.137734
30	1	0	2.213088	-2.552816	0.778795
31	1	0	4.044126	0.831768	0.979158
32	1	0	1.430610	-0.060656	-2.322691
33	1	0	2.817861	1.358627	-3.802307
34	1	0	4.814230	2.534220	-2.890133
35	1	0	5.409684	2.264708	-0.489329
36	1	0	3.157066	-2.150681	-0.494939
37	1	0	-3.872825	-3.853409	-0.063049
38	1	0	-3.674034	-3.559754	-1.811115
39	1	0	-1.319856	-3.136898	-1.462438
40	1	0	-1.520364	-3.422897	0.272174
41	1	0	-5.072838	1.396937	1.085571
42	1	0	-5.440688	-0.310265	0.753140
43	1	0	-4.145203	0.114263	1.892322
44	1	0	-5.161539	0.103901	-1.751536
45	1	0	-4.810290	1.814781	-1.419459
46	1	0	-3.678440	0.847176	-2.387701
47	1	0	-0.020214	2.955804	-0.273471
48	1	0	-0.242286	2.672502	1.457075
49	1	0	-1.981992	4.369848	-0.308448
50	1	0	-2.199526	4.098454	1.440625
51	8	0	4.687659	-2.107898	-0.909798
52	1	0	4.932953	-2.550976	-1.738378
53	1	0	4.934968	-1.171873	-1.017548

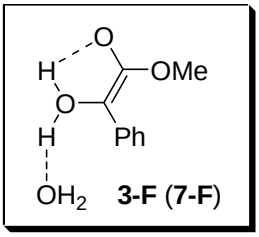


3-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.633628	-2.596233	1.272447
2	7	0	2.338345	-1.311069	0.607357
3	6	0	3.445663	-0.681322	0.460644
4	8	0	4.563293	-1.290475	0.908396
5	6	0	4.168794	-2.580299	1.455539
6	29	0	0.477340	-0.650306	-0.091178
7	7	0	1.276293	1.069162	-0.745398
8	6	0	2.508985	1.425737	-0.667480
9	8	0	2.814652	2.653156	-1.129886
10	6	0	1.581132	3.276148	-1.587256
11	6	0	0.516722	2.180499	-1.359131
12	6	0	3.727965	0.681922	-0.146891
13	6	0	4.709022	0.485539	-1.341183
14	8	0	-1.077661	-1.815463	0.083459
15	6	0	-2.252491	-1.710796	-0.375800
16	8	0	-2.820596	-2.796569	-1.036227
17	6	0	-1.960617	-3.905497	-1.341539
18	6	0	-3.116955	-0.636946	-0.319728
19	8	0	-4.376494	-0.889698	-1.069290
20	6	0	-3.049592	0.661341	0.303390
21	6	0	-3.915923	1.712232	-0.086527
22	6	0	-3.862540	2.957027	0.544282
23	6	0	-2.946720	3.198571	1.569748
24	6	0	-2.085661	2.168903	1.964241
25	6	0	-2.136920	0.917083	1.355369
26	6	0	4.403843	1.561852	0.945797
27	1	0	4.691364	-3.353673	0.888304
28	1	0	4.493517	-2.610840	2.497584
29	1	0	2.090905	-2.647366	2.221287
30	1	0	2.287942	-3.421920	0.643590
31	1	0	-0.283132	2.491316	-0.681908

32	1	0	0.057981	1.832984	-2.289834
33	1	0	1.425376	4.176137	-0.988229
34	1	0	1.719787	3.554138	-2.633830
35	1	0	5.306657	1.067043	1.308535
36	1	0	4.673730	2.531962	0.524733
37	1	0	3.729209	1.723412	1.793371
38	1	0	4.970656	1.456412	-1.766961
39	1	0	5.619015	-0.006128	-0.991574
40	1	0	4.256492	-0.131389	-2.124821
41	1	0	-4.251017	-1.807201	-1.433490
42	1	0	-4.597971	1.569152	-0.920619
43	1	0	-1.495868	0.116218	1.706891
44	1	0	-1.529373	-4.315689	-0.426385
45	1	0	-1.159788	-3.597513	-2.019930
46	1	0	-2.599937	-4.644491	-1.825133
47	1	0	-4.535802	3.745428	0.218224
48	1	0	-1.380441	2.333487	2.775003
49	1	0	-2.909722	4.166926	2.059100
50	1	0	-5.177557	-0.850671	-0.394775
51	8	0	-6.183815	-0.474411	0.645033
52	1	0	-6.210235	-1.026274	1.444961
53	1	0	-5.902149	0.413875	0.938940



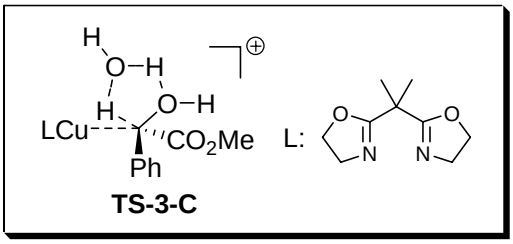
3-F (7-F)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.899343	0.602219	-0.626238
2	6	0	3.183277	0.073417	-0.465629
3	6	0	3.370422	-1.212235	0.037223
4	6	0	2.239559	-1.973326	0.364716
5	6	0	0.955940	-1.465850	0.218043
6	6	0	0.744407	-0.151706	-0.279973
7	6	0	-0.567340	0.398824	-0.390354
8	8	0	-0.654467	1.848526	-0.736093
9	6	0	-1.892203	0.004142	-0.182883

10	8	0	-2.824691	0.851372	-0.321691
11	8	0	-2.132242	-1.286704	0.148534
12	6	0	-3.514614	-1.635991	0.286310
13	8	0	0.684568	2.720921	1.306566
14	1	0	-1.659174	1.908819	-0.704834
15	1	0	1.428570	2.121256	1.084497
16	1	0	-4.054919	-1.470218	-0.650004
17	1	0	-3.991174	-1.049866	1.077340
18	1	0	-3.520001	-2.696228	0.544257
19	1	0	1.783657	1.574464	-1.099368
20	1	0	4.040814	0.677144	-0.754158
21	1	0	4.368892	-1.620360	0.162208
22	1	0	2.362595	-2.983650	0.748375
23	1	0	0.096690	-2.070804	0.483020
24	1	0	-0.249100	2.361028	0.052346
25	1	0	0.295059	2.338543	2.110503

* This structure was optimized as the distance between atom 8 and atom 14 was frozen at 1.007 Å.

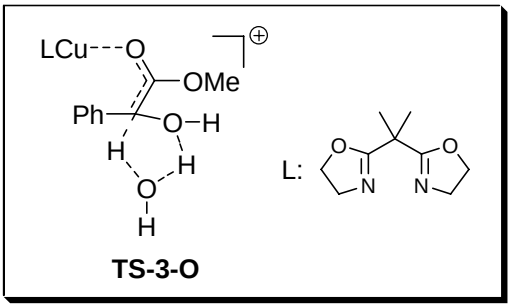


TS-3-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.191651	4.631144	-0.431284
2	6	0	-1.931722	3.866834	0.302696
3	6	0	-0.681270	3.037581	-0.059883
4	8	0	-3.000323	2.878398	0.307653
5	1	0	-1.892180	4.313667	1.298698
6	7	0	-1.176005	1.643122	-0.096241
7	1	0	0.118782	3.129173	0.679437
8	1	0	-0.269195	3.300209	-1.039565
9	6	0	-2.448321	1.671722	0.099857
10	29	0	-0.027034	-0.009684	-0.360343
11	6	0	-3.470901	0.550041	0.143957
12	7	0	-1.717328	-1.229262	-0.351539
13	6	0	-2.922561	-0.836732	-0.140443
14	6	0	-4.568759	0.860679	-0.917357

15	6	0	-4.107393	0.534784	1.566218
16	6	0	-1.764082	-2.683465	-0.634727
17	8	0	-3.883827	-1.776948	-0.164879
18	1	0	-5.343674	0.093451	-0.877164
19	1	0	-5.018527	1.832955	-0.708989
20	1	0	-4.146892	0.878755	-1.927878
21	1	0	-4.556784	1.506552	1.780188
22	1	0	-4.883210	-0.232252	1.610873
23	1	0	-3.355756	0.318612	2.332969
24	6	0	-3.226962	-3.067052	-0.338128
25	1	0	-1.037555	-3.211012	-0.014072
26	1	0	-1.490845	-2.847024	-1.683034
27	1	0	-3.354417	-3.627098	0.592073
28	1	0	-3.732408	-3.589034	-1.151459
29	1	0	0.134020	-2.574447	2.768050
30	6	0	1.123439	-2.134043	2.914047
31	8	0	1.431824	-1.222288	1.835883
32	1	0	1.872397	-2.926750	2.962904
33	1	0	1.144954	-1.525649	3.817145
34	6	0	1.551853	-1.766811	0.618710
35	6	0	1.940237	-0.791002	-0.466417
36	8	0	1.354437	-2.952733	0.375466
37	6	0	3.139121	0.075599	-0.105996
38	8	0	2.248631	-1.610043	-1.627626
39	6	0	2.989603	1.187231	0.737463
40	6	0	4.412734	-0.212545	-0.619162
41	1	0	1.958175	-2.520801	-1.400337
42	1	0	1.947619	-0.487447	-2.790500
43	6	0	4.086096	1.978837	1.075227
44	1	0	2.008836	1.420135	1.144610
45	6	0	5.507841	0.592627	-0.292321
46	1	0	4.543834	-1.072482	-1.267233
47	8	0	1.633639	0.481755	-2.754360
48	6	0	5.350874	1.688290	0.556032
49	1	0	3.952752	2.828625	1.739162
50	1	0	6.486863	0.353688	-0.698343
51	1	0	2.442548	1.033827	-2.760845
52	1	0	1.342645	0.344897	-1.617207
53	1	0	6.202993	2.311559	0.810472

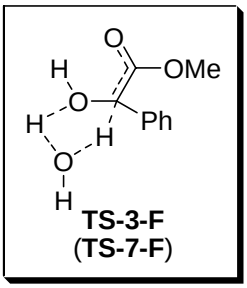


TS-3-O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.092056	-1.023648	-0.496801
2	7	0	-1.899694	-1.472316	-0.654813
3	6	0	-1.990346	-2.747824	-1.395088
4	6	0	-3.505590	-2.935399	-1.636227
5	8	0	-4.096886	-1.763853	-1.007535
6	29	0	-0.201257	-0.645947	0.196651
7	7	0	-1.250933	0.918260	0.938694
8	6	0	-2.510816	1.120183	0.793026
9	8	0	-3.000444	2.279557	1.275031
10	6	0	-1.888073	3.027815	1.842045
11	6	0	-0.676896	2.092226	1.629852
12	6	0	-3.589942	0.242338	0.180725
13	1	0	-3.926899	-3.818815	-1.152047
14	1	0	-3.792620	-2.925200	-2.689817
15	1	0	-1.417652	-2.672824	-2.324477
16	1	0	-1.551696	-3.550119	-0.794243
17	1	0	0.103210	2.534979	1.004852
18	1	0	-0.219952	1.769820	2.570625
19	1	0	-1.817137	3.973606	1.300487
20	1	0	-2.122452	3.224659	2.890174
21	6	0	-4.563710	-0.170716	1.324800
22	6	0	-4.359318	1.079006	-0.883616
23	1	0	-5.171637	0.482086	-1.302315
24	1	0	-4.777564	1.973752	-0.419427
25	1	0	-3.694669	1.386348	-1.698078
26	1	0	-4.967679	0.723570	1.804000
27	1	0	-5.388193	-0.756630	0.913856
28	1	0	-4.048681	-0.772018	2.081520
29	1	0	4.682332	-0.352093	1.448214
30	8	0	4.640169	0.156079	0.610778
31	6	0	3.358067	-0.191862	-0.039448

32	1	0	5.422814	-0.392649	-0.294308
33	6	0	2.675410	-1.250221	0.621517
34	6	0	2.674988	0.968633	-0.639130
35	8	0	5.474040	-1.003337	-1.268963
36	8	0	1.500942	-1.635632	0.427400
37	8	0	3.468373	-1.906042	1.516752
38	6	0	3.034676	2.289484	-0.311183
39	6	0	1.655173	0.774751	-1.595564
40	1	0	5.779113	-0.443235	-2.007801
41	1	0	4.409345	-0.971230	-1.243786
42	6	0	2.896692	-3.043422	2.192090
43	6	0	2.384572	3.373206	-0.903907
44	1	0	3.828898	2.463176	0.406985
45	6	0	0.999982	1.864076	-2.173195
46	1	0	1.414547	-0.232159	-1.925378
47	1	0	2.620881	-3.813098	1.467706
48	1	0	2.015526	-2.747020	2.765481
49	1	0	3.680833	-3.407317	2.855578
50	6	0	1.357999	3.169960	-1.830298
51	1	0	2.686350	4.383452	-0.640130
52	1	0	0.226543	1.687562	-2.916161
53	1	0	0.862857	4.016557	-2.296849

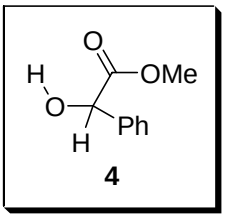


TS-3-F
(TS-7-F)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.586059	-1.483976	0.665572
2	6	0	1.262507	-1.051048	0.696372
3	6	0	0.863117	0.097624	-0.016059
4	6	0	1.844347	0.802648	-0.736459
5	6	0	3.170235	0.367004	-0.754479
6	6	0	3.552176	-0.779040	-0.057252
7	6	0	-0.536746	0.574169	0.057707

8	6	0	-1.699596	-0.240652	-0.262298
9	8	0	-1.695084	-1.488179	0.232737
10	6	0	-2.873109	-2.266198	-0.035352
11	8	0	-0.755454	1.842988	-0.723559
12	1	0	-1.642657	1.641609	-1.154418
13	8	0	-2.654429	0.225803	-0.902946
14	8	0	-1.059931	2.567758	1.503320
15	1	0	-0.250032	2.946800	1.885972
16	1	0	-3.023196	-2.380470	-1.111924
17	1	0	-3.755646	-1.790283	0.400100
18	1	0	-2.690694	-3.235025	0.430521
19	1	0	1.562053	1.689179	-1.294005
20	1	0	3.906260	0.928916	-1.324594
21	1	0	4.584802	-1.116644	-0.072571
22	1	0	2.865119	-2.377464	1.218907
23	1	0	0.527504	-1.605095	1.269563
24	1	0	-0.943627	2.517425	0.209072
25	1	0	-0.834638	1.470912	1.320455

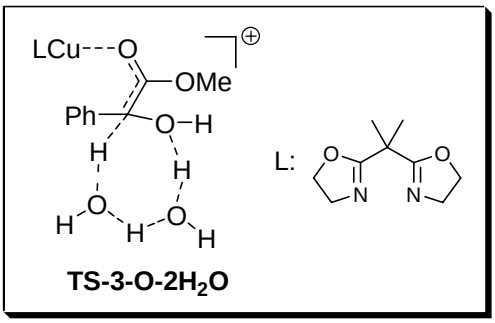


4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.194815	-0.926430	0.861001
2	6	0	-0.738104	0.307376	0.382093
3	6	0	-1.536610	1.037110	-0.502933
4	6	0	-2.774835	0.536371	-0.909689
5	6	0	-3.224890	-0.696778	-0.435065
6	6	0	-2.431515	-1.426701	0.453613
7	6	0	0.625826	0.852493	0.810935
8	6	0	1.743394	0.206610	-0.019829
9	8	0	1.901335	-1.095631	0.232429
10	6	0	2.908729	-1.767353	-0.548853
11	8	0	0.722800	2.248750	0.665375
12	1	0	1.380836	2.396369	-0.041305
13	8	0	2.405358	0.841366	-0.818780

14	1	0	0.799186	0.581381	1.862347
15	1	0	-1.189610	2.005396	-0.847408
16	1	0	-3.390033	1.113819	-1.594908
17	1	0	-4.190478	-1.084336	-0.749006
18	1	0	-2.778572	-2.383401	0.835317
19	1	0	-0.580699	-1.497273	1.552795
20	1	0	2.904000	-2.800329	-0.201679
21	1	0	3.886241	-1.307492	-0.384235
22	1	0	2.660110	-1.716209	-1.611746

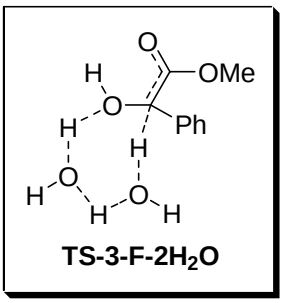


TS-3-O-2H$_2$O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.683837	3.335200	1.621972
2	6	0	-2.599050	3.403511	0.567742
3	6	0	-3.045486	2.244072	-0.066564
4	6	0	-2.584063	0.973904	0.337517
5	6	0	-1.675123	0.916459	1.419925
6	6	0	-1.228628	2.082927	2.042817
7	6	0	-3.078188	-0.250664	-0.305340
8	6	0	-2.284055	-1.362102	-0.642054
9	8	0	-2.885607	-2.171992	-1.574789
10	6	0	-2.173642	-3.357782	-1.963290
11	8	0	-4.209746	-0.034159	-1.191874
12	8	0	-1.161811	-1.691677	-0.166865
13	29	0	0.522667	-0.680981	-0.159646
14	7	0	1.472600	0.981407	-0.799977
15	6	0	2.719767	1.253219	-0.657267
16	8	0	3.127847	2.469606	-1.069907
17	6	0	1.955514	3.190258	-1.545331
18	6	0	0.817570	2.153680	-1.419777
19	6	0	3.860765	0.411865	-0.110184
20	6	0	4.562516	1.216065	1.023689

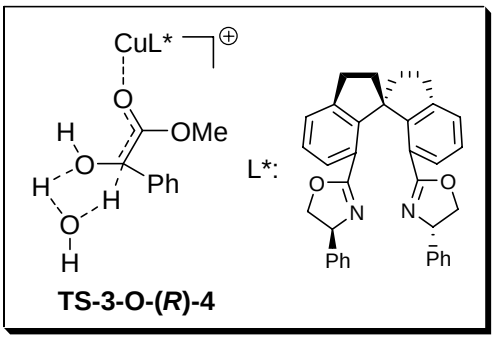
21	7	0	2.299738	-1.479400	0.576060
22	6	0	3.456820	-0.937404	0.459449
23	8	0	4.513300	-1.643432	0.913106
24	6	0	4.007180	-2.904121	1.434460
25	6	0	2.480246	-2.797958	1.217134
26	6	0	4.865944	0.165915	-1.274938
27	8	0	-4.644782	-1.127759	1.888928
28	1	0	4.481058	-3.709714	0.869471
29	1	0	4.303843	-2.971351	2.483231
30	1	0	1.913201	-2.828677	2.152510
31	1	0	2.087527	-3.580456	0.561139
32	1	0	-0.003627	2.493390	-0.784142
33	1	0	0.401286	1.860323	-2.388751
34	1	0	1.825494	4.065469	-0.904546
35	1	0	2.158467	3.513279	-2.568093
36	1	0	5.414219	0.648352	1.403052
37	1	0	4.916454	2.172091	0.633923
38	1	0	3.873635	1.409848	1.852824
39	1	0	5.207129	1.123268	-1.674362
40	1	0	5.728083	-0.392718	-0.905368
41	1	0	4.398386	-0.405404	-2.083937
42	1	0	-4.095255	-0.658792	-1.934486
43	1	0	-5.491672	-0.196153	-0.487215
44	1	0	-4.490697	-0.515056	2.630035
45	1	0	-3.883738	-0.964542	1.222193
46	1	0	-3.753261	2.314895	-0.885051
47	1	0	-1.339831	-0.048341	1.788026
48	1	0	-2.022463	-4.013929	-1.102581
49	1	0	-1.204691	-3.104157	-2.400850
50	1	0	-2.807035	-3.845236	-2.705025
51	1	0	-2.973337	4.368250	0.235053
52	1	0	-0.534653	2.007983	2.876347
53	1	0	-1.347496	4.239974	2.119730
54	8	0	-6.247033	-0.351641	0.239697
55	1	0	-6.869514	-1.035180	-0.067052
56	1	0	-5.638063	-0.726852	1.114951



TS-3-F-2H_2O

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.660243	-0.760079	0.007126
2	6	0	2.726558	-1.402511	0.825223
3	6	0	1.373757	-1.078533	0.754172
4	6	0	0.907490	-0.109227	-0.158893
5	6	0	1.858207	0.532535	-0.975026
6	6	0	3.213551	0.209162	-0.891150
7	6	0	-0.523875	0.276431	-0.184268
8	8	0	-0.790407	1.363860	-1.161663
9	6	0	-1.604255	-0.675341	-0.391958
10	8	0	-2.581408	-0.397698	-1.103340
11	8	0	-1.507036	-1.832724	0.289223
12	6	0	-2.608805	-2.738119	0.127374
13	8	0	-0.935098	1.704875	2.036903
14	1	0	-1.657952	1.061058	-1.556431
15	1	0	-0.105479	1.677657	2.542393
16	1	0	-2.724650	-3.024103	-0.921389
17	1	0	-3.538695	-2.281024	0.476389
18	1	0	-2.359195	-3.608845	0.734940
19	1	0	1.525937	1.276476	-1.691286
20	1	0	3.922514	0.717569	-1.540739
21	1	0	4.715619	-1.010363	0.071404
22	1	0	3.054396	-2.160531	1.532798
23	1	0	0.664726	-1.584570	1.400604
24	1	0	-0.929155	2.429412	-0.541880
25	1	0	-0.801161	0.960890	1.220581
26	8	0	-1.012303	3.336042	0.223397
27	1	0	-0.969529	2.753828	1.167953
28	1	0	-0.204588	3.871796	0.152902



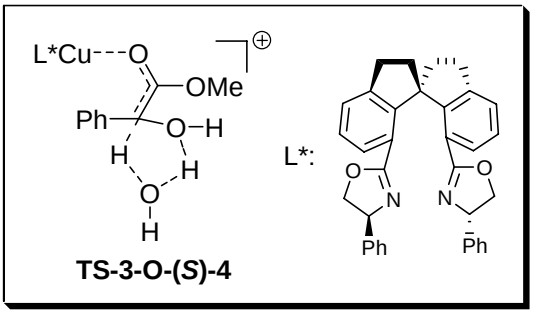
TS-3-O-(*R*)-4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.033419	0.648364	-1.120307
2	6	0	5.632024	0.708949	0.371116
3	6	0	4.570387	-0.428584	0.569462
4	6	0	3.999915	-0.593334	-0.837984
5	6	0	4.816600	0.042682	-1.784395
6	6	0	5.244437	-1.738464	1.110203
7	6	0	5.056041	-1.700069	2.642888
8	6	0	3.804550	-0.868246	2.815053
9	6	0	3.545480	-0.115943	1.659547
10	6	0	2.826667	-1.245356	-1.259972
11	6	0	2.478067	-1.212107	-2.621659
12	6	0	3.298086	-0.573449	-3.552183
13	6	0	4.477910	0.050383	-3.137459
14	6	0	2.969984	-0.787434	3.929567
15	6	0	1.847196	0.043548	3.885640
16	6	0	1.581153	0.801801	2.745577
17	6	0	2.435210	0.748603	1.629433
18	6	0	1.920777	-1.981790	-0.345572
19	6	0	2.108000	1.648637	0.497734
20	8	0	3.027003	2.578812	0.168876
21	6	0	2.500610	3.302747	-0.978644
22	6	0	1.010549	2.881703	-1.033790
23	7	0	0.986365	1.688123	-0.140076
24	7	0	0.672995	-1.717440	-0.148793
25	6	0	0.104429	-2.765178	0.747532
26	6	0	1.363338	-3.583459	1.141458
27	8	0	2.418587	-3.059066	0.286432
28	29	0	-0.179348	0.035695	-0.536903
29	1	0	6.297742	1.631479	-1.524692
30	1	0	6.906395	-0.000388	-1.276392

31	1	0	6.482498	0.580571	1.047124
32	1	0	5.179614	1.678254	0.587504
33	1	0	4.730342	-2.611536	0.703734
34	1	0	6.294508	-1.800053	0.809561
35	1	0	4.971739	-2.700098	3.081794
36	1	0	5.903445	-1.208137	3.140335
37	1	0	1.568822	-1.708917	-2.947159
38	1	0	3.019545	-0.570965	-4.601901
39	1	0	5.122565	0.539117	-3.863556
40	1	0	3.186286	-1.368602	4.822444
41	1	0	1.183472	0.110220	4.742709
42	1	0	0.718565	1.460657	2.717869
43	1	0	2.660080	4.366851	-0.803079
44	1	0	3.063338	2.978311	-1.858435
45	1	0	0.736851	2.565807	-2.043572
46	1	0	-0.310721	-2.262808	1.626012
47	1	0	1.668586	-3.419213	2.177611
48	1	0	1.276632	-4.652474	0.944101
49	6	0	0.018228	3.930924	-0.563099
50	6	0	-1.112327	4.225458	-1.334490
51	6	0	0.211933	4.615154	0.646731
52	6	0	-2.029059	5.193625	-0.913027
53	1	0	-1.273417	3.700012	-2.272632
54	6	0	-0.702066	5.579444	1.069941
55	1	0	1.085101	4.402492	1.259680
56	6	0	-1.824641	5.872182	0.289763
57	1	0	-2.896389	5.416703	-1.527336
58	1	0	-0.535592	6.107301	2.004647
59	1	0	-2.529814	6.631869	0.615001
60	6	0	-1.002314	-3.540646	0.058957
61	6	0	-2.330101	-3.375066	0.468036
62	6	0	-0.721346	-4.409320	-1.006444
63	6	0	-3.363251	-4.065581	-0.170526
64	1	0	-2.562913	-2.704718	1.292411
65	6	0	-1.750158	-5.104401	-1.641502
66	1	0	0.304536	-4.549844	-1.340785
67	6	0	-3.074005	-4.933364	-1.224211
68	1	0	-4.387963	-3.919274	0.157483
69	1	0	-1.519486	-5.782430	-2.458449
70	1	0	-3.873721	-5.479384	-1.716599
71	8	0	-1.918577	0.766090	-1.320633
72	6	0	-3.078247	0.269625	-1.150009
73	6	0	-3.986013	0.834195	-0.213425
74	8	0	-3.528146	-0.751365	-1.884311

75	6	0	-4.995822	0.109167	0.588809
76	8	0	-3.287100	1.891472	0.549726
77	6	0	-2.660307	-1.272511	-2.906217
78	6	0	-5.874843	-0.815367	-0.011691
79	6	0	-5.138747	0.364537	1.965867
80	1	0	-2.383156	1.921154	0.149617
81	1	0	-3.979749	2.877504	0.067893
82	1	0	-1.771150	-1.726054	-2.461409
83	1	0	-2.369996	-0.481869	-3.602830
84	1	0	-3.249802	-2.033918	-3.415588
85	1	0	-5.800146	-1.013797	-1.074650
86	6	0	-6.838616	-1.475069	0.748476
87	6	0	-6.113500	-0.295561	2.716656
88	1	0	-4.478303	1.075777	2.450303
89	8	0	-4.802116	3.194397	-0.704452
90	6	0	-6.967374	-1.220704	2.116793
91	1	0	-7.504924	-2.182784	0.262012
92	1	0	-6.200226	-0.082872	3.779016
93	1	0	-5.635469	3.393795	-0.237764
94	1	0	-4.815854	2.135402	-0.938910
95	1	0	-7.727021	-1.730145	2.702245

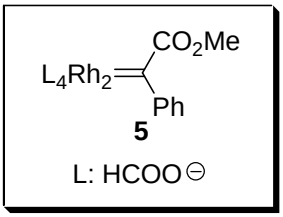


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.698860	1.586869	3.565729
2	6	0	3.870302	2.090864	2.993990
3	6	0	4.359102	1.569051	1.795927
4	6	0	3.691106	0.516575	1.142708
5	6	0	2.531620	-0.011607	1.747144
6	6	0	2.035237	0.532296	2.935233
7	6	0	4.194820	-0.049856	-0.124042
8	6	0	3.426531	-0.078663	-1.327589

9	8	0	2.192838	-0.189042	-1.444641
10	29	0	0.537693	0.145535	-0.278038
11	7	0	-0.721701	1.694182	-0.139393
12	6	0	-1.958106	1.657431	-0.504643
13	8	0	-2.767037	2.611135	-0.000318
14	6	0	-1.983485	3.348514	0.980204
15	6	0	-0.523775	2.908041	0.703943
16	6	0	-2.538873	0.726490	-1.501350
17	6	0	-3.623204	-0.131581	-1.243077
18	6	0	-4.132114	-0.934350	-2.274891
19	6	0	-3.572820	-0.904740	-3.552087
20	6	0	-2.477430	-0.073000	-3.800964
21	6	0	-1.962824	0.731667	-2.784545
22	6	0	-5.306688	-1.753111	-1.787332
23	6	0	-5.157060	-1.707736	-0.250050
24	6	0	-4.378373	-0.380979	0.060254
25	6	0	-3.515172	-0.483377	1.316912
26	6	0	-4.121195	0.189022	2.389074
27	6	0	-5.454286	0.770327	1.972519
28	6	0	-5.370541	0.775965	0.429764
29	6	0	-2.272835	-1.116180	1.506451
30	6	0	-1.654433	-1.037837	2.766577
31	6	0	-2.268114	-0.368286	3.824953
32	6	0	-3.510324	0.245320	3.641207
33	6	0	-1.573607	-1.905250	0.463202
34	8	0	-2.222672	-2.988968	-0.012260
35	6	0	-1.372675	-3.574969	-1.035627
36	6	0	-0.015381	-2.844596	-0.860092
37	7	0	-0.374625	-1.705168	0.031142
38	6	0	1.099056	-3.683585	-0.258847
39	6	0	2.325557	-3.803335	-0.922106
40	6	0	3.355822	-4.579378	-0.383346
41	6	0	3.167934	-5.241709	0.831220
42	6	0	1.947346	-5.126122	1.502715
43	6	0	0.921199	-4.352059	0.961456
44	6	0	0.338304	3.932883	-0.011902
45	6	0	1.608062	4.249203	0.482581
46	6	0	2.409479	5.188540	-0.171579
47	6	0	1.948110	5.818921	-1.327567
48	6	0	0.680759	5.507327	-1.828871
49	6	0	-0.118074	4.569950	-1.175539
50	8	0	5.616977	0.297098	-0.375645
51	8	0	4.216136	-0.029547	-2.444810
52	6	0	3.549534	-0.068120	-3.719023

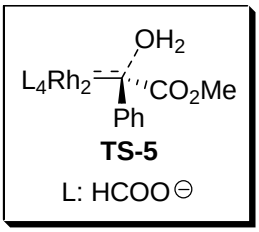
53	8	0	5.835959	-2.016205	0.015676
54	1	0	-5.308592	-2.776118	-2.179055
55	1	0	-6.247942	-1.289863	-2.114234
56	1	0	-6.117375	-1.736207	0.273332
57	1	0	-4.570815	-2.565586	0.084302
58	1	0	-4.964833	1.731137	0.091492
59	1	0	-6.342938	0.636538	-0.051995
60	1	0	-5.635961	1.767707	2.387489
61	1	0	-6.271184	0.127554	2.329066
62	1	0	-1.119690	1.387310	-2.980348
63	1	0	-2.028805	-0.043061	-4.789695
64	1	0	-3.981650	-1.524210	-4.346420
65	1	0	-3.994034	0.760740	4.467107
66	1	0	-1.781103	-0.333530	4.795229
67	1	0	-1.327885	-4.649805	-0.856416
68	1	0	-1.837876	-3.374614	-2.004789
69	1	0	0.329067	-2.438649	-1.814296
70	1	0	-0.026107	2.607529	1.629183
71	1	0	-2.335171	3.050240	1.972039
72	1	0	-2.165593	4.411356	0.820318
73	1	0	2.471902	-3.291298	-1.870077
74	1	0	-0.026380	-4.275497	1.490073
75	1	0	4.298104	-4.671207	-0.916601
76	1	0	1.792926	-5.644585	2.444803
77	1	0	3.962261	-5.854487	1.248384
78	1	0	1.973101	3.760023	1.382213
79	1	0	-1.104507	4.339377	-1.572199
80	1	0	3.390988	5.430091	0.226990
81	1	0	0.313486	5.998721	-2.725525
82	1	0	2.567970	6.553651	-1.833644
83	1	0	5.683691	0.560046	-1.318609
84	1	0	6.081966	-0.891364	-0.205255
85	1	0	6.118852	-2.256684	0.917600
86	1	0	4.820255	-1.673103	0.075029
87	1	0	5.265833	1.975665	1.361361
88	1	0	2.057141	-0.893011	1.323227
89	1	0	4.409418	2.898529	3.482169
90	1	0	1.140174	0.107421	3.380946
91	1	0	2.999665	-1.005450	-3.832951
92	1	0	2.860399	0.773797	-3.817030
93	1	0	4.343673	-0.001417	-4.462610
94	1	0	2.324448	1.993220	4.500851
95	1	0	-0.697414	-1.529261	2.913209



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.853288	0.417667	0.180387
2	6	0	2.216274	1.840993	0.392412
3	8	0	2.287728	2.561908	-0.733782
4	6	0	2.479592	3.979216	-0.552482
5	45	0	-0.139997	0.057142	0.077373
6	45	0	-2.583022	-0.356814	-0.107519
7	8	0	-2.646085	1.114876	-1.567599
8	6	0	-1.570381	1.698451	-1.861381
9	8	0	-0.405359	1.512250	-1.387129
10	8	0	-0.603656	1.470193	1.524465
11	6	0	-1.825288	1.657885	1.822700
12	8	0	-2.847882	1.090175	1.356067
13	8	0	0.099766	-1.395573	-1.400074
14	6	0	-0.938914	-1.961620	-1.871677
15	8	0	-2.143934	-1.774063	-1.567518
16	8	0	-0.115374	-1.439797	1.528639
17	6	0	-1.213799	-2.005960	1.839312
18	8	0	-2.363164	-1.802026	1.373116
19	8	0	2.395979	2.268246	1.516023
20	1	0	-1.997898	2.421427	2.595491
21	1	0	-0.740974	-2.714960	-2.649031
22	1	0	-1.129970	-2.775416	2.621365
23	1	0	-1.633563	2.479426	-2.633898
24	6	0	2.923417	-0.525636	0.087679
25	1	0	3.429629	4.178922	-0.049849
26	1	0	1.662166	4.396037	0.040564
27	1	0	2.480000	4.399633	-1.557646
28	6	0	4.273377	-0.091235	-0.058246
29	6	0	5.304293	-1.006060	-0.195330
30	6	0	5.021915	-2.378909	-0.171702
31	6	0	3.708865	-2.833633	-0.012105
32	6	0	2.666876	-1.924223	0.111116

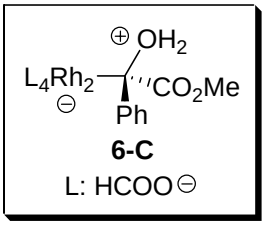
33	1	0	4.492590	0.971238	-0.075337
34	1	0	6.326943	-0.662020	-0.317206
35	1	0	5.832269	-3.095735	-0.275717
36	1	0	3.503291	-3.899541	0.013301
37	1	0	1.650121	-2.264921	0.242743



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.611413	-1.929430	-0.358055
2	6	0	2.871685	-0.562764	-0.067552
3	6	0	4.229917	-0.144097	0.041159
4	6	0	5.267295	-1.045096	-0.126037
5	6	0	4.981995	-2.384724	-0.426032
6	6	0	3.658903	-2.821203	-0.545895
7	6	0	1.801266	0.368997	0.086526
8	45	0	-0.218694	0.028336	0.036115
9	8	0	-0.126832	-1.857084	0.915630
10	6	0	-1.208107	-2.510597	1.076880
11	8	0	-2.379864	-2.183504	0.758565
12	45	0	-2.671048	-0.332070	-0.140032
13	8	0	-2.800549	1.548896	-1.010490
14	6	0	-1.743337	2.217318	-1.143018
15	8	0	-0.552139	1.896544	-0.831306
16	6	0	2.161262	1.818732	0.112011
17	8	0	2.322027	2.275246	-1.137298
18	6	0	2.440619	3.705629	-1.271878
19	8	0	2.264838	2.502415	1.114566
20	8	0	-0.066366	-0.855157	-1.837775
21	6	0	-1.133057	-1.239996	-2.417888
22	8	0	-2.319906	-1.173312	-2.008528
23	8	0	-0.623670	0.845335	1.916660
24	6	0	-1.827652	0.898359	2.334102
25	8	0	-2.870643	0.528111	1.740908
26	8	0	1.992992	0.373992	3.007952

27	1	0	1.107021	0.533547	2.638443
28	1	0	1.586373	-2.259779	-0.439606
29	1	0	3.449261	-3.860698	-0.779431
30	1	0	5.797567	-3.089374	-0.565902
31	1	0	6.297398	-0.716173	-0.028032
32	1	0	4.450638	0.890440	0.283703
33	1	0	-0.979607	-1.691058	-3.409448
34	1	0	3.310958	4.073325	-0.723062
35	1	0	1.536630	4.187167	-0.892572
36	1	0	2.553606	3.884436	-2.340673
37	1	0	-1.951039	1.326719	3.338743
38	1	0	-1.850811	3.216996	-1.589934
39	1	0	-1.086273	-3.491273	1.559980
40	1	0	2.424359	1.225127	2.827045



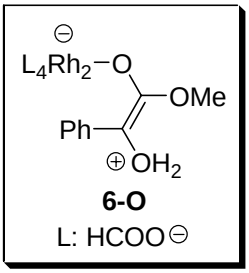
6-C

L: $HCOO^{\ominus}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.123013	-0.669800	-1.133413
2	6	0	2.861119	-0.494675	0.238160
3	6	0	3.512465	-1.329428	1.160070
4	6	0	4.410415	-2.303840	0.723030
5	6	0	4.675614	-2.463973	-0.636770
6	6	0	4.025461	-1.641223	-1.559701
7	6	0	1.879389	0.543017	0.670456
8	8	0	1.847894	0.635597	2.198225
9	1	0	0.904502	0.407966	2.480265
10	6	0	2.141027	1.970645	0.340603
11	8	0	2.116430	2.821084	1.247026
12	45	0	-0.215751	0.092533	0.123424
13	8	0	0.119158	-1.946776	0.336162
14	6	0	-0.865023	-2.739143	0.206277
15	8	0	-2.074469	-2.465980	-0.027484
16	45	0	-2.595851	-0.466693	-0.248097
17	8	0	-2.145083	-0.580695	-2.266388

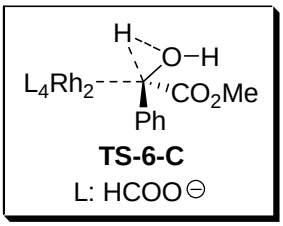
18	6	0	-0.959545	-0.353977	-2.631157
19	8	0	0.050769	-0.052381	-1.921523
20	8	0	2.359487	2.254907	-0.927890
21	6	0	2.479464	3.655421	-1.255158
22	8	0	-0.741913	2.101325	-0.107211
23	6	0	-1.964244	2.369838	-0.333866
24	8	0	-2.938340	1.578876	-0.443531
25	8	0	-0.665181	0.191566	2.171588
26	6	0	-1.867806	-0.043464	2.559440
27	8	0	-2.849893	-0.313929	1.839815
28	1	0	-2.029187	0.008531	3.645209
29	1	0	-0.764316	-0.423884	-3.711426
30	1	0	-0.621570	-3.806410	0.315729
31	1	0	-2.194079	3.440308	-0.446396
32	1	0	3.317506	4.101314	-0.714848
33	1	0	1.552970	4.172267	-0.997600
34	1	0	2.653067	3.681430	-2.330119
35	1	0	3.320065	-1.218081	2.220990
36	1	0	4.904005	-2.938776	1.454288
37	1	0	5.375199	-3.223550	-0.974800
38	1	0	4.213503	-1.760730	-2.623609
39	1	0	2.598657	-0.061877	-1.859841
40	1	0	1.952761	1.673509	2.274319



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.317625	-2.735131	-0.219496
2	6	0	5.918745	-1.714378	0.515011
3	6	0	5.290801	-0.476469	0.653870
4	6	0	4.041904	-0.229445	0.044043
5	6	0	3.434712	-1.273171	-0.693943
6	6	0	4.071158	-2.503075	-0.812496
7	6	0	3.402413	1.054726	0.139478

8	8	0	4.245262	2.137045	0.786601
9	1	0	5.064183	2.272546	0.259500
10	6	0	2.238428	1.617671	-0.343614
11	8	0	1.328191	1.095712	-1.018965
12	45	0	-0.632216	0.254762	-0.280318
13	8	0	-0.134465	-1.589722	-1.090929
14	6	0	-0.977217	-2.529240	-0.984597
15	8	0	-2.117380	-2.503864	-0.438606
16	45	0	-2.745090	-0.725670	0.413656
17	8	0	-1.828235	-1.254770	2.198260
18	6	0	-0.612974	-0.941566	2.354750
19	8	0	0.152791	-0.328251	1.552519
20	8	0	-1.553501	0.784253	-2.064693
21	6	0	-2.771237	0.470718	-2.216651
22	8	0	-3.535561	-0.135107	-1.410624
23	8	0	-1.278089	2.043970	0.578842
24	6	0	-2.421613	2.058403	1.129198
25	8	0	-3.252022	1.114678	1.233885
26	8	0	2.185958	2.995353	0.004597
27	6	0	1.219002	3.814934	-0.683906
28	1	0	-0.676609	-3.490941	-1.425470
29	1	0	-2.724635	3.019222	1.571415
30	1	0	-3.222182	0.765213	-3.175814
31	1	0	-0.158898	-1.238015	3.311698
32	1	0	0.213530	3.501220	-0.404586
33	1	0	1.355574	3.734394	-1.765733
34	1	0	1.413566	4.834827	-0.348393
35	1	0	3.599605	2.931160	0.630465
36	1	0	5.761335	0.283667	1.272643
37	1	0	2.468144	-1.109676	-1.155810
38	1	0	6.879409	-1.879038	0.996377
39	1	0	3.585645	-3.292119	-1.380904
40	1	0	5.806022	-3.699823	-0.322604



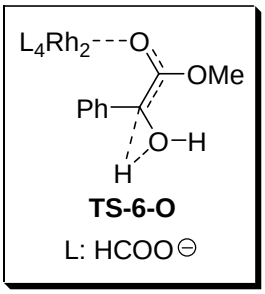
TS-6-C

L: $HCOO^{\ominus}$

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	2.058793	0.480950	0.735330
2	6	0	2.160986	1.935269	0.403946
3	8	0	2.392798	2.177651	-0.883423
4	6	0	2.328997	3.561734	-1.278682
5	45	0	-0.290032	0.030408	0.215214
6	45	0	-2.632271	-0.373635	-0.361498
7	8	0	-2.634685	1.427682	-1.374678
8	6	0	-1.568619	2.100960	-1.380924
9	8	0	-0.454118	1.819054	-0.843096
10	8	0	-0.964493	1.003637	1.924636
11	6	0	-2.219593	1.070002	2.116386
12	8	0	-3.145901	0.615957	1.392572
13	8	0	0.218911	-0.960474	-1.533160
14	6	0	-0.719538	-1.402194	-2.263556
15	8	0	-1.966670	-1.328212	-2.073551
16	8	0	-0.343056	-1.782984	1.241888
17	6	0	-1.426018	-2.449124	1.240675
18	8	0	-2.519476	-2.158093	0.687777
19	8	0	2.017840	2.801151	1.258768
20	1	0	-2.527130	1.592998	3.032979
21	1	0	-0.399479	-1.916305	-3.181206
22	1	0	-1.394658	-3.398145	1.794536
23	1	0	-1.603556	3.057349	-1.922740
24	6	0	3.043239	-0.509831	0.230544
25	1	0	3.084525	4.145429	-0.747255
26	1	0	1.335756	3.958878	-1.062827
27	1	0	2.523056	3.561364	-2.350831
28	6	0	4.271230	-0.104034	-0.319872
29	6	0	5.213597	-1.047516	-0.725478
30	6	0	4.951885	-2.410302	-0.575657
31	6	0	3.738701	-2.824192	-0.021806
32	6	0	2.789520	-1.884329	0.374056
33	1	0	4.491420	0.950530	-0.440830
34	1	0	6.156030	-0.715286	-1.152200
35	1	0	5.688892	-3.144977	-0.888799
36	1	0	3.526745	-3.883206	0.097522
37	1	0	1.844919	-2.210681	0.793937
38	8	0	2.133579	0.476349	2.354176
39	1	0	1.172707	0.164442	1.653312
40	1	0	1.987516	1.444717	2.532120



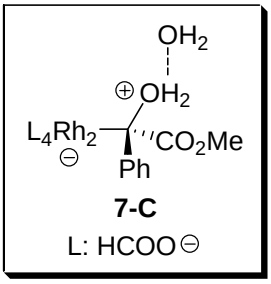
TS-6-O

L: $HCOO^{\ominus}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.511382	-2.558354	-0.502831
2	6	0	5.529164	-2.092891	0.815713
3	6	0	4.793965	-0.964297	1.162608
4	6	0	4.053967	-0.258920	0.192040
5	6	0	4.055302	-0.734730	-1.135478
6	6	0	4.765530	-1.883553	-1.472952
7	6	0	3.305405	0.922902	0.585155
8	6	0	2.325219	1.593740	-0.220451
9	8	0	1.436791	0.982708	-0.828943
10	45	0	-0.649112	0.202466	-0.249481
11	8	0	-1.167235	1.969850	0.733758
12	6	0	-2.314070	2.027457	1.273938
13	8	0	-3.210484	1.138837	1.301383
14	45	0	-2.825669	-0.667742	0.356855
15	8	0	-1.975462	-1.401002	2.097149
16	6	0	-0.741800	-1.190436	2.283453
17	8	0	0.072055	-0.574625	1.533331
18	8	0	-0.276180	-1.602994	-1.188746
19	6	0	-1.182253	-2.486575	-1.158297
20	8	0	-2.324534	-2.421391	-0.616772
21	8	0	-1.510904	0.936297	-1.991216
22	6	0	-2.745881	0.721419	-2.173425
23	8	0	-3.556293	0.109252	-1.418779
24	8	0	2.388522	2.946570	-0.203617
25	6	0	1.314182	3.650362	-0.870268
26	8	0	4.520044	2.212952	1.118840
27	1	0	4.062955	3.011595	0.776767
28	1	0	-3.167047	1.119730	-3.107916
29	1	0	-0.320480	-1.592634	3.216028
30	1	0	-2.555848	2.972331	1.782186
31	1	0	-0.944844	-3.431234	-1.668086

32	1	0	0.372024	3.461716	-0.353310
33	1	0	1.238771	3.323371	-1.909354
34	1	0	1.590889	4.703339	-0.815093
35	1	0	4.782872	-0.613882	2.190702
36	1	0	3.471450	-0.217375	-1.889050
37	1	0	6.101903	-2.620822	1.572930
38	1	0	4.745742	-2.247868	-2.496248
39	1	0	6.072337	-3.449513	-0.771487
40	1	0	3.723200	1.670258	1.673761



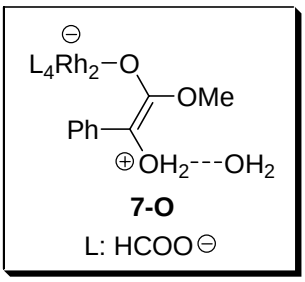
7-C

L: $HCOO^{\ominus}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.143980	-2.540160	-0.990858
2	6	0	-3.360664	-1.401551	-1.180743
3	6	0	-2.726094	-0.769834	-0.095735
4	6	0	-2.883914	-1.337567	1.183928
5	6	0	-3.669360	-2.473505	1.364902
6	6	0	-4.309714	-3.081740	0.282978
7	6	0	-1.880116	0.449666	-0.296334
8	45	0	0.310909	0.049152	-0.037448
9	8	0	0.587385	0.988237	-1.892060
10	6	0	1.766870	1.034868	-2.398681
11	8	0	2.820362	0.598766	-1.892331
12	45	0	2.751834	-0.355182	-0.011716
13	8	0	2.956304	1.492616	0.925999
14	6	0	1.914242	2.153530	1.181255
15	8	0	0.703225	1.858247	0.935195
16	8	0	-1.940834	0.841899	-1.744289
17	6	0	-2.135750	1.671805	0.513823
18	8	0	-2.204903	1.418958	1.823684
19	6	0	-2.275757	2.565965	2.686915
20	8	0	-2.224422	2.819708	0.069875
21	8	0	0.123703	-1.776250	-1.015885

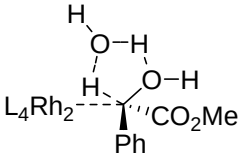
22	6	0	1.174846	-2.455323	-1.229856
23	8	0	2.371669	-2.170031	-0.950156
24	8	0	0.222575	-0.906225	1.794330
25	6	0	1.309221	-1.333189	2.294433
26	8	0	2.479558	-1.262579	1.827862
27	1	0	-2.587180	1.620298	-2.000163
28	1	0	1.835877	1.519706	-3.382481
29	1	0	1.208430	-1.831399	3.270069
30	1	0	1.011807	-3.421779	-1.729930
31	1	0	2.066558	3.120495	1.684727
32	1	0	-3.160570	3.166709	2.461838
33	1	0	-1.377276	3.174382	2.566437
34	1	0	-2.334590	2.159233	3.696428
35	1	0	-2.369582	-0.901244	2.028545
36	1	0	-3.772690	-2.891071	2.363289
37	1	0	-4.919667	-3.968870	0.430276
38	1	0	-4.622554	-3.004712	-1.849439
39	1	0	-3.233254	-1.011414	-2.183386
40	1	0	-1.004274	1.041594	-2.059874
41	8	0	-3.375930	2.864080	-2.300217
42	1	0	-4.332343	2.728609	-2.199199
43	1	0	-3.060631	3.233617	-1.436989



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.976390	-1.474098	-0.682860
2	6	0	3.453461	-2.769663	-0.841235
3	6	0	4.612529	-3.208483	-0.188350
4	6	0	5.282984	-2.324487	0.654255
5	6	0	4.817893	-1.017693	0.831935
6	6	0	3.656890	-0.558711	0.158147
7	6	0	3.207913	0.800888	0.282294
8	8	0	4.163530	1.703152	0.999935

9	6	0	2.138776	1.510991	-0.238828
10	8	0	1.198077	1.092589	-0.952992
11	45	0	-0.805474	0.296631	-0.274509
12	8	0	-0.034287	-0.481296	1.489873
13	6	0	-0.819436	-1.124596	2.248150
14	8	0	-2.050458	-1.364555	2.084986
15	45	0	-2.958265	-0.638036	0.367028
16	8	0	-2.429166	-2.370596	-0.637401
17	6	0	-1.299970	-2.401456	-1.204477
18	8	0	-0.415034	-1.496083	-1.247226
19	8	0	2.234167	2.871481	0.094302
20	6	0	1.219806	3.747847	-0.429688
21	8	0	-1.354897	2.032197	0.749589
22	6	0	-2.493956	2.056021	1.307849
23	8	0	-3.371029	1.149384	1.336919
24	8	0	-1.721197	1.026086	-1.990701
25	6	0	-2.953386	0.781243	-2.151171
26	8	0	-3.735761	0.140368	-1.390823
27	8	0	6.148787	1.397678	-0.579957
28	1	0	5.013011	1.755563	0.404876
29	1	0	-1.051388	-3.335012	-1.730494
30	1	0	-2.746916	2.988774	1.833690
31	1	0	-3.401201	1.179710	-3.073666
32	1	0	-0.368917	-1.524975	3.168279
33	1	0	0.245388	3.489656	-0.013504
34	1	0	1.186523	3.677597	-1.519981
35	1	0	1.520643	4.750977	-0.122150
36	1	0	3.673940	2.576007	0.970235
37	1	0	5.312883	-0.376943	1.557904
38	1	0	2.074698	-1.159383	-1.193209
39	1	0	6.168356	-2.648771	1.195825
40	1	0	2.909259	-3.449885	-1.491683
41	1	0	4.974481	-4.223134	-0.325878
42	1	0	6.143265	0.423891	-0.454707
43	1	0	5.852988	1.529122	-1.497042



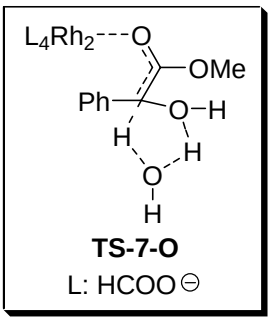
TS-7-C

L: $HCOO^{\ominus}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.014022	-1.356541	-1.933332
2	6	0	3.045402	-0.607641	-1.268645
3	6	0	3.231399	-0.235419	0.075772
4	6	0	4.404875	-0.653293	0.730645
5	6	0	5.366567	-1.413838	0.059038
6	6	0	5.177122	-1.769070	-1.275676
7	6	0	2.173242	0.541679	0.826319
8	6	0	1.975258	1.969554	0.395593
9	8	0	1.961421	2.172159	-0.921959
10	6	0	1.704510	3.521897	-1.342255
11	8	0	2.510682	0.622272	2.228421
12	1	0	2.242456	1.534135	2.487793
13	8	0	1.875745	2.863908	1.227076
14	8	0	1.541086	-1.639088	2.070015
15	8	0	-0.089104	-2.049930	-0.094529
16	6	0	-1.094371	-2.759023	-0.409747
17	8	0	-2.289199	-2.394329	-0.577166
18	45	0	-2.736644	-0.381133	-0.335428
19	8	0	-3.055332	-0.684894	1.691494
20	6	0	-2.077682	-0.544701	2.476330
21	8	0	-0.872686	-0.261761	2.193476
22	45	0	-0.372959	-0.001938	0.193669
23	8	0	-0.864392	2.009322	0.393418
24	6	0	-2.071589	2.361340	0.229313
25	8	0	-3.065641	1.642604	-0.069059
26	8	0	-0.085333	0.254764	-1.855788
27	6	0	-1.087530	0.172511	-2.628738
28	8	0	-2.293768	-0.054338	-2.331824
29	1	0	2.278435	-2.147060	1.673836
30	1	0	-2.290451	-0.683592	3.546245
31	1	0	-0.873899	0.320648	-3.697564
32	1	0	-0.888602	-3.829628	-0.555342
33	1	0	-2.273042	3.433857	0.365132
34	1	0	2.469189	4.197903	-0.951290
35	1	0	0.721012	3.839253	-0.989910
36	1	0	1.735833	3.494536	-2.431565
37	1	0	4.572218	-0.351144	1.759122
38	1	0	6.269536	-1.717488	0.583014
39	1	0	5.923970	-2.359959	-1.798937

40	1	0	3.853557	-1.628865	-2.973478
41	1	0	2.140323	-0.311035	-1.784811
42	1	0	1.964241	-0.948266	2.665546
43	1	0	1.332171	-0.815328	1.245100



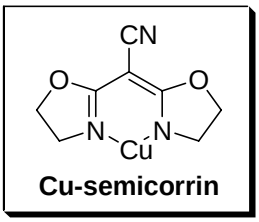
TS-7-O

L: $HCOO^{\ominus}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.682023	-2.568302	-1.064811
2	6	0	3.064769	-1.329381	-0.913153
3	6	0	3.700526	-0.299911	-0.185310
4	6	0	4.963918	-0.570517	0.382329
5	6	0	5.567798	-1.818706	0.225816
6	6	0	4.932287	-2.828855	-0.495671
7	6	0	3.065154	1.004867	0.036866
8	6	0	2.038993	1.610086	-0.717204
9	8	0	2.038215	2.980030	-0.588475
10	6	0	1.016447	3.700730	-1.302856
11	8	0	3.917744	1.949097	0.759412
12	1	0	3.663500	2.833607	0.425035
13	8	0	1.178775	1.029401	-1.422170
14	45	0	-0.677037	0.212343	-0.437402
15	8	0	-0.442513	-1.603911	-1.407932
16	6	0	-1.311257	-2.503960	-1.205050
17	8	0	-2.336808	-2.454318	-0.466043
18	45	0	-2.693912	-0.701112	0.574271
19	8	0	-2.936213	1.111160	1.558655
20	6	0	-2.080680	2.016468	1.355250
21	8	0	-1.049551	1.974917	0.615607
22	8	0	-1.861104	0.889477	-1.990796
23	6	0	-3.105011	0.654730	-1.936127
24	8	0	-3.751210	0.043142	-1.036862
25	8	0	0.386847	-0.510155	1.222014

26	6	0	-0.270022	-1.150573	2.103238
27	8	0	-1.503580	-1.399117	2.132535
28	8	0	2.562099	1.044100	2.539465
29	1	0	3.001967	0.258246	2.918522
30	1	0	0.036085	3.485506	-0.875972
31	1	0	1.028463	3.429468	-2.360759
32	1	0	1.269908	4.754436	-1.175245
33	1	0	5.489960	0.213883	0.916800
34	1	0	6.547356	-1.993856	0.664625
35	1	0	5.403304	-3.800350	-0.617514
36	1	0	3.174726	-3.340379	-1.638042
37	1	0	2.094750	-1.151274	-1.358964
38	1	0	3.321225	1.638816	2.054942
39	1	0	2.225512	0.723437	1.550324
40	1	0	-2.245820	2.964857	1.887591
41	1	0	-1.150028	-3.449564	-1.742469
42	1	0	0.317669	-1.536591	2.950300
43	1	0	-3.697190	1.033692	-2.781425

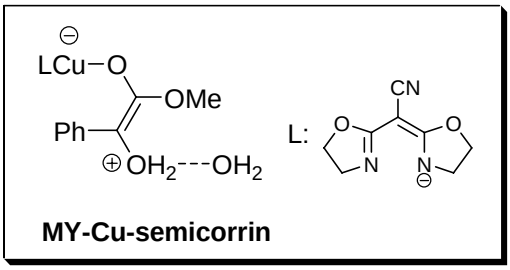


Cu-semicorrin

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.350263	1.301744	-0.078300
2	6	0	-1.276124	0.473786	-0.025777
3	7	0	-1.585740	-0.812932	0.010559
4	6	0	-3.041602	-0.942495	-0.110856
5	6	0	-3.533762	0.499449	0.112117
6	6	0	0.000028	1.116897	-0.017231
7	6	0	0.000044	2.542368	0.007277
8	7	0	0.000089	3.707508	0.029583
9	29	0	-0.000037	-1.889788	0.039448
10	7	0	1.585758	-0.813028	0.009515
11	6	0	3.041637	-0.942495	-0.111426
12	6	0	3.533708	0.499339	0.112566
13	8	0	2.350267	1.301759	-0.077607

14	6	0	1.276127	0.473726	-0.025860
15	1	0	4.286521	0.835071	-0.603059
16	1	0	3.899710	0.667913	1.131620
17	1	0	3.437534	-1.639744	0.633362
18	1	0	3.310071	-1.322603	-1.106528
19	1	0	-3.437761	-1.639354	0.634150
20	1	0	-3.309686	-1.323093	-1.105865
21	1	0	-3.899967	0.668684	1.130989
22	1	0	-4.286462	0.834654	-0.603873

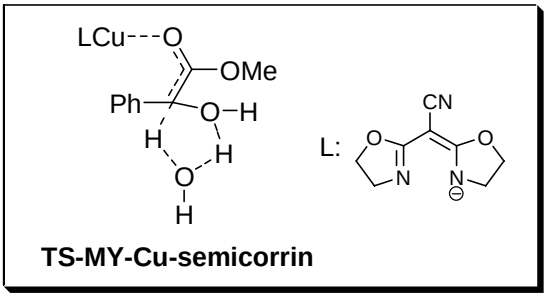


MY-Cu-semicorrin

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.494619	0.715772	1.631366
2	6	0	-3.273666	0.588217	0.453982
3	6	0	-4.323652	1.521441	0.255841
4	6	0	-4.582599	2.521929	1.197639
5	6	0	-3.812214	2.628838	2.353786
6	6	0	-2.763454	1.722250	2.551512
7	6	0	-3.022615	-0.473674	-0.481563
8	8	0	-4.068975	-0.631683	-1.537830
9	6	0	-2.051866	-1.457386	-0.567435
10	8	0	-2.315779	-2.339149	-1.630224
11	6	0	-1.264087	-3.251846	-1.977239
12	8	0	-1.046499	-1.634380	0.157921
13	29	0	0.764803	-0.754145	0.099207
14	7	0	1.300777	0.904497	-0.897423
15	6	0	2.551071	1.306200	-0.865518
16	8	0	2.813242	2.430161	-1.595651
17	6	0	1.549365	2.957404	-2.037169
18	6	0	0.563244	1.797920	-1.795476
19	6	0	3.665626	0.734344	-0.187289
20	7	0	2.543766	-1.206070	0.866381
21	6	0	2.962667	-2.223063	1.836615

22	6	0	4.497904	-2.101316	1.838372
23	8	0	4.738264	-0.817997	1.233688
24	6	0	3.580996	-0.436995	0.617420
25	8	0	-6.060692	-1.054357	-0.011825
26	1	0	4.982880	-2.869517	1.223252
27	1	0	4.950774	-2.099637	2.832547
28	1	0	2.531755	-2.008509	2.825347
29	1	0	2.622106	-3.219683	1.536221
30	1	0	-0.372372	2.132663	-1.335257
31	1	0	0.306587	1.275372	-2.729152
32	1	0	1.314898	3.842662	-1.433499
33	1	0	1.650802	3.254270	-3.083854
34	1	0	-3.703546	-1.382653	-2.084782
35	1	0	-4.887892	1.514323	-0.673783
36	1	0	-1.684783	0.017332	1.804634
37	1	0	-0.991257	-3.862857	-1.114585
38	1	0	-0.382114	-2.708155	-2.328871
39	1	0	-1.667727	-3.875604	-2.776055
40	1	0	-5.386245	3.229407	1.008586
41	1	0	-2.144982	1.796759	3.442308
42	1	0	-4.014202	3.407780	3.082701
43	1	0	-4.938442	-0.927745	-1.048346
44	1	0	-5.875668	-1.764241	0.626472
45	1	0	-5.907198	-0.221850	0.484809
46	6	0	4.929065	1.373914	-0.312608
47	7	0	5.966010	1.898092	-0.417205

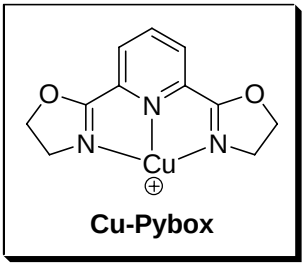


TS-MY-Cu-semicorrin

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.454698	2.120677	-0.214238
2	6	0	2.610778	1.057933	-0.322909
3	7	0	1.615292	1.227338	-1.164653

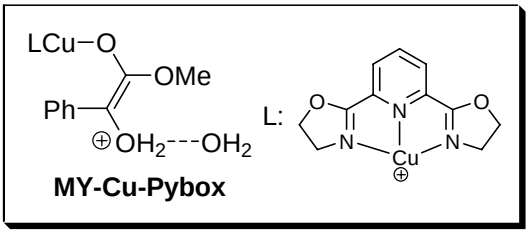
4	6	0	1.781631	2.536197	-1.807102
5	6	0	2.877315	3.210546	-0.959827
6	6	0	2.935258	-0.073282	0.483638
7	6	0	4.050075	0.025392	1.361292
8	7	0	4.954167	0.105274	2.093880
9	29	0	0.238719	-0.145134	-1.374477
10	7	0	1.094661	-1.592525	-0.172039
11	6	0	2.225165	-1.304678	0.438929
12	8	0	2.789745	-2.343505	1.124445
13	6	0	1.848719	-3.432476	1.091898
14	6	0	0.891520	-3.041662	-0.045807
15	8	0	-1.676413	-0.710882	-1.792955
16	6	0	-2.339410	-1.079883	-0.796768
17	8	0	-2.941204	-2.317436	-0.790428
18	6	0	-2.750962	-3.125621	-1.963239
19	6	0	-2.501996	-0.387976	0.427951
20	8	0	-3.282559	-1.128554	1.437157
21	6	0	-2.559184	1.069638	0.617539
22	6	0	-2.218089	1.976768	-0.407876
23	6	0	-2.248329	3.351700	-0.180258
24	6	0	-2.617685	3.866663	1.064062
25	6	0	-2.970560	2.979835	2.082123
26	6	0	-2.940774	1.602887	1.866152
27	8	0	-1.075667	-1.539928	2.229221
28	1	0	-3.706944	-1.871347	0.961405
29	1	0	-0.758211	-0.913447	2.907461
30	1	0	-1.690440	-3.341594	-2.114196
31	1	0	-3.144627	-2.618540	-2.847004
32	1	0	-3.304385	-4.046106	-1.773123
33	1	0	-3.248280	0.935177	2.665219
34	1	0	-3.277290	3.358956	3.053814
35	1	0	-2.638367	4.939220	1.234702
36	1	0	-1.992050	4.026631	-0.993438
37	1	0	-1.951244	1.599314	-1.387417
38	1	0	-2.190448	-1.526914	2.170143
39	1	0	-1.076654	-1.003233	1.291143
40	1	0	1.148663	-3.548292	-0.987708
41	1	0	-0.152089	-3.279226	0.186575
42	1	0	1.342774	-3.485677	2.064255
43	1	0	2.404806	-4.356898	0.922647
44	1	0	2.473514	3.938035	-0.245889
45	1	0	3.672353	3.680829	-1.542552
46	1	0	2.086426	2.410490	-2.855291
47	1	0	0.841169	3.096013	-1.795624



Cu-Pybox

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.223644	2.649633	-0.000017
2	6	0	1.166265	1.252888	-0.000622
3	7	0	0.000063	0.627408	-0.001150
4	6	0	-1.166213	1.252764	-0.000536
5	6	0	-1.223707	2.649533	0.000089
6	6	0	-0.000066	3.336118	0.000179
7	6	0	-2.267789	0.253126	-0.000167
8	6	0	2.267901	0.253189	-0.000296
9	8	0	3.528322	0.670275	0.000076
10	6	0	4.369512	-0.533668	0.001888
11	6	0	3.345436	-1.698977	-0.000214
12	7	0	2.032665	-1.021394	-0.000283
13	7	0	-2.032669	-1.021485	0.000241
14	6	0	-3.345525	-1.698969	0.000484
15	6	0	-4.369454	-0.533531	0.001194
16	8	0	-3.528188	0.670282	-0.000089
17	29	0	-0.000039	-1.496226	-0.000477
18	1	0	2.169277	3.180418	0.000291
19	1	0	-2.169437	3.180149	0.000516
20	1	0	-0.000071	4.421557	0.000606
21	1	0	4.993261	-0.489095	0.896036
22	1	0	4.997221	-0.489123	-0.889450
23	1	0	3.430465	-2.337267	0.884195
24	1	0	3.431508	-2.334885	-0.886276
25	1	0	-3.430856	-2.336317	0.885550
26	1	0	-3.431340	-2.335790	-0.884929
27	1	0	-4.994155	-0.488711	0.894661
28	1	0	-4.996246	-0.489186	-0.890811

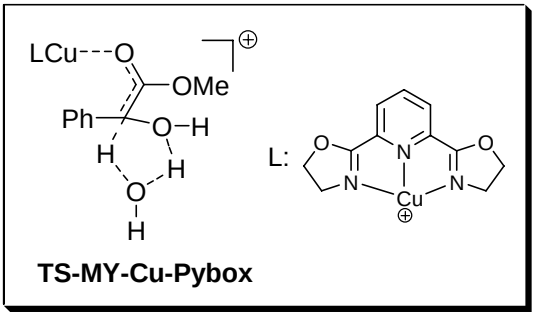


MY-Cu-Pybox

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	4.529336	-3.581016	2.212586
2	6	0	4.337225	-3.315185	1.171065
3	6	0	2.843357	-3.415540	0.757501
4	8	0	4.645164	-1.895304	1.015075
5	1	0	5.015561	-3.871957	0.520872
6	7	0	2.472537	-2.039825	0.386560
7	1	0	2.684147	-4.082517	-0.095743
8	1	0	2.200176	-3.761123	1.573382
9	6	0	3.513037	-1.319203	0.567934
10	6	0	3.548491	0.134666	0.309288
11	7	0	2.387234	0.656825	-0.119430
12	6	0	4.697353	0.907966	0.494194
13	6	0	2.327494	1.970851	-0.389225
14	6	0	4.627779	2.273651	0.219527
15	1	0	5.610903	0.441767	0.843898
16	6	0	3.426438	2.820095	-0.230508
17	6	0	1.014346	2.448968	-0.867820
18	1	0	5.500765	2.904597	0.353195
19	1	0	3.329007	3.874977	-0.458057
20	8	0	0.877739	3.776941	-1.054190
21	7	0	0.023406	1.677323	-1.105294
22	6	0	-0.489245	3.975739	-1.527768
23	6	0	-1.088559	2.543171	-1.532825
24	1	0	-0.431644	4.435759	-2.516972
25	1	0	-0.981099	4.660990	-0.834375
26	1	0	-1.435645	2.235599	-2.524606
27	1	0	-1.923749	2.428443	-0.834508
28	29	0	0.734574	-0.557612	-0.369872
29	8	0	-5.923886	-1.522347	0.534644
30	1	0	-5.801008	-2.411929	0.907104
31	1	0	-5.706681	-0.897552	1.254768
32	1	0	-4.977127	-1.130624	-0.558701
33	8	0	-4.229958	-0.695425	-1.150445

34	6	0	-2.958235	-0.718040	-0.374463
35	1	0	-4.023476	-1.265262	-1.940804
36	6	0	-2.995027	0.047818	0.845407
37	6	0	-2.000984	-1.514676	-0.971394
38	6	0	-2.017232	-0.137957	1.853066
39	6	0	-4.027101	0.986827	1.096439
40	8	0	-2.491289	-2.129397	-2.124617
41	8	0	-0.814353	-1.738321	-0.605658
42	6	0	-2.072362	0.588498	3.038662
43	1	0	-1.235474	-0.873420	1.701803
44	6	0	-4.073701	1.698827	2.298074
45	1	0	-4.767736	1.197548	0.328816
46	6	0	-1.554611	-2.868246	-2.923100
47	6	0	-3.099218	1.508431	3.277450
48	1	0	-1.310894	0.420048	3.795896
49	1	0	-4.875132	2.415528	2.457661
50	1	0	-1.081898	-3.652576	-2.328665
51	1	0	-0.786251	-2.204273	-3.329465
52	1	0	-2.141347	-3.304226	-3.732182
53	1	0	-3.138406	2.062589	4.210038

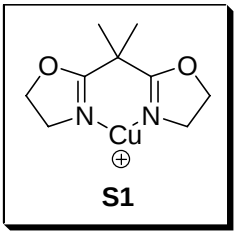


TS-MY-Cu-Pybox

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.015666	1.576097	1.804344
2	8	0	-4.275021	1.359035	0.883396
3	6	0	-3.238225	0.442583	0.343522
4	1	0	-4.033846	2.318523	0.097829
5	6	0	-2.105478	0.351851	1.197363
6	6	0	-3.807448	-0.672521	-0.445252
7	8	0	-3.357613	2.706627	-0.808738
8	8	0	-1.152270	-0.446636	1.070640
9	8	0	-2.130969	1.274531	2.208322

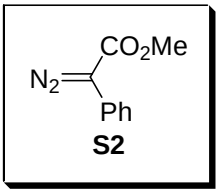
10	6	0	-2.967645	-1.581470	-1.118434
11	6	0	-5.199011	-0.817652	-0.588163
12	1	0	-3.878828	2.701059	-1.633470
13	1	0	-2.906390	1.715082	-0.698272
14	6	0	-1.044473	1.258955	3.151286
15	6	0	-3.509452	-2.607514	-1.889730
16	1	0	-1.892011	-1.485178	-1.027554
17	6	0	-5.731265	-1.845666	-1.367450
18	1	0	-5.866777	-0.134086	-0.075514
19	1	0	-0.109734	1.534460	2.655989
20	1	0	-0.948045	0.271683	3.608976
21	1	0	-1.307183	2.001660	3.904854
22	6	0	-4.892884	-2.747467	-2.022359
23	1	0	-2.842602	-3.300618	-2.396174
24	1	0	-6.810131	-1.941433	-1.454993
25	1	0	-5.309713	-3.546380	-2.628398
26	1	0	0.840741	4.876876	-1.715606
27	6	0	1.219499	4.525398	-0.752950
28	6	0	0.218172	3.632682	0.026942
29	8	0	2.338999	3.630075	-1.020720
30	1	0	1.602076	5.373019	-0.180800
31	7	0	0.854178	2.302024	0.064443
32	1	0	0.052240	3.984802	1.051143
33	1	0	-0.760037	3.566160	-0.459618
34	6	0	1.983533	2.427055	-0.521421
35	6	0	2.970338	1.338428	-0.692921
36	7	0	2.592622	0.127057	-0.256272
37	6	0	4.226236	1.566496	-1.267753
38	6	0	3.457150	-0.898383	-0.360511
39	6	0	5.113340	0.497702	-1.381172
40	1	0	4.486982	2.560553	-1.610387
41	6	0	4.729253	-0.760954	-0.918073
42	6	0	2.948412	-2.179869	0.170424
43	1	0	6.094047	0.643943	-1.822544
44	1	0	5.387979	-1.619190	-0.981253
45	8	0	3.738654	-3.259483	0.075683
46	7	0	1.795019	-2.296028	0.715148
47	6	0	2.988053	-4.363281	0.677897
48	6	0	1.649351	-3.706731	1.112860
49	1	0	3.584065	-4.749161	1.507261
50	1	0	2.876954	-5.136446	-0.084743
51	1	0	1.477696	-3.768907	2.191954
52	1	0	0.779538	-4.142041	0.611251
53	29	0	0.740239	-0.327686	0.561352



S1

Standard orientation:

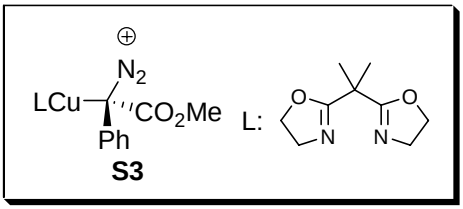
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.314481	0.506854	-0.000751
2	7	0	-1.560993	-0.762304	-0.000694
3	6	0	-3.027888	-0.957785	-0.002563
4	6	0	-3.583073	0.483427	-0.002076
5	8	0	-2.381201	1.312953	-0.001937
6	29	0	0.000177	-1.933870	0.001121
7	7	0	1.560880	-0.762050	0.000016
8	6	0	1.314483	0.507127	-0.000777
9	8	0	2.381185	1.313147	-0.002639
10	6	0	3.583050	0.483544	-0.002541
11	6	0	3.027784	-0.957653	-0.001798
12	6	0	-0.000050	1.291648	0.001460
13	1	0	-4.155714	0.740092	0.890603
14	1	0	-4.155946	0.740703	-0.894403
15	1	0	-3.319808	-1.527001	-0.889458
16	1	0	-3.321985	-1.528412	0.882684
17	1	0	3.319654	-1.527598	-0.888235
18	1	0	3.321877	-1.527536	0.883929
19	1	0	4.155618	0.740145	-0.895259
20	1	0	4.155977	0.740863	0.889759
21	6	0	-0.000160	2.186213	1.280335
22	6	0	-0.000159	2.194541	-1.271513
23	1	0	-0.888493	2.828190	-1.271534
24	1	0	0.887226	2.829531	-1.270649
25	1	0	0.000793	1.590320	-2.184843
26	1	0	0.887256	2.821214	1.283635
27	1	0	-0.888488	2.819895	1.284305
28	1	0	0.000797	1.575989	2.189672



S2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.753212	-1.539438	-0.000046
2	6	0	1.387645	-1.256143	-0.000268
3	6	0	0.942967	0.078738	-0.000094
4	6	0	1.904606	1.107249	0.000306
5	6	0	3.265151	0.811615	0.000516
6	6	0	3.700291	-0.515019	0.000342
7	1	0	3.074645	-2.577711	-0.000186
8	1	0	0.662415	-2.058568	-0.000566
9	1	0	1.595083	2.148824	0.000460
10	1	0	3.985915	1.624914	0.000824
11	1	0	4.761950	-0.745215	0.000509
12	6	0	-0.500590	0.401737	-0.000334
13	6	0	-1.621381	-0.551082	-0.000520
14	8	0	-2.815676	0.093908	-0.000026
15	6	0	-3.970738	-0.758636	0.000456
16	1	0	-4.827236	-0.083928	0.000804
17	1	0	-3.981358	-1.393151	-0.889704
18	1	0	-3.980634	-1.393143	0.890630
19	8	0	-1.517228	-1.763127	-0.000087
20	7	0	-0.849215	1.672908	-0.000302
21	7	0	-1.121431	2.778179	-0.000274



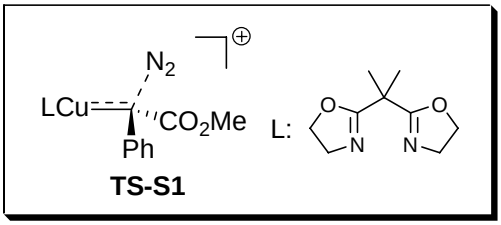
S3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.161561	-0.766936	0.154778
2	7	0	-2.411048	-2.050687	-0.219118
3	7	0	-2.590921	-3.111144	-0.556175
4	6	0	-2.320203	-0.557694	1.633740
5	8	0	-2.308376	0.534168	2.165231
6	8	0	-2.443061	-1.725409	2.283244
7	6	0	-2.578598	-1.641034	3.721809
8	1	0	-2.687817	-2.671174	4.057225
9	1	0	-3.460214	-1.051901	3.981205
10	1	0	-1.687923	-1.182489	4.157205
11	6	0	-2.550578	0.257176	-0.886170
12	6	0	-2.267858	0.005717	-2.241740
13	1	0	-1.772954	-0.917101	-2.536787
14	6	0	-2.632690	0.925944	-3.223157
15	1	0	-2.416130	0.710896	-4.265310
16	6	0	-3.272279	2.114619	-2.866545
17	1	0	-3.556340	2.832477	-3.629904
18	6	0	-3.549696	2.369824	-1.522299
19	1	0	-4.056836	3.286791	-1.236262
20	6	0	-3.199944	1.450989	-0.531834
21	1	0	-3.423732	1.659401	0.506317
22	1	0	1.399785	4.320457	0.917652
23	6	0	1.419134	3.384465	1.478922
24	6	0	0.221941	2.451744	1.194263
25	8	0	2.569804	2.619089	1.011015
26	1	0	1.575509	3.596757	2.538589
27	7	0	0.848365	1.241441	0.617412
28	1	0	-0.484391	2.869267	0.470858
29	1	0	-0.342499	2.177511	2.088085
30	6	0	2.116587	1.438165	0.557923
31	29	0	-0.072763	-0.461978	-0.010529
32	6	0	3.231893	0.544051	0.040487
33	7	0	1.635960	-1.358593	-0.580512
34	6	0	2.802136	-0.820252	-0.476888
35	6	0	4.244872	0.316895	1.202670
36	6	0	3.937543	1.293359	-1.130189
37	6	0	1.806411	-2.711460	-1.155851
38	8	0	3.843466	-1.558711	-0.892526
39	1	0	5.096749	-0.262752	0.842584
40	1	0	4.600936	1.280821	1.570604
41	1	0	3.778134	-0.223739	2.033024
42	1	0	4.308882	2.256763	-0.775964
43	1	0	4.778752	0.700351	-1.494007
44	1	0	3.245121	1.468839	-1.960379

45	6	0	3.330160	-2.831871	-1.377462
46	1	0	1.236217	-2.789402	-2.086321
47	1	0	1.418925	-3.458054	-0.456118
48	1	0	3.620862	-2.926232	-2.425493
49	1	0	3.804316	-3.622551	-0.793155



TS-S1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.417823	-2.979122	-1.065388
2	6	0	1.903686	-2.793595	-0.823449
3	7	0	1.772250	-1.365707	-0.456583
4	6	0	2.951501	-0.847864	-0.455611
5	8	0	3.969254	-1.663424	-0.775270
6	29	0	0.041904	-0.415700	-0.017406
7	7	0	1.034893	1.366967	0.247633
8	6	0	0.407420	2.664277	0.586055
9	6	0	1.611288	3.589291	0.863654
10	8	0	2.762095	2.774081	0.487150
11	6	0	2.305847	1.541703	0.203737
12	6	0	3.415096	0.562942	-0.135142
13	6	0	4.178135	1.115640	-1.375780
14	6	0	-1.911626	-0.517877	0.269854
15	6	0	-2.789604	0.125871	-0.740768
16	6	0	-2.379197	0.154072	-2.088394
17	6	0	-3.173009	0.751738	-3.063014
18	6	0	-4.388282	1.341392	-2.702792
19	6	0	-4.807886	1.325899	-1.369083
20	6	0	-4.022822	0.714240	-0.395839
21	7	0	-2.334770	-2.203015	0.170152
22	7	0	-2.375208	-3.259417	-0.172014
23	6	0	-2.141096	-0.200612	1.715912
24	8	0	-2.251547	-1.270085	2.517998
25	6	0	-2.357843	-0.987532	3.933198
26	8	0	-2.131875	0.954010	2.099866

27	6	0	4.381883	0.482246	1.083718
28	1	0	-2.472005	-1.959830	4.410254
29	1	0	-3.226448	-0.355126	4.126885
30	1	0	-1.453892	-0.485437	4.285426
31	1	0	-1.432182	-0.303959	-2.365126
32	1	0	-2.845710	0.763274	-4.098229
33	1	0	-5.007425	1.813271	-3.460152
34	1	0	-5.751213	1.785311	-1.089941
35	1	0	-4.353999	0.714555	0.637389
36	1	0	1.635681	4.493826	0.254302
37	1	0	1.729525	3.853483	1.917346
38	1	0	-0.197673	2.997208	-0.263515
39	1	0	-0.259075	2.540081	1.441911
40	1	0	5.218498	-0.179211	0.850301
41	1	0	4.768238	1.477826	1.309970
42	1	0	3.866770	0.097416	1.970372
43	1	0	4.562477	2.113140	-1.154441
44	1	0	5.014742	0.458059	-1.619204
45	1	0	3.517847	1.181332	-2.247139
46	1	0	1.304124	-3.001891	-1.714440
47	1	0	1.525624	-3.415928	-0.006566
48	1	0	3.675743	-3.224044	-2.097697
49	1	0	3.893696	-3.692785	-0.390423

N_2

Standard orientation:

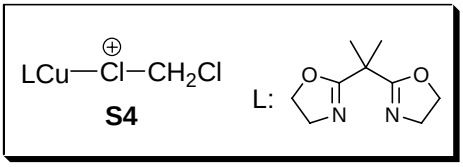
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.552659
2	7	0	0.000000	0.000000	-0.552659

CH_2Cl_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.767875
2	1	0	-0.899012	0.000000	1.380265
3	1	0	0.899012	0.000000	1.380265

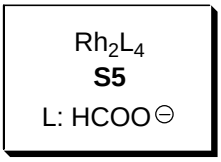
4	17	0	0.000000	-1.495284	-0.216699
5	17	0	0.000000	1.495284	-0.216699



Standard orientation:

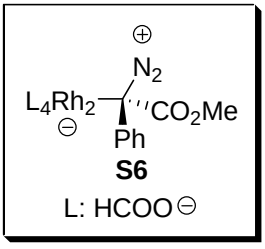
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.298416	1.546029	-0.075706
2	7	0	-0.034604	1.325346	-0.199993
3	6	0	0.648853	2.631232	-0.334177
4	6	0	-0.495823	3.660391	-0.213858
5	8	0	-1.686236	2.829379	-0.084134
6	29	0	0.745462	-0.510633	-0.196917
7	7	0	-1.000536	-1.500984	-0.011103
8	6	0	-2.131899	-0.894335	0.091100
9	8	0	-3.219026	-1.667620	0.228681
10	6	0	-2.786075	-3.059727	0.215687
11	6	0	-1.252580	-2.957583	0.060242
12	6	0	-2.470800	0.588874	0.085304
13	1	0	-0.627887	4.287562	-1.097019
14	1	0	-0.436363	4.288629	0.677073
15	1	0	1.400671	2.734211	0.452407
16	1	0	1.160367	2.676177	-1.300352
17	1	0	-0.710017	-3.381128	0.910603
18	1	0	-0.885845	-3.438411	-0.851281
19	1	0	-3.109969	-3.512962	1.154219
20	1	0	-3.286192	-3.550789	-0.621088
21	6	0	-3.458032	0.845279	-1.093909
22	6	0	-3.171871	0.920604	1.437898
23	1	0	-3.481581	1.967203	1.443818
24	1	0	-4.053707	0.288737	1.557718
25	1	0	-2.498814	0.748416	2.284457
26	1	0	-4.340637	0.214139	-0.976364
27	1	0	-3.767365	1.891888	-1.093660
28	1	0	-2.990010	0.617815	-2.057547
29	1	0	5.067511	-1.183205	0.109176
30	6	0	4.264432	-0.559842	-0.277466

31	1	0	4.447770	-0.228669	-1.296903
32	17	0	4.026121	0.835235	0.778021
33	17	0	2.791232	-1.658846	-0.344730



Standard orientation:

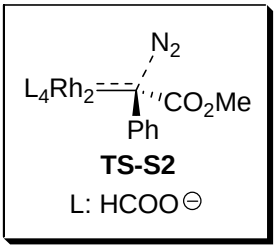
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.000000	0.000000	1.199783
2	45	0	0.000000	0.000000	-1.199783
3	6	0	0.000000	2.622295	0.000000
4	6	0	-2.622295	0.000000	0.000000
5	6	0	0.000000	-2.622295	0.000000
6	6	0	2.622295	0.000000	0.000000
7	1	0	0.000000	3.720534	0.000000
8	1	0	-3.720534	0.000000	0.000000
9	1	0	0.000000	-3.720534	0.000000
10	1	0	3.720534	0.000000	0.000000
11	8	0	0.000000	2.066448	1.138346
12	8	0	-2.066448	0.000000	1.138346
13	8	0	0.000000	-2.066448	1.138346
14	8	0	2.066448	0.000000	1.138346
15	8	0	0.000000	2.066448	-1.138346
16	8	0	-2.066448	0.000000	-1.138346
17	8	0	0.000000	-2.066448	-1.138346
18	8	0	2.066448	0.000000	-1.138346



Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.145571	0.784384	0.407542
2	45	0	0.255638	0.121307	0.122354
3	8	0	-0.087116	-1.636595	1.165324
4	6	0	0.867406	-2.465817	1.268150
5	1	0	0.637069	-3.388545	1.819388
6	8	0	2.044077	-2.364783	0.819102
7	45	0	2.542378	-0.637277	-0.210045
8	8	0	3.029700	0.294317	1.578963
9	6	0	2.112299	0.891683	2.207649
10	1	0	2.404697	1.374731	3.150901
11	8	0	0.888701	1.007353	1.889692
12	8	0	2.915555	1.126943	-1.225716
13	6	0	1.965399	1.950085	-1.348441
14	1	0	2.197171	2.874595	-1.896594
15	8	0	0.776243	1.849304	-0.918964
16	8	0	1.929719	-1.523506	-1.973877
17	6	0	0.710999	-1.411124	-2.293002
18	1	0	0.412628	-1.892470	-3.234955
19	8	0	-0.213372	-0.814291	-1.665362
20	7	0	-2.029716	1.087381	1.718865
21	7	0	-1.892774	1.303976	2.816099
22	6	0	-2.149062	2.009754	-0.459608
23	8	0	-2.420248	2.014038	-1.639045
24	8	0	-1.798473	3.103039	0.245397
25	6	0	-1.632365	4.305160	-0.528340
26	1	0	-1.364287	5.075920	0.194029
27	1	0	-2.562590	4.561565	-1.040880
28	1	0	-0.834151	4.163101	-1.259396
29	6	0	-2.963828	-0.435686	0.112618
30	6	0	-3.349994	-1.307880	1.144685
31	1	0	-3.054447	-1.116328	2.171692
32	6	0	-4.109705	-2.441919	0.868433
33	1	0	-4.399130	-3.099749	1.683332
34	6	0	-4.495352	-2.730673	-0.441486
35	1	0	-5.088536	-3.615111	-0.656559
36	6	0	-4.108422	-1.871665	-1.470180
37	1	0	-4.397528	-2.084379	-2.495923
38	6	0	-3.347319	-0.733484	-1.205844
39	1	0	-3.049339	-0.077597	-2.010882



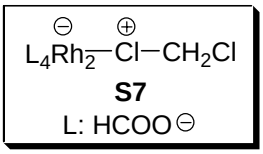
TS-S2

L: $HCOO^{\ominus}$

Standard orientation:

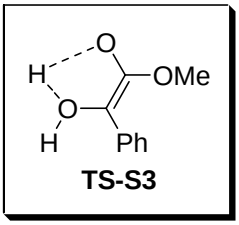
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.892918	0.522077	0.196751
2	45	0	0.237730	0.044657	0.061319
3	8	0	0.219535	-1.347164	1.620231
4	6	0	1.302295	-1.960598	1.892374
5	1	0	1.235197	-2.679803	2.722188
6	8	0	2.425808	-1.848546	1.338611
7	45	0	2.629792	-0.482922	-0.219462
8	8	0	3.033428	1.015334	1.164960
9	6	0	2.062035	1.638835	1.669097
10	1	0	2.312389	2.417226	2.405256
11	8	0	0.820035	1.489904	1.442493
12	8	0	2.687977	0.912670	-1.747861
13	6	0	1.624628	1.532137	-2.020077
14	1	0	1.685254	2.268244	-2.835007
15	8	0	0.482092	1.422454	-1.476712
16	8	0	2.074169	-1.936678	-1.588899
17	6	0	0.844024	-2.085895	-1.824552
18	1	0	0.580902	-2.862144	-2.558089
19	8	0	-0.141140	-1.459561	-1.325452
20	7	0	-1.976118	0.872712	1.933269
21	7	0	-1.728241	0.761695	3.009624
22	6	0	-2.113194	1.872367	-0.418849
23	8	0	-2.432574	1.986106	-1.584039
24	8	0	-1.830528	2.903434	0.395661
25	6	0	-1.811588	4.194710	-0.240449
26	1	0	-1.576216	4.903147	0.553477
27	1	0	-2.784640	4.419262	-0.684398
28	1	0	-1.044032	4.212678	-1.017399
29	6	0	-2.938287	-0.509408	0.000444
30	6	0	-2.702426	-1.828328	0.438405
31	1	0	-1.759123	-2.066858	0.914403
32	6	0	-3.672461	-2.812618	0.272658

33	1	0	-3.477722	-3.823234	0.620283
34	6	0	-4.884756	-2.506806	-0.350611
35	1	0	-5.636384	-3.279386	-0.489413
36	6	0	-5.129282	-1.205627	-0.797082
37	1	0	-6.069222	-0.963135	-1.284724
38	6	0	-4.173813	-0.210810	-0.612987
39	1	0	-4.370338	0.791246	-0.973042



Standard orientation:

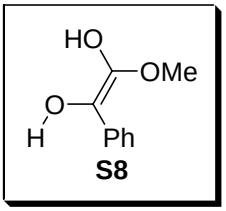
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.234285	-0.369971	-0.068138
2	45	0	2.022397	0.473437	0.063278
3	6	0	1.189286	-1.088764	2.342598
4	6	0	0.021643	2.237755	1.176881
5	6	0	0.615573	1.195389	-2.345197
6	6	0	1.777464	-2.115900	-1.175354
7	1	0	1.311381	-1.566114	3.324912
8	1	0	-0.345944	3.151047	1.664917
9	1	0	0.495157	1.670092	-3.328770
10	1	0	2.144372	-3.027493	-1.666547
11	8	0	0.058564	-1.242325	1.790579
12	8	0	-0.863302	1.380176	0.866760
13	8	0	-0.389222	0.555053	-1.914842
14	8	0	0.525232	-2.056386	-0.988357
15	8	0	2.192919	-0.454581	1.905061
16	8	0	1.267864	2.166185	0.992167
17	8	0	1.738069	1.358134	-1.782628
18	8	0	2.654692	-1.257079	-0.867687
19	1	0	-3.014822	0.758891	0.997807
20	6	0	-3.736813	-0.011177	0.736234
21	1	0	-4.181720	-0.483576	1.608855
22	17	0	-2.821099	-1.298368	-0.150094
23	17	0	-5.035073	0.706834	-0.250016



TS-S3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.246680	0.628321	0.000210
2	6	0	-1.939243	1.110342	-0.000021
3	6	0	-0.837819	0.224240	-0.000243
4	6	0	-1.113702	-1.165758	-0.000245
5	6	0	-2.424814	-1.628628	0.000002
6	6	0	-3.506529	-0.742412	0.000235
7	6	0	0.521547	0.684200	-0.000440
8	6	0	1.833645	0.202379	-0.000069
9	8	0	1.984885	-1.148480	-0.000260
10	6	0	3.340838	-1.608465	0.000276
11	8	0	0.681501	2.208395	-0.000057
12	8	0	2.815243	0.993560	0.000280
13	1	0	1.308833	2.363260	-0.750138
14	1	0	3.874125	-1.260375	0.889621
15	1	0	3.874715	-1.260689	-0.888842
16	1	0	3.275327	-2.697683	0.000436
17	1	0	-0.287934	-1.867461	-0.000433
18	1	0	-2.602190	-2.701660	0.000004
19	1	0	-4.527391	-1.113371	0.000423
20	1	0	-4.069912	1.339077	0.000381
21	1	0	-1.770139	2.182658	-0.000035
22	1	0	1.308066	2.363134	0.750645

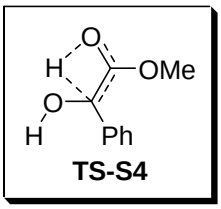


S8

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.170168	0.608092	0.360805
2	6	0	-1.864371	1.093563	0.314314
3	6	0	-0.788212	0.255241	-0.043923
4	6	0	-1.076062	-1.090798	-0.356872
5	6	0	-2.382519	-1.568790	-0.300222
6	6	0	-3.439994	-0.726357	0.054968
7	6	0	0.559666	0.818882	-0.102528
8	6	0	1.762362	0.190629	-0.135133
9	8	0	1.910165	-1.145354	-0.156585
10	6	0	3.055997	-1.682256	0.521551
11	8	0	0.686616	2.225041	-0.071364
12	8	0	2.923153	0.891212	-0.161086
13	1	0	0.204776	2.588337	-0.834477
14	1	0	3.049481	-1.399353	1.580326
15	1	0	3.984399	-1.341926	0.056732
16	1	0	2.964885	-2.765244	0.427724
17	1	0	-0.271443	-1.754653	-0.648037
18	1	0	-2.577472	-2.609830	-0.546310
19	1	0	-4.457674	-1.105393	0.091513
20	1	0	-3.978722	1.277192	0.645019
21	1	0	-1.663495	2.126366	0.580807
22	1	0	2.645595	1.828075	-0.118776

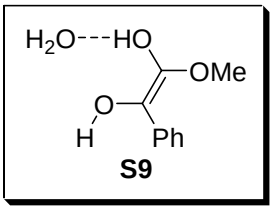


TS-S4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.460520	-0.722041	-0.283393
2	6	0	-3.219514	0.642051	-0.130318
3	6	0	-1.924126	1.115526	0.088033
4	6	0	-0.829996	0.231927	0.153280
5	6	0	-1.088321	-1.146163	-0.000547
6	6	0	-2.382400	-1.610841	-0.211932
7	6	0	0.526808	0.807463	0.377203

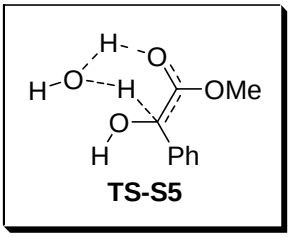
8	8	0	0.697293	2.141522	-0.010891
9	6	0	1.686911	-0.040124	0.202728
10	8	0	1.810739	-0.838459	1.213997
11	8	0	2.583927	0.043656	-0.744330
12	6	0	3.826758	-0.675648	-0.560754
13	1	0	0.211979	2.284650	-0.844833
14	1	0	3.678986	-1.729294	-0.807498
15	1	0	4.163920	-0.581983	0.473509
16	1	0	4.534481	-0.217417	-1.251434
17	1	0	-0.271620	-1.860911	0.050597
18	1	0	-2.549874	-2.678586	-0.331128
19	1	0	-4.468402	-1.090583	-0.452147
20	1	0	-4.043474	1.350240	-0.173974
21	1	0	-1.756265	2.177991	0.234143
22	1	0	0.950998	-0.040751	1.626758



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.856049	0.040109	0.198492
2	6	0	3.239612	-1.207606	0.299671
3	6	0	1.859263	-1.328529	0.151953
4	6	0	1.046162	-0.202595	-0.102939
5	6	0	1.686804	1.051366	-0.212736
6	6	0	3.066432	1.163892	-0.057387
7	6	0	-0.398416	-0.400649	-0.269707
8	8	0	-0.812756	-1.741610	-0.458985
9	6	0	-1.400288	0.523671	-0.227981
10	8	0	-2.713379	0.274200	-0.329695
11	8	0	-1.110463	1.837474	-0.099873
12	6	0	-2.123558	2.689664	0.447441
13	1	0	-0.481141	-2.043830	-1.321589
14	1	0	-2.441417	2.342383	1.436675
15	1	0	-2.992994	2.747325	-0.211643
16	1	0	-1.652758	3.670307	0.534320

17	1	0	1.099042	1.933740	-0.427384
18	1	0	3.530182	2.143294	-0.148556
19	1	0	4.932347	0.135823	0.313369
20	1	0	3.834056	-2.095777	0.500537
21	1	0	1.393389	-2.303144	0.252090
22	1	0	-2.949082	-0.670822	-0.123729
23	8	0	-3.307301	-2.262223	0.419039
24	1	0	-2.368707	-2.450328	0.202892
25	1	0	-3.344078	-2.247629	1.388292



TS-S5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.324272	-0.686447	-0.426405
2	6	0	-1.980013	-1.046650	-0.525893
3	6	0	-0.961027	-0.211022	-0.031526
4	6	0	-1.351121	0.993626	0.589397
5	6	0	-2.693614	1.350671	0.683763
6	6	0	-3.692936	0.516863	0.174303
7	6	0	0.451632	-0.650237	-0.112748
8	6	0	1.576836	0.219769	-0.308194
9	8	0	1.368498	1.540738	-0.389255
10	6	0	2.527874	2.385444	-0.288107
11	8	0	0.652822	-1.944301	-0.701396
12	1	0	0.659395	-1.846571	-1.668629
13	8	0	2.774985	-0.219557	-0.282596
14	8	0	2.179711	-1.810498	1.437640
15	1	0	3.063735	2.199547	0.646552
16	1	0	3.204646	2.213239	-1.128220
17	1	0	2.140740	3.404600	-0.312247
18	1	0	-4.085817	-1.355137	-0.820870
19	1	0	-1.708683	-1.995657	-0.975111
20	1	0	-0.596884	1.655844	0.998301
21	1	0	-2.961298	2.288136	1.165573
22	1	0	-4.739508	0.798845	0.251907

23	1	0	1.977340	-2.668425	1.017284
24	1	0	1.228382	-1.242226	1.166787
25	1	0	2.689670	-1.215363	0.615997

7. Computed Energies of All Stationary Points

Table S3. Sum of electronic and thermal enthalpies (*H*, in a.u.), sum of electronic and thermal free energies (*G*, in a.u.), thermal correction to Enthalpy (*TCH*, in a.u.), thermal correction to Gibbs free energy (*TCGFE*, in a.u.), and total free energy in solution (E_S, in a.u., solvent = dichloromethane)

Structure	*H*	*G*	*TCH*	*TCGFE*	E_S
1	-1305.098058	-1305.185575	0.409446	0.321929	-1305.537411
H_2O	-76.382115	-76.404215	0.024908	0.002808	-76.415872
TS-1	-1381.48748	-1381.580285	0.435947	0.343142	-1381.956946
2-C	-1381.487203	-1381.579995	0.43669	0.343898	-1381.958728
2-O	-1381.469074	-1381.562571	0.437347	0.343851	-1381.946331
2-F (6-F)	-574.36436	-574.413194	0.186106	0.137273	-574.56294
TS-2-C	-1381.453837	-1381.543045	0.43207	0.342862	-1381.919305
TS-2-O	-1381.444266	-1381.537013	0.432743	0.339995	-1381.906104
TS-2-F (TS-6-F)	-574.339827	-574.3896	0.182862	0.133089	-574.524271
3-C	-1457.89615	-1457.994413	0.464923	0.36666	-1458.393036
3-O	-1457.885689	-1457.984981	0.465004	0.365712	-1458.386356 -1458.430454[c]
3-F (7-F)	-650.77337	-650.829167	0.215249	0.159452	-650.996739 -651.032807[c]
TS-3-C	-1457.865883	-1457.959764	0.460147	0.366266	-1458.364724
TS-3-O	-1457.87733	-1457.97318	0.460485	0.364635	-1458.374699 -2902.631329[b] -1458.416152[c]
TS-3-F (TS-7-F)	-650.76849	-650.821763	0.209498	0.156225	-650.985979 -651.020454[b,c]
4	-574.447405	-574.498067	0.189075	0.138413	-574.639422
TS-3-O-2H_2O	-1534.295251	-1534.396004	0.488657	0.387904	-1534.825316
TS-3-F-2H_2O	-727.182362	-727.241105	0.235119	0.176376	-727.432397
TS-3-O-(*R*)-4	-2457.938217	-2458.073021	0.817448	0.682643	-2458.768932[a] -2458.839162[a,c]
TS-3-O-(*S*)-4	-2457.938698	-2458.072659	0.817398	0.683436	-2458.767041[a] -2458.837467[a,c]
5	-1473.70523	-1473.788234	0.277647	0.194643	-1473.994173
TS-5	-1550.100768	-1550.187641	0.304492	0.217619	-1550.416276
6-C	-1550.120767	-1550.20445	0.305685	0.222002	-1550.433695
6-O	-1550.074368	-1550.161859	0.305229	0.217738	-1550.4046
TS-6-C	-1550.066609	-1550.151341	0.30103	0.216298	-1550.37693
TS-6-O	-1550.050762	-1550.140366	0.300803	0.211199	-1550.362272
7-C	-1626.521884	-1626.611256	0.333659	0.244287	-1626.867414
7-O	-1626.488366	-1626.580708	0.333787	0.241445	-1626.842552 -1626.899114[c]

TS-7-C	-1626.476139	-1626.564353	0.32936	0.241146	-1626.820795
TS-7-O	-1626.483774	-1626.573361	0.329565	0.239979	-1626.834862 -1626.889636[c]
Cu-semicorrin	-820.339558	-820.393327	0.175834	0.122066	-820.526831 -820.551552[c]
MY-Cu-semicorrin	-1471.135639	-1471.23388	0.392589	0.294348	-1471.545946 -1471.601637[c]
TS-MY-Cu-semicorrin	-1471.128297	-1471.218902	0.38786	0.297255	-1471.534177 -1471.586829[c]
Cu-Pybox	-936.2436	-936.302337	0.232728	0.173991	-936.527062 -936.545781[c]
MY-Cu-Pybox	-1587.052792	-1587.154589	0.449377	0.347581	-1587.540777 -1587.590079[c]
TS-MY-Cu-Pybox	-1587.04032	-1587.138156	0.444238	0.346402	-1587.52855 -1587.575075[c]
S1	-807.056525	-807.114491	0.248202	0.190236	-807.355216 -2251.574859[b] -807.369398[c]
S2	-607.498958	-607.550969	0.171365	0.119353	-607.66899
S3	-1414.58745	-1414.68101	0.42092	0.327359	-1415.036607
TS-S1	-1414.575433	-1414.66806	0.418541	0.325914	-1415.02056
N_2	-109.511814	-109.533568	0.008905	-0.01285	-109.518183
CH_2Cl_2	-959.654717	-959.685405	0.034143	0.003454	-959.691334
S4	-1766.73469	-1766.8092	0.28416	0.20965	-1767.059282
S5	-975.695757	-975.748967	0.11651	0.0633	-975.837526 -975.864966[c]
S6	-1583.204829	-1583.292864	0.289365	0.20133	-1583.500968
TS-S2	-1583.18859	-1583.275122	0.287091	0.200559	-1583.482599
S7	-1935.361114	-1935.431869	0.152731	0.081976	-1935.527613
TS-S3	-574.35072	-574.401501	0.186995	0.136214	-574.554585
S8	-574.406287	-574.456477	0.18851	0.13832	-574.60188
TS-S4	-574.331338	-574.380927	0.182434	0.132845	-574.519022
S9	-650.80498	-650.861606	0.216145	0.159518	-651.030692
TS-S5	-650.769431	-650.822498	0.209648	0.156581	-650.98946

[a] solvent = trichloromethane

[b] CPCM-B3LYP/6-31+G(d)//B3LYP/6-31LAN

[c] CPCM-B3LYP/6-31+LAN//B3LYP/6-31LAN