Supporting Information

Theoretical Study of Aromatic Hydroxylation in $[Cu_2(H\text{-}XYL)O_2]^{2+}$ Complex Mediated by a Side-on Peroxo Dicopper Core and the Cu-ligands Effects

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1Computational details

For completeness, both antiferromagnetic and ferromagnetic couplings of the unpaired spins on the complex were investigated. Open-shell calculations for the singlet (S = 0) states resulted in a significant degree of spin contamination due to the high spin state (triplet state), with $\langle S^2 \rangle_S$ = 0.9-1.0(0 for a pure singlet, the S subscript stands for singlet), and the high-spin triplet (S = 1) states are contaminated by all the higher spin states (quintet, septet, etc.), with $\langle S^2 \rangle_T$ =2.0-2.3(2 for a pure triplet, the T subscript stands for triplet). In the present study, for the **TS1**^{1} singlet state, spin contamination result in $\langle S^2 \rangle_S$ =0.8, and spin contamination was observed for the**TS1**^{3} triplet, with $\langle S^2 \rangle_T$=2.1. However, for other intermediates and transition states, the triplet states are pure spin states. In addition, the singlet states are contaminated only by the triplet component. Thus, the singlet-triplet gap for pure triplet states can be estimated by a simple spin projection technique,[1] which is obtained from the broken symmetry (BS) approach:[2]

$$\Delta_{ST}^{BS} = \frac{2_{pure\ triplet} - 0_{pure\ singlet}}{2_{pure\ triplet} - \left\langle S^2 \right\rangle_S} \Delta_{unr,ST} \tag{1}$$

where $\Delta_{unr,\,ST}$ is the singlet-triplet energy gap from the unrestricted calculations and the value of $\langle S^2 \rangle_S$ implies that the singlet states in particular suffer from admixtures of higher spin states (triplet). For **TS1**, however, the high-spin states obtained here are not pure triplet states either. Assuming that the contributions from all the higher spin states (quintet, septet, etc.) for both the singlet and triplet are equal, a corrected expression that accounts for this can be written as

$$\Delta_{ST} = \frac{2_{pure\ triplet} - 0_{pure\ singlet}}{\left\langle S^2 \right\rangle_T - \left\langle S^2 \right\rangle_S} \Delta_{unr,ST} \tag{2}$$

The low-spin $E_{\text{cc-pVTZ(-f)}}$energies for all states were corrected using Eq. 2. The singlet-triplet gap correction

$$\delta_{ST} = \Delta_{ST} - \Delta_{unr,ST} \tag{3}$$

is normally small (see Table S1).

Table S1. Singlet-triplet splittings, for all states in the whole reaction at the B3LYP*/cc-pVTZ(-f) level: E_S and E_T energies are "actual" ground state for singlet and triplet states from the DFT calculation. $\Delta_{unr,ST}$ from the unrestricted calculations, Δ_{ST} from the broken symmetry (or spin projection) approach (See Eq. 2), and the final singlet-triplet gap correction δ_{ST} (see Eq. 1), The low-spin $E_{cc\text{-}pVTZ(\text{-}f)}$ energies for all states were corrected using Eq. 2. $\langle S^2\rangle_S$ = 0.9-1.0(0 for a pure singlet, the S subscript stands for singlet), and the high-spin triplet (S = 1) states are contaminated by all the higher spin states (quintet, septet, etc.), with $\langle S^2\rangle_T$ =2.0-2.3(2 for a pure triplet, the T subscript stands for triplet).

	$\langle S^2\rangle_S$	$\langle S^2\rangle_T$	E_S (Hartree)	E_T (Hartree)	$\Delta_{unr,ST}$ (Hartree)	$\Delta_{unr,ST}$ (Kcal mol^{-1})	Δ_{ST} (Hartree)	Δ_{ST} (Kcal mol^{-1})	δ_{ST} (Hartree)	δ_{ST} (Kcal mol^{-1})	$E_{cc\text{-}pVTZ(\text{-}f)}^{BS}$ (Hartree)	$E_{cc\text{-}pVTZ(\text{-}f)}^{BS}$ (Kcal mol^{-1})
1	0.902325	2.010914	-5154.715372	-5154.71569	-0.00032	0	-0.00057	0	-0.00026	0	-5154.72	
TS1	0.768032	2.145799	-5154.679828	-5154.670887	0.008941	5.809488	0.012978	8.503395	0.004038	2.693908	-5154.68	19.61081
2	1.252772	2.039932	-5154.702394	-5154.69584	0.006554	4.311872	0.016652	10.80879	0.010098	6.496918	-5154.71	1.647346
TS3	0.976457	2.007181	-5154.704158	-5154.705398	-0.00124	-0.57888	-0.00241	-1.15039	-0.00117	-0.57151	-5154.7	7.608786
4	0.933069	2.007733	-5154.756231	-5154.756132	9.85E-05	0.260981	0.000183	0.474355	8.48E-05	0.213374	-5154.76	-25.8522
TS9	0.991309	2.007627	-5154.746695	-5154.747653	-0.00096	-0.40173	-0.00188	-0.82319	-0.00093	-0.42145	-5154.75	-19.2339
3	0.920008	2.004826	-5154.847279	-5154.843816	0.003464	2.372741	0.006386	4.366576	0.002922	1.993835	-5154.85	-84.7667
TS3'	0.982165	2.007066	-5154.69836	-5154.704202	-0.00584	-3.46668	-0.0114	-6.79425	-0.00556	-3.32757	-5154.69	14.00321
4'	0.922689	2.007175	-5154.75879	-5154.757527	0.001263	0.99178	0.002329	1.821045	0.001066	0.829266	-5154.76	-28.074
TS4	0.945745	2.007026	-5154.666565	-5154.666593	-2.8E-05	0.181288	-5.4E-05	0.325622	-2.5E-05	0.144334	-5154.67	30.48305
5	0.922024	2.007686	-5154.774196	-5154.781502	-0.00731	-4.38529	-0.01346	-8.08614	-0.00615	-3.70085	-5154.77	-33.2117
TS6	0.911584	2.008928	-5154.777397	-5154.776403	0.000994	0.822917	0.001812	1.496151	0.000818	0.673235	-5154.78	-39.5945
TS5	0.92571	2.007991	-5154.680033	-5154.679074	0.000959	0.801079	0.001773	1.471619	0.000813	0.67054	-5154.68	21.50529

3 Results

3.1 The properties of the $[Cu_2(H\text{-}XYL)O_2]^{2+}$ complex

Table S2. Calculated geometric parameters for the μ-η^2:η^2-peroxo dicopper (II) complex, $[Cu_2(H\text{-}XYL)O_2]^{2+}$ (**1**), studied in the present study. Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Distances (Å)									
		$Cu\text{-}O_{ave}$	$Cu_A\text{-}Cu_B$	$O_A\text{-}O_B$	$O_A\text{-}C_A$	$Cu_A\text{-}N_A$	$Cu_A\text{-}N_B$	$Cu_B\text{-}N_C$	$Cu_B\text{-}N_D$	$Cu_B\text{-}N_E$	$Cu_B\text{-}N_F$
1	so[a]	2.06	3.57	1.39	2.80	2.14	2.20	2.05	2.11	2.09	2.14
	t[a]	2.39	4.29	1.30	3.09	2.15	2.06	2.09	2.15	2.02	2.06
1	so[b]	2.04	3.57	1.42	2.79	2.18	2.04	2.18	2.10	2.11	2.13
	so[c]	2.07	3.57	1.39	2.80	2.14	2.20	2.05	2.11	2.09	2.15
1	so[d]	2.00	3.23	1.43	2.69	2.02	2.01	-	2.02	2.01	-
1	so[e]	1.98	3.63	1.46	-	2.04	2.05	-	2.04	2.05	-

[a] The structure is shown in Figure 1.

[b] Geometrical parameters for the $\mathbf{P^{NO2-XYL}}$ structure(**1**) determined by Qayyum *et al.* [3]

[c] Geometrical parameters for the $\mathbf{P^{NO2-XYL}}$ structure(**1**) calculatedat the same level in this work.

[d]Geometrical parameters for structure(**1**) determined by Sander *et al.*[4]

[e]Geometrical parameters for the $\mathbf{P^{DBED}}$ structure(**1**) determined by Liu*et al.*[5]

Table S3. Spin populations for the μ-η^2:η^2-peroxo dicopper (II) complex $[Cu_2(H\text{-}XYL)O_2]^{2+}$ (**1**) studied in the present study. Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Spin populations				
		Cu_A	Cu_B	O_A	O_B	Substrate
1	so[a]	0.42	-0.42	-0.01	0.01	-
	t[a]	0.40	0.40	0.48	0.49	-
1	so[b]	0.44	-0.44	0.02	-0.01	-
1	so[c]	0.40	-0.40	-	-	-
1	so[d]	0.43	-0.43	0	0	-

[a] The spin populations are shown in Figure 1.

[b] Spin populations for the $\mathbf{P^{NO2-XYL}}$ structure(**1**)determined by Qayyum *et al.*[3]

[c]Spin populations for the $\mathbf{P^{NO2-XYL}}$ structure(**1**) calculatedat the same level in this work.

[d]Spin populations for the $\mathbf{P^{DBED}}$ structure (**1**) determined by Liu*et al.*[5]

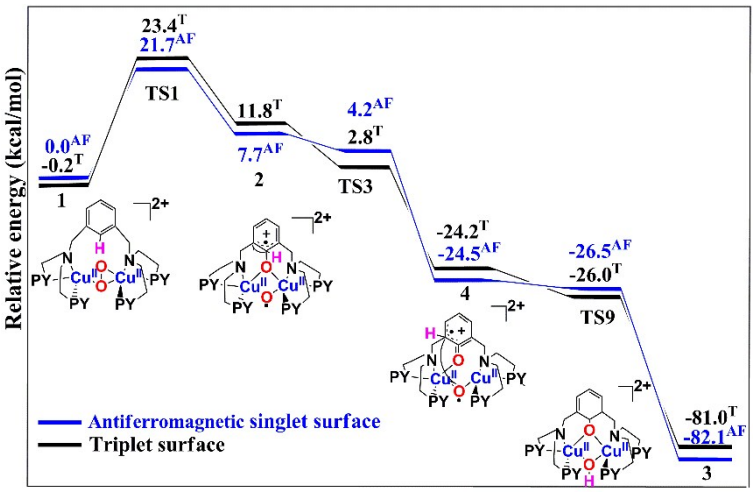

Fig. S1 Calculated free-energy profiles for mechanism**A** in the open-shell singlet and triplet statesat the B3LYP* level of theory. The energies (*G*, in kcal mol^{-1}) are relative to structure**1** without broken symmetry (BS) corrections. Note: AF: Antiferromagnetic singlet; T: triplet.

Table S4.Calculated geometric parameters for the O-O bond cleavage and C-O bond formation transition state (**TS1**) and complex **2**. Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Distances (Å)									
		Cu_A-O_{ava}	Cu_A-Cu_B	O_A-O_B	O_A-C_A	Cu_A-N_A	Cu_A-N_B	Cu_B-N_C	Cu_B-N_D	Cu_B-N_E	Cu_B-N_F
TS1	so[a]	1.94	3.28	1.95	1.89	2.15	2.23	2.07	2.15	2.31	2.05
	t[a]	1.96	3.21	1.97	1.91	2.15	2.25	2.08	2.17	2.29	2.07
TS1	so[b]	1.94	3.29	1.97	1.88	2.14	2.05	2.22	2.14	2.04	2.32
TS1	so[c]	1.92	3.14	1.91	1.95	2.03	2.00	-	2.02	2.00	-
2	so[a]	1.96	3.04	246	1.42	2.13	2.26	2.09	2.16	2.30	2.06
	t[a]	1.98	3.02	2.56	1.41	2.12	2.12	2.24	2.17	2.28	2.09
2	so[b]	1.98	3.08	2.49	1.41	2.12	2.09	2.24	2.16	2.05	2.26
2	so[c]	1.90	2.86	2.48	1.42	1.99	2.02		1.97	1.96	

[a] The structures are shown in Figures3.

[b] Geometrical parameters for **TSG (TS1)** andintermediate **K (2)** determined by Qayyum *et al.*[3]

[c]Geometrical parameters for **TS1** and **2** determined by Sander *et al.*[4]

Table S5. Spin populations for the O-O bond cleavage and C-O bond formation transition state (**TS1**) and the diradical complex **2**. Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Spin populations				
		Cu_A	Cu_B	O_A	O_B	Substrate
TS1	so[a]	0.48	-0.47	-0.09	0.23	0.01
	t[a]	0.54	0.55	0.33	0.03	0.24
TS1	so[b]	0.52	-0.52	-0.21	0.52	-0.31
2	so[a]	0.55	-0.41	0.02	0.45	-0.58
	t[a]	0.54	0.21	0.08	0.46	0.31
2	so[b]	0.59	-0.57	-0.03	0.96	-0.98

[a] The spin populations are shown in Figures 3.

[b] Spin populations forTS G **(TS1)** andintermediateK **(2)** determined by Qayyum *et al.*[3]

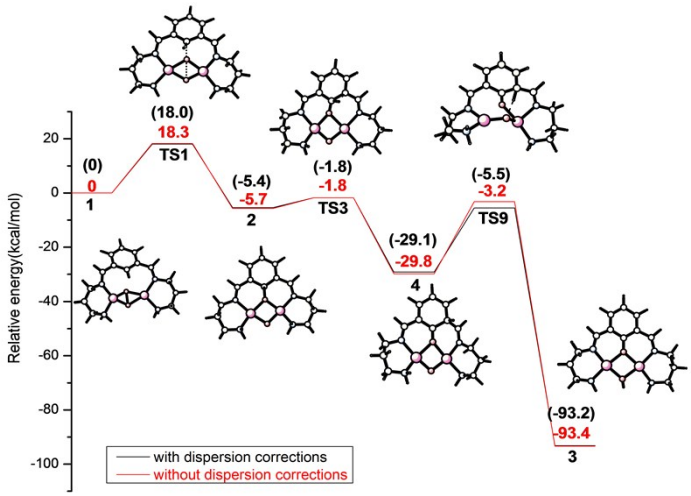

Fig. S2 The free-energy profile of the energetically most favorable route of $[Cu_2(DAPA)O_2]^{2+}$ from the model by Holthausen and co-workers. [11]

Table S6:Spin populations for transition states (**TS3 and TS9**) and complex **4** and **3**. Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Spin populations				
		Cu_A	Cu_B	O_A	O_B	Substrate
TS3	so[a]	0.55	-0.52	0.01	-0.04	-
	t[a]	0.54	0.51	0.05	0.64	-
4	so[a]	0.55	-0.52	0.02	-0.02	-
	t[a]	0.54	0.51	0.03	0.61	-
TS9	so[a]	0.57	-0.55	0.03	-0.04	-
	t[a]	0.57	0.54	0.09	0.44	-
3	so [a]	0.58	-0.58	-0.01	0.01	-
	t[a]	0.61	0.61	0.14	0.18	0.05

[a] The structures are shown in Figures 4.

Table S7. Geometrical parameters for product complex **3** $[Cu_2(H\text{-}XYL\text{-}O\text{-})(OH)]^{2+}$ studied in the present study and by Karlin *et al.* [7] Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Distances (Å)									
		$Cu\text{-}O_{ave}$	$Cu_A\text{-}Cu_B$	$O_A\text{-}O_B$	$O_A\text{-}C_A$	$Cu_A\text{-}N_A$	$Cu_A\text{-}N_B$	$Cu_B\text{-}N_C$	$Cu_B\text{-}N_D$	$Cu_B\text{-}N_E$	$Cu_B\text{-}N_F$
3	so[a]	1.99	3.13	2.45	1.34	2.15	2.26	2.05	2.15	2.27	2.05
	t[a]	1.99	3.09	2.51	1.34	2.15	2.26	2.05	2.15	2.27	2.06
3	so[b]	1.96	3.08	2.43	1.34	2.03	2.26	2.01	2.03	2.03	2.15
3	so[c]	2.01	3.19	2.43	1.33	2.12	2.06	2.25	2.12	2.06	2.26
3	so[d]	1.98	3.04	2.50	1.31	1.98	2.02	-	1.98	2.02	-

[a] The structures are shown in Figure 4.

[b] Crystal structure for $[Cu_2(H\text{-}XYL\text{-}O\text{-})(OH)]^{2+}$ (**3**) determined by Karlin *et al.*[6]

[c] Geometrical parameters for $[Cu_2(NO_2\text{-}XYL\text{-}O\text{-})(OH)]^{2+}$ (**3**) determined by Qayyum *et al.*[3]

[d]Geometrical parameters for **3** determined by Sander *et al.*[4]

Table S8. Big basis Energy (E, including the dispersion Correction and solvent Correction), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Free Energies (G_{total}, Including the ZPE Correction) and Relative Total Energies (ΔG_{total}) at 298.15 K of all structures in Pathway**A** at the B3LYP* levelof theory. Note: AF: Antiferromagnetic singlet; T: triplet.

	E (Hartree)	Gtc(Hartree)	G_{total} (Hartree)	ΔG_{total}(Kcal/mol)
1^{AF}	-5155.055786	0.634572	-5154.421214	0
$TS1^{AF}$	-5155.029025	0.638095	-5154.39093	19.0
2^{AF}	-5155.055722	0.636442	-5154.41928	1.2
$TS3^{AF}$	-5155.048116	0.634492	-5154.413624	4.8
4^{AF}	-5155.100404	0.639858	-5154.460546	-24.7
$TS9^{AF}$	-5155.097216	0.634376	-5154.46284	-26.17
3^{AF}	-5155.194701	0.639513	-5154.555188	-84.1

	E (Hartree)	Gtc(Hartree)	G_{total} (Hartree)	ΔG_{total}(Kcal/mol)
1^{AF}	-5155.055786	0.634572	-5154.421214	0
1^{T}	-5155.05598	0.634255	-5154.421725	-0.3
$TS1^{T}$	-5155.020773	0.636578	-5154.384195	23.2
2^{T}	-5155.037712	0.635059	-5154.402653	11.6
$TS3^{T}$	-5155.050234	0.633284	-5154.41695	2.7
4^{T}	-5155.098603	0.638582	-5154.460021	-24.4
$TS9^{T}$	-5155.099444	0.636492	-5154.462952	-26.2
3^{T}	-5155.188489	0.637946	-5154.550543	-81.2

Table S9: Calculated geometrical parameters for transition states (**ATS3 and ATS9**) and complex A**4**. Notation: so is the open-shell singlet state and t is the triplet state.

Structure	Multiplicity	Distances (Å)								
		Cu_A-O_A	Cu_A-O_B	Cu_B-O_A	Cu_B-O_B	Cu_A-Cu_B	O_A-O_B	O_A-C_A	H_A-O_B	H_A-$C_{Cor\,C}$
TS3	so[a]	2.13	1.88	2.14	1.89	3.02	2.64	1.31	4.08	1.65
	t[a]	2.13	1.89	2.13	1.90	3.02	2.65	1.31	4.08	1.64
TS3	so[b]	2.05	1.86	2.05	1.85	2.87	2.61	1.31	4.09	1.61
4	so[a]	2.20	1.88	2.37	1.88	3.15	2.69	1.26	3.62	1.11
	t[a]	2.19	1.90	2.32	1.90	3.14	2.69	1.26	3.64	1.11
4	so[b]	2.07	1.86	2.08	1.85	2.92	2.61	1.25	4.98	1.12
TS9	so[a]	2.14	1.93	2.71	1.91	3.08	2.69	1.28	1.54	1.25
	t[a]	2.13	1.93	2.70	1.91	3.07	2.68	1.29	1.53	1.25
TS9	t[b]	3.16	1.81	2.01	1.97	3.26	2.67	1.26	1.60	1.25

[a] The structures are shown in Figures 4.

[b] Geometrical parameters for **TS3, 4** and**TS9** determined by Sander *et al.*[4]

Table S10. Big basis Energy (E, including the dispersion Correction and solvent Correction), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Free Energies (G_{total}, Including the ZPE Correction) and Relative Total Energies (ΔG_{total}) at 298.15 K of all structures in Pathway**B and B'** at the B3LYP* levelof theory. Note: AF: Antiferromagnetic singlet; T: triplet.

	E (Hartree)	Gtc(Hartree)	G_{total} (Hartree)	ΔG_{total}(Kcal/mol)
1^{AF}	-5155.055786	0.634572	-5154.421214	0
$TS1^{AF}$	-5155.029025	0.638095	-5154.39093	19.0
2^{AF}	-5155.055722	0.636442	-5154.41928	1.2
$TS4^{AF}$	-5155.004902	0.631718	-5154.373184	30.3
5^{AF}	-5155.111743	0.639976	-5154.471767	-31.7
$TS6^{AF}$	-5155.118842	0.637423	-5154.481419	-37.8
$TS5^{AF}$	-5155.023318	0.633724	-5154.389594	19.8
3^{AF}	-5155.194701	0.639513	-5154.555188	-84.1

	E (Hartree)	Gtc(Hartree)	G_{total} (Hartree)	ΔG_{total}(Kcal/mol)
1^{AF}	-5155.055786	0.634572	-5154.421214	0
1^{T}	-5155.05598	0.634255	-5154.421725	-0.3
$TS1^{T}$	-5155.020773	0.636578	-5154.384195	23.2
2^{T}	-5155.037712	0.635059	-5154.402653	11.6
$TS4^{T}$	-5155.004824	0.630028	-5154.374796	29.1
5^{T}	-5155.112696	0.640698	-5154.471998	-31.9
$TS6^{T}$	-5155.109359	0.634276	-5154.475083	-33.8
$TS5^{T}$	-5155.021186	0.632677	-5154.388509	20.5
3^{T}	-5155.188489	0.637946	-5154.550543	-81.2

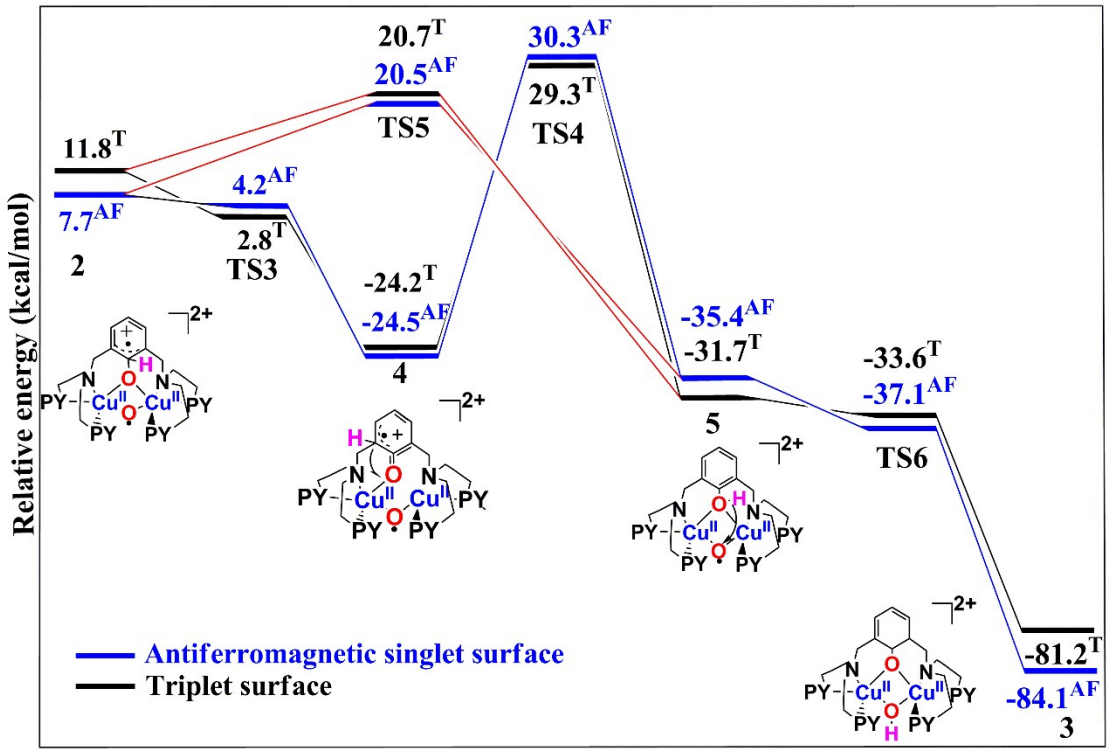

Fig. S3 Calculated free-energy profile obtained for mechanisms **B** and **C** in the open-shell singlet and triplet states at the B3LYP* level of theory. The free energies (*G*, in kcal mol^{-1}) are relative to structure **1** without broken symmetry (BS) corrections.Note: AF: Antiferromagnetic singlet; T: triplet.

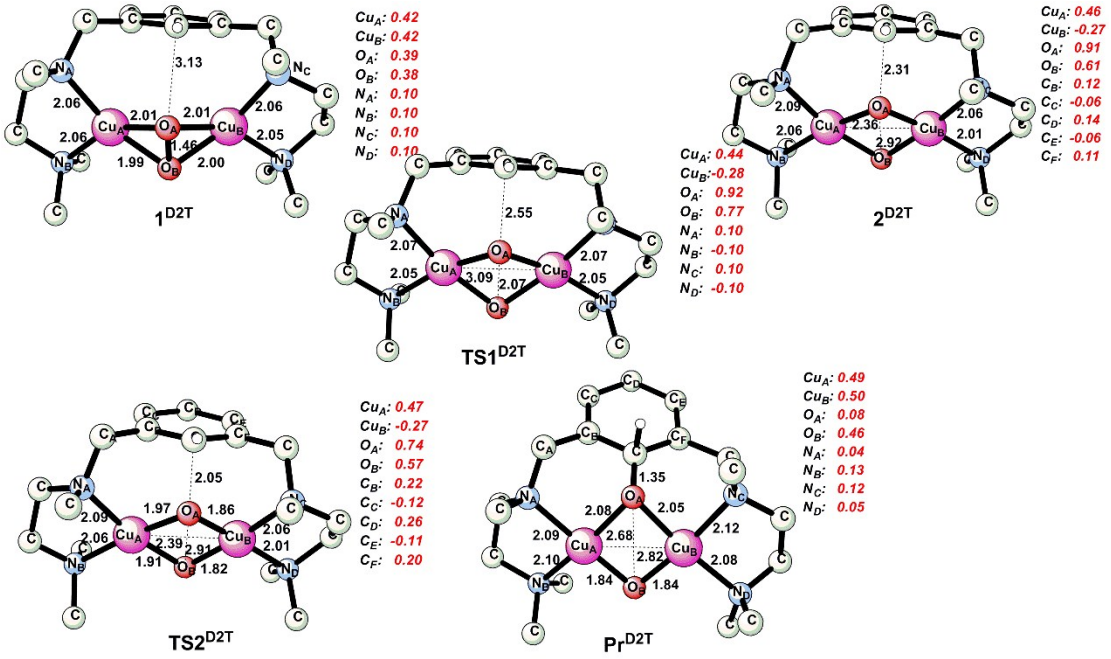

Fig. S4 The optimized structures for complex $\mathbf{1^{D2}}$, $\mathbf{TS1^{D2}}$, $\mathbf{2^{D2}}$, $\mathbf{TS2^{D2}}$ **and** $\mathbf{Pr^{D2}}$ in prefer spin states; Distances are given in [Å] and important Mulliken spin densities are shown in red font. For clarity, unimportant hydrogen atoms are not shown.

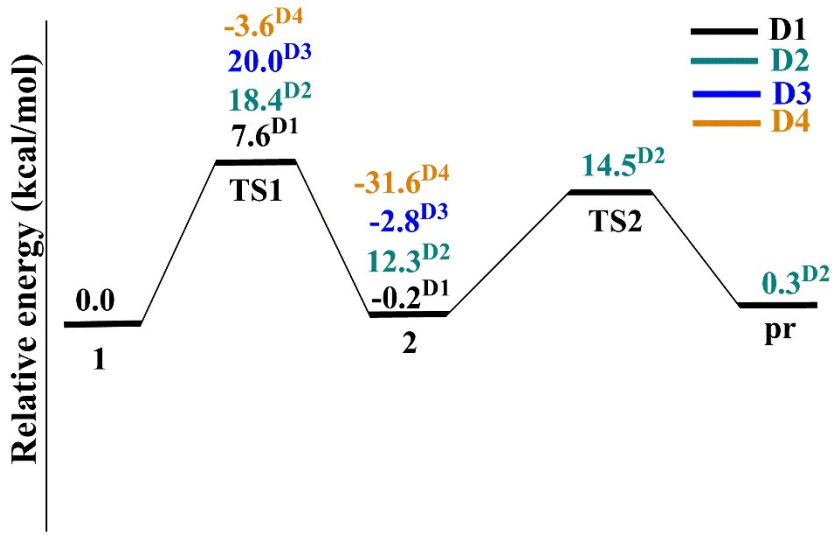

Fig. S5 Calculated free-energy profiles for mechanism **D1, D2, D3 and D4** at the B3LYP* level of theory. The energies (*G*, in kcal mol^{-1}) are relative to structure **1** without broken symmetry (BS) corrections.

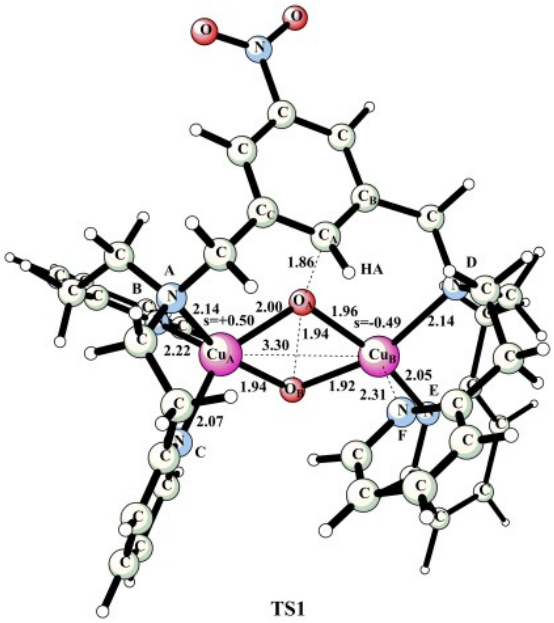

Fig. S6 Optimized structure of the O-O bond cleavage and C-O bond formation transition state (**TS1**, open-shell singlet**)**for$[Cu_2(NO_2\text{-}XYL)O_2]^{2+}$ complex reported by Karlin and co-workers; Selected distances [Å] and important spin populations are indicated.

Table S11. Big basis Energy (E, including the dispersion Correction and solvent Correction), Thermal Correction to the Gibbs Free Energy (G_{tc}), Total Free Energies (G_{total}, Including the ZPE Correction) and Relative Total Energies (ΔG_{total}) at 298.15 K of all structures at the B3LYP* levelof theory. Note: AF: Antiferromagnetic singlet; T: triplet.

	E (Hartree)	Gtc(Hartree)	G_{total} (Hartree)	ΔG_{total}(Kcal/mol)
1^{D1T}	-4502.180114	0.368523	-4501.989486	0
$TS1^{D1T}$	-4502.164577	0.368672	-4501.973264	7.6
2^{D1T}	-4502.175233	0.369969	-4501.985922	-0.2
1^{D2T}	-4355.849982	0.463001	-4355.578831	0
$TS1^{D2T}$	-4355.819717	0.463113	-4355.546362	18.4
2^{D2T}	-4355.830094	0.465013	-4355.554167	12.3
$TS2^{D2T}$	-4355.828822	0.466062	-4355.551338	14.5
pr^{D2T}	-4355.846547	0.463544	-4355.576699	0.3
1^{D3T}	-4353.423942	0.426624	-4353.193942	0
$TS1^{D3T}$	-4353.392199	0.425987	-4353.158557	20.0
2^{D3T}	-4353.424337	0.425123	-4353.197117	-2.8
1^{D4T}	-4314.515179	0.346842	-4314.335769	0
$TS1^{D4T}$	-4314.482745	0.347442	-4314.339916	-3.6
2^{D4T}	-4314.518377	0.346355	-4314.386215	-31.6

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Cartesian coordinates of stationary points optimized at the B3LYP/6-31G /LANL2DZ level**

1 (open-shell triplet)

Cu	2.40775200	5.78358500	8.63236500
Cu	3.18642400	8.91329100	10.15859000
O	3.63759600	6.94270400	9.89067100
O	2.29801700	7.02561500	10.25576800
N	3.07024300	5.20746600	6.68314700
N	0.38949000	5.50247100	8.37696300
N	3.09201300	4.02568700	9.76516900
N	4.96977700	9.98473700	9.82285000
N	2.64257500	9.61689100	12.05256100
N	1.93529400	9.87629800	8.70876900
C	3.83333500	6.28914500	5.93228700
C	5.08815700	6.80524600	6.59578900
C	6.34538800	6.31865400	6.22312000
C	7.49350600	6.78328000	6.86357500
C	7.38741800	7.71240900	7.89410700
C	6.13812400	8.21705700	8.28746000
C	5.00387200	7.78625000	7.59393500
C	6.14640100	9.10941200	9.52291100
C	-0.34230400	5.21372900	9.47355000
C	-1.69927400	4.92277100	9.40545500
C	-2.31697800	4.92946600	8.15389400
C	-1.55719000	5.22712700	7.02421700
C	-0.19701100	5.51232100	7.16111000
C	0.68369300	5.82147200	5.97268100
C	1.87947400	4.86028300	5.83715800
C	3.17766700	4.11142800	11.10757100
C	3.68246600	3.08691200	11.89909600
C	4.13772100	1.92882600	11.26981900
C	4.06213900	1.84283500	9.88147100
C	3.52565600	2.90720800	9.15136200
C	3.37751200	2.81560400	7.64690400
C	3.94343700	3.98979700	6.82186900
C	1.35706900	9.66571000	12.45065800
C	0.98550100	10.06018800	13.73030500
C	1.98907400	10.41727500	14.63140600
C	3.31994800	10.36849300	14.21890200
C	3.62177700	9.96189000	12.91632600
C	5.04527300	9.90117300	12.40275300

C	5.27312000	10.70983300	11.10766300
C	0.81077800	9.26812500	8.27942900
C	-0.02859400	9.82244300	7.32059800
C	0.31876500	11.05722900	6.77113900
C	1.47835200	11.68824200	7.21417200
C	2.26890300	11.08215700	8.19722200
C	3.48995000	11.79017000	8.74525800
C	4.80789500	10.99236100	8.72424300
H	3.13121400	7.11287000	5.77415500
H	4.08427500	5.88261300	4.94220400
H	6.43149300	5.58477500	5.42558800
H	8.47066300	6.41613000	6.56483500
H	8.28742900	8.04791300	8.40466500
H	6.28552600	8.46292700	10.39548400
H	7.03378600	9.75889800	9.47387100
H	0.19057900	5.22259000	10.41902400
H	-2.25247600	4.69301600	10.31009700
H	-3.37444900	4.70162200	8.05816800
H	-2.01007500	5.23201000	6.03815500
H	1.02941500	6.86226000	6.02840900
H	0.08595600	5.74795800	5.05900300
H	1.54840100	3.85472700	6.09943700
H	2.20063200	4.82279700	4.78730100
H	2.82616100	5.04113600	11.54415300
H	3.72063900	3.19822200	12.97799800
H	4.54617600	1.10664500	11.84986500
H	4.40962600	0.95448500	9.36394900
H	2.32135800	2.63570200	7.40871900
H	3.90299400	1.91729000	7.30717300
H	4.88383500	4.31972600	7.26679900
H	4.17050200	3.62532300	5.80852200
H	0.61601900	9.37835900	11.71106500
H	-0.06213300	10.08869200	14.01046900
H	1.73949700	10.73330700	15.64005300
H	4.12038500	10.64430600	14.89813200
H	5.71579400	10.30233600	13.16915500
H	5.34058400	8.85194200	12.26620900
H	6.31747400	11.04743500	11.06338000
H	4.65079200	11.60542400	11.14298300
H	-0.30513100	11.52535900	6.01524100
H	1.76906000	12.65323800	6.81076700
H	3.65587200	12.69407900	8.15017100

H	5.64689400	11.69970000	8.78921700
H	4.02839400	8.19622700	7.83135700
H	-0.93252300	9.30300700	7.01931900
H	0.59411700	8.30710800	8.73470100
H	3.26920800	12.14233700	9.76062000
H	4.90452300	10.46809100	7.77194100

1 (open-shell singlet)

Cu	2.40775200	5.78358500	8.63236500
Cu	3.18642400	8.91329100	10.15859000
O	3.63759600	6.94270400	9.89067100
O	2.29801700	7.02561500	10.25576800
N	3.07024300	5.20746600	6.68314700
N	0.38949000	5.50247100	8.37696300
N	3.09201300	4.02568700	9.76516900
N	4.96977700	9.98473700	9.82285000
N	2.64257500	9.61689100	12.05256100
N	1.93529400	9.87629800	8.70876900
C	3.83333500	6.28914500	5.93228700
C	5.08815700	6.80524600	6.59578900
C	6.34538800	6.31865400	6.22312000
C	7.49350600	6.78328000	6.86357500
C	7.38741800	7.71240900	7.89410700
C	6.13812400	8.21705700	8.28746000
C	5.00387200	7.78625000	7.59393500
C	6.14640100	9.10941200	9.52291100
C	-0.34230400	5.21372900	9.47355000
C	-1.69927400	4.92277100	9.40545500
C	-2.31697800	4.92946600	8.15389400
C	-1.55719000	5.22712700	7.02421700
C	-0.19701100	5.51232100	7.16111000
C	0.68369300	5.82147200	5.97268100
C	1.87947400	4.86028300	5.83715800
C	3.17766700	4.11142800	11.10757100
C	3.68246600	3.08691200	11.89909600
C	4.13772100	1.92882600	11.26981900
C	4.06213900	1.84283500	9.88147100
C	3.52565600	2.90720800	9.15136200
C	3.37751200	2.81560400	7.64690400
C	3.94343700	3.98979700	6.82186900
C	1.35706900	9.66571000	12.45065800
C	0.98550100	10.06018800	13.73030500
C	1.98907400	10.41727500	14.63140600

C	3.31994800	10.36849300	14.21890200
C	3.62177700	9.96189000	12.91632600
C	5.04527300	9.90117300	12.40275300
C	5.27312000	10.70983300	11.10766300
C	0.81077800	9.26812500	8.27942900
C	-0.02859400	9.82244300	7.32059800
C	0.31876500	11.05722900	6.77113900
C	1.47835200	11.68824200	7.21417200
C	2.26890300	11.08215700	8.19722200
C	3.48995000	11.79017000	8.74525800
C	4.80789500	10.99236100	8.72424300
H	3.13121400	7.11287000	5.77415500
H	4.08427500	5.88261300	4.94220400
H	6.43149300	5.58477500	5.42558800
H	8.47066300	6.41613000	6.56483500
H	8.28742900	8.04791300	8.40466500
H	6.28552600	8.46292700	10.39548400
H	7.03378600	9.75889800	9.47387100
H	0.19057900	5.22259000	10.41902400
H	-2.25247600	4.69301600	10.31009700
H	-3.37444900	4.70162200	8.05816800
H	-2.01007500	5.23201000	6.03815500
H	1.02941500	6.86226000	6.02840900
H	0.08595600	5.74795800	5.05900300
H	1.54840100	3.85472700	6.09943700
H	2.20063200	4.82279700	4.78730100
H	2.82616100	5.04113600	11.54415300
H	3.72063900	3.19822200	12.97799800
H	4.54617600	1.10664500	11.84986500
H	4.40962600	0.95448500	9.36394900
H	2.32135800	2.63570200	7.40871900
H	3.90299400	1.91729000	7.30717300
H	4.88383500	4.31972600	7.26679900
H	4.17050200	3.62532300	5.80852200
H	0.61601900	9.37835900	11.71106500
H	-0.06213300	10.08869200	14.01046900
H	1.73949700	10.73330700	15.64005300
H	4.12038500	10.64430600	14.89813200
H	5.71579400	10.30233600	13.16915500
H	5.34058400	8.85194200	12.26620900
H	6.31747400	11.04743500	11.06338000
H	4.65079200	11.60542400	11.14298300

H	-0.30513100	11.52535900	6.01524100
H	1.76906000	12.65323800	6.81076700
H	3.65587200	12.69407900	8.15017100
H	5.64689400	11.69970000	8.78921700
H	4.02839400	8.19622700	7.83135700
H	-0.93252300	9.30300700	7.01931900
H	0.59411700	8.30710800	8.73470100
H	3.26920800	12.14233700	9.76062000
H	4.90452300	10.46809100	7.77194100

TS1 (open-shell singlet)

Cu	2.50448000	5.92181600	8.61516300
Cu	3.31296300	8.74857900	10.06031200
O	3.94048800	7.23380500	9.01324100
O	2.35719000	7.09111700	10.14768900
N	3.05540600	5.23445300	6.65986200
N	0.48651300	5.51991300	8.41062800
N	3.20055900	4.09739400	9.69697300
N	4.94343500	10.11527700	9.74058200
N	2.71198700	9.48354500	11.87835000
N	1.92295100	9.93628600	8.65023600
C	3.95069300	6.25365000	5.98020800
C	5.16139500	6.69558700	6.76857000
C	6.36435300	6.01333200	6.67922600
C	7.47127000	6.41472000	7.44485700
C	7.36466900	7.48954900	8.32508500
C	6.18598800	8.23121400	8.41595100
C	5.06092700	7.84348200	7.62582700
C	6.19706700	9.35616700	9.43788200
C	-0.21077200	5.15200300	9.50253600
C	-1.57585300	4.89059200	9.46002200
C	-2.23943300	5.01984500	8.23940800
C	-1.51483500	5.40416200	7.11107700
C	-0.14439600	5.65082800	7.22368100
C	0.70436400	6.04412200	6.03740200
C	1.85401600	5.05601500	5.77546800
C	3.45744600	4.21730300	11.01146100
C	3.90814700	3.15371500	11.78835200
C	4.10832800	1.91924100	11.17049600
C	3.85391600	1.79770000	9.80450600
C	3.39649300	2.90991300	9.09275300
C	3.09723000	2.83408300	7.61121400
C	3.78245200	3.92469700	6.76318100

C	1.41807200	9.36318900	12.22909200
C	0.94679400	9.74694900	13.47896500
C	1.85569200	10.26717800	14.40076100
C	3.19673800	10.38337200	14.03719500
C	3.60209200	9.97974100	12.76331700
C	5.03843300	10.08435800	12.30875400
C	5.20671400	10.88569500	11.00654600
C	0.78762800	9.30866400	8.29281200
C	-0.16669500	9.88057600	7.45684500
C	0.07408300	11.16118100	6.95681700
C	1.24923300	11.81391500	7.32252000
C	2.15267400	11.17797400	8.18284600
C	3.39642400	11.89575400	8.65801400
C	4.71145500	11.10157400	8.62774800
H	3.32021500	7.11842400	5.75461400
H	4.27153500	5.82329400	5.02065100
H	6.46644700	5.17182500	6.00005400
H	8.41015200	5.87639800	7.36020700
H	8.22055500	7.76207600	8.93774500
H	6.53144300	8.91221500	10.37997200
H	6.97420400	10.08477100	9.15482500
H	0.35656600	5.07324600	10.42361600
H	-2.10007500	4.59174300	10.36132400
H	-3.30441900	4.82141600	8.16493000
H	-2.00351900	5.50795200	6.14756800
H	1.09471400	7.06132300	6.17854800
H	0.07511600	6.07809900	5.14261900
H	1.47732400	4.04080600	5.90845000
H	2.17848400	5.13538700	4.72948900
H	3.28404000	5.20654500	11.42551300
H	4.09773100	3.29219100	12.84761000
H	4.46105200	1.06451400	11.74003300
H	4.00651000	0.85152000	9.29476300
H	2.01000500	2.84256300	7.46158900
H	3.43899600	1.86569300	7.23219000
H	4.76407200	4.13086100	7.19042800
H	3.93712400	3.54616300	5.74198300
H	0.76130600	8.93662900	11.47913500
H	-0.10490600	9.63754200	13.72028000
H	1.52692400	10.57779200	15.38785500
H	3.92765200	10.78148700	14.73349600
H	5.62220400	10.58388400	13.08790300

H	5.46726400	9.07761200	12.20921300
H	6.22513000	11.29384100	10.95237600
H	4.52655900	11.73769600	11.03332300
H	-0.64079700	11.64546500	6.29828100
H	1.46412100	12.81220700	6.95422700
H	3.55133900	12.77682600	8.02647300
H	5.54605200	11.81739700	8.65154000
H	4.30916200	8.57931300	7.36595100
H	-1.07471000	9.33937200	7.21126800
H	0.65959300	8.31536200	8.71330400
H	3.20585300	12.29371000	9.66283200
H	4.79080900	10.56366700	7.68108400

2 (open-shell singlet)

Cu	2.37559000	6.05106300	8.58121900
Cu	3.24818000	8.64138200	9.91013400
O	4.01491400	7.28234200	8.67141700
O	1.92695100	7.28015700	9.97830300
N	2.99175300	5.11238900	6.77126500
N	0.34806000	5.56665000	8.38085000
N	3.12805900	4.38823900	9.91087700
N	5.03951000	9.84877100	9.85163000
N	2.66768300	9.25826000	11.79168300
N	2.12524000	10.11590600	8.55317900
C	3.67133300	6.15381300	5.91692900
C	4.92345400	6.78026300	6.47022200
C	6.13172000	6.57995200	5.84754000
C	7.30270400	7.23797100	6.28299600
C	7.28246200	8.06400700	7.42719900
C	6.11499000	8.28899800	8.11352700
C	4.79741800	7.77427100	7.59470300
C	6.17005400	8.93660200	9.47138700
C	-0.36293300	5.45741200	9.52074900

C	-1.71264500	5.12492200	9.52699000
C	-2.35057400	4.90466900	8.30639700
C	-1.61434900	5.02523700	7.12875100
C	-0.25910300	5.35813500	7.19409700
C	0.59053900	5.48248900	5.95309400
C	1.83609600	4.58163400	5.97889300
C	3.16802900	4.66776400	11.22663000
C	3.67551300	3.78242700	12.17213500
C	4.17454400	2.55678500	11.73134300
C	4.14015100	2.26758900	10.36895500
C	3.60270600	3.20459600	9.47975300
C	3.50219700	2.89449000	8.00200400
C	3.96566900	4.00120900	7.04040100
C	1.34969400	9.30076200	12.05695600
C	0.85792800	9.63404600	13.31341700
C	1.76885200	9.91511900	14.33200400
C	3.13386700	9.85707200	14.05501100
C	3.55992800	9.52418200	12.76733900
C	5.01946800	9.47078000	12.39044800
C	5.35553900	10.39904100	11.21261500
C	0.98315900	9.65171000	8.01283100
C	0.17370100	10.41629300	7.17880800
C	0.57038300	11.72154700	6.88649200
C	1.74912900	12.20761400	7.44793700
C	2.50433100	11.38101600	8.28732800
C	3.75529100	11.89969100	8.96170300
C	4.99112500	10.99108700	8.87748800
H	2.93361300	6.94119400	5.72487400

H	3.91182000	5.69320400	4.94889900
H	6.19562200	5.90963400	4.99461200
H	8.23744400	7.07139600	5.75772900
H	8.21859500	8.47832900	7.79182700
H	6.19347400	8.13445200	10.21798300
H	7.11749300	9.48639400	9.56076300
H	0.18321800	5.66094300	10.43416200
H	-2.24555000	5.04159000	10.46759700
H	-3.40308700	4.64154500	8.27038800
H	-2.08101100	4.85968600	6.16347100
H	0.86919800	6.53259400	5.79878800
H	-0.00847200	5.20094400	5.08266600
H	1.55291900	3.61465200	6.39494900
H	2.17679000	4.39707500	4.95081400
H	2.76551100	5.63903900	11.50100200
H	3.67730600	4.04731900	13.22394600
H	4.58330700	1.83779200	12.43456300
H	4.52002000	1.32239300	9.99494000
H	2.47618300	2.57843200	7.77777800
H	4.12234900	2.01804900	7.79086500
H	4.87379200	4.45977500	7.43636500
H	4.22501600	3.54147700	6.07524800
H	0.69533200	9.03918600	11.23361100
H	-0.21195300	9.66698900	13.48584000
H	1.42288700	10.17494500	15.32754900
H	3.86685900	10.06695300	14.82665800
H	5.62307400	9.77983600	13.24809800
H	5.31143500	8.43583300	12.17065700

H	6.42234600	10.65732100	11.23823900
H	4.80293300	11.33096400	11.33818200
H	-0.02908600	12.35240500	6.23754900
H	2.08079800	13.22079900	7.24554800
H	4.02791400	12.85427700	8.50214000
H	5.89233500	11.60063700	9.03379500
H	4.25908700	8.64223800	7.14254500
H	-0.74425900	10.00216500	6.77582000
H	0.72342300	8.63334000	8.28984800
H	3.51759600	12.13749900	10.00592300
H	5.06575100	10.57682500	7.87024600

TS3 (open-shell triplet)

Cu	2.25821900	6.07502700	8.62534100
Cu	3.15946100	8.65060300	9.90902700
O	4.06326500	7.20949100	8.60953200
O	1.72391600	7.42120000	9.82246600
N	3.12240100	4.95721400	6.98497100
N	0.24031400	5.67148900	8.06983700
N	2.94041600	4.54736800	10.10650400
N	5.11909200	9.79765100	9.79837100
N	2.91335100	8.93472300	11.97606300
N	2.14063000	10.21243600	8.68310900
C	3.61999800	5.92033700	5.95974200
C	4.81359400	6.77756100	6.32788900
C	5.84107200	6.98611300	5.39388400
C	6.91534500	7.81751600	5.68383200
C	7.00530600	8.50600300	6.91269700
C	6.03472400	8.35791900	7.88153100

C	4.84324500	7.53080000	7.60815200
C	6.20595000	8.91515500	9.27235100
C	-0.65168500	5.98436400	9.03232800
C	-2.00344700	5.67333300	8.93167800
C	-2.45315100	5.01431100	7.78872500
C	-1.53343600	4.70109100	6.78956500
C	-0.18843300	5.04386700	6.95399700
C	0.81538800	4.74460100	5.86366000
C	2.11334100	4.06924500	6.33043600
C	2.58064300	4.87058400	11.36485500
C	2.85849900	4.05913800	12.45941600
C	3.55205700	2.86748000	12.24415400
C	3.93958800	2.54176200	10.94711000
C	3.61249900	3.40207300	9.89173400
C	3.99629100	3.01715100	8.47563300
C	4.28461900	4.14304600	7.47375200
C	1.64498200	8.89913000	12.42645100
C	1.32269900	9.10514700	13.76399100
C	2.35649100	9.34495400	14.66895200
C	3.67061700	9.36525300	14.20259600
C	3.92125800	9.15606700	12.84414600
C	5.32396900	9.17181800	12.28459200
C	5.53418100	10.21932100	11.17686200
C	0.96602300	9.81569600	8.15681500
C	0.15423900	10.66136400	7.40597700
C	0.57639000	11.97307000	7.19230400
C	1.78517900	12.38869600	7.74879700
C	2.54434300	11.48619500	8.50011500

C	3.82587800	11.92671600	9.17081100
C	5.04105900	11.01749200	8.93329800
H	2.79194700	6.58210300	5.68541700
H	3.89355900	5.36969700	5.04622100
H	5.79958800	6.47086200	4.43893400
H	7.70184600	7.94634200	4.94601100
H	7.87603200	9.12513600	7.11003800
H	6.28261200	8.05313700	9.94534700
H	7.16363300	9.45511900	9.31236500
H	-0.23176100	6.51944800	9.87780300
H	-2.68212700	5.94269200	9.73394900
H	-3.49985500	4.74912500	7.67377200
H	-1.85224600	4.19491700	5.88394400
H	1.01992200	5.66098800	5.29421300
H	0.34955800	4.06267700	5.14508500
H	1.84888800	3.29252600	7.04811700
H	2.58895300	3.57320900	5.46942700
H	2.06607000	5.82395300	11.45099400
H	2.53893200	4.35519300	13.45318900
H	3.79196900	2.20545900	13.07092300
H	4.48833600	1.62612700	10.74795000
H	3.25139000	2.31725800	8.07695300
H	4.92010400	2.42895400	8.52610500
H	4.98909600	4.84237200	7.93267400
H	4.77787500	3.69095200	6.59836800
H	0.89662400	8.67080200	11.67581100
H	0.28654000	9.07505000	14.08371700
H	2.14579200	9.51082900	15.72122900

H	4.49763100	9.54089300	14.88317300
H	6.02557200	9.39816000	13.09343500
H	5.58768200	8.16670300	11.92957100
H	6.59399200	10.51366500	11.14593500
H	4.96812500	11.11575800	11.43503200
H	-0.02637200	12.66491500	6.61134600
H	2.13509700	13.40732100	7.61330800
H	4.08900000	12.92348000	8.80249100
H	5.96247700	11.60319900	9.07630000
H	4.33310300	8.28063800	6.80993200
H	-0.78849800	10.30004900	7.00820200
H	0.69976500	8.78965400	8.39625500
H	3.63812300	12.05140900	10.24474900
H	5.03305100	10.68890500	7.89008900

4 (open-shell singlet)

Cu	2.46025100	5.93322900	8.72367800
Cu	3.22976100	8.76038200	9.87157200
O	4.36354500	7.04262200	8.69797900
O	1.89168400	7.45548600	9.66913700
N	3.45620700	4.60227700	7.31528700
N	0.54100500	5.74686500	7.76011800
N	2.68400700	4.57817700	10.41579200
N	5.13749500	9.91001700	9.68216600
N	3.23789800	8.73126900	11.96746600
N	2.10770600	10.24373100	8.78411800
C	4.33062200	5.33616000	6.33215500
C	4.22885100	6.88941800	6.30667800
C	4.84137900	7.44466000	5.05283700

C	5.73156500	8.45551000	5.08137100
C	6.14457700	9.04405100	6.33910200
C	5.67570500	8.62479000	7.55263300
C	4.75469800	7.50509300	7.58924900
C	6.16359900	9.16299900	8.87480400
C	-0.47484400	6.23809100	8.50048100
C	-1.80611000	6.12758500	8.11522200
C	-2.10171100	5.48346200	6.91453700
C	-1.05306900	4.97948900	6.14838500
C	0.26400400	5.12648100	6.59404300
C	1.41497900	4.58894500	5.77459000
C	2.44951400	3.78379100	6.57300900
C	2.20419600	5.09211000	11.56682900
C	2.24371700	4.40287400	12.77256100
C	2.80917400	3.12796600	12.79238900
C	3.30560700	2.59763800	11.60524500
C	3.22409300	3.34470300	10.42461000
C	3.72451500	2.74904800	9.12815100
C	4.36524600	3.69785800	8.11016700
C	2.03172200	8.64673500	12.56128800
C	1.88026000	8.64621400	13.94342200
C	3.02514900	8.72472600	14.73734600
C	4.27221500	8.80831000	14.11999500
C	4.35019200	8.81485700	12.72480500
C	5.66695600	8.93798700	11.99786900
C	5.72341300	10.14385100	11.04235200
C	0.98645100	9.82220700	8.16954000
C	0.11861600	10.69218700	7.51804700

C	0.41673400	12.05399200	7.51517500
C	1.57204600	12.49069700	8.16111500
C	2.40446400	11.56082400	8.78921600
C	3.66465700	11.99024800	9.50002600
C	4.91876600	11.23891900	9.02907700
H	4.11654100	4.97259400	5.32264500
H	5.37383800	5.07852400	6.52975200
H	4.52575900	7.01160900	4.10713400
H	6.15490300	8.84857500	4.16316600
H	6.87244300	9.85216400	6.30345700
H	6.50806400	8.32300800	9.48248100
H	7.02709300	9.82137800	8.70630600
H	-0.16804600	6.74659300	9.40866800
H	-2.58795700	6.53481800	8.74680600
H	-3.12850600	5.37230500	6.58023600
H	-1.24840000	4.47041700	5.21034100
H	1.89109900	5.40891200	5.22159100
H	1.00815200	3.92444000	5.00705300
H	1.91251100	3.17318500	7.29951800
H	2.98017300	3.09825600	5.89636900
H	1.79365800	6.09147900	11.46925200
H	1.84170200	4.85729600	13.67136500
H	2.86613900	2.55755200	13.71428600
H	3.75095000	1.60821800	11.58533600
H	2.92198200	2.16073400	8.66804600
H	4.49605600	2.01188700	9.37390900
H	5.07821700	4.34875800	8.62280100
H	4.92914200	3.07919800	7.39751000

H	1.18671800	8.55798000	11.88684300
H	0.89000300	8.58806300	14.38156000
H	2.94906600	8.72636200	15.82027500
H	5.17968300	8.87702700	14.71051900
H	6.46897800	9.05233300	12.73219300
H	5.87540100	8.00494800	11.46027100
H	6.76642600	10.46843300	10.92013200
H	5.18803800	10.97882700	11.49882800
H	-0.23815900	12.76611300	7.02268300
H	1.83035600	13.54422200	8.18270700
H	3.82231400	13.05829700	9.32692900
H	5.80927400	11.86129900	9.19794500
H	3.15680600	7.15816400	6.28810400
H	-0.77378100	10.30875500	7.03564200
H	0.81147800	8.75479000	8.25518400
H	3.52970600	11.87880000	10.58305300
H	4.84347500	11.07099200	7.95225000

TS9 (open-shell triplet)

Cu	2.68633200	6.00368300	9.02811700
Cu	3.13686300	9.02763100	9.23701500
O	4.65618400	6.81172500	9.05402300
O	2.27829300	7.69155500	8.17542000
N	3.16368900	4.72228500	7.14409000
N	0.67704300	5.43432600	9.05456900
N	3.24010700	4.49508200	10.36994500
N	4.96442200	9.98412400	9.90623800
N	2.36494900	8.63506900	11.15752900
N	2.40770600	10.63491000	8.10998900

C	4.26642100	5.44121600	6.44864000
C	4.41682000	6.96912500	6.68332700
C	4.86418500	7.68736000	5.49008600
C	5.70749700	8.75697800	5.55502300
C	6.17324700	9.20092500	6.82600000
C	5.81072200	8.59061300	8.00980400
C	5.01966200	7.38704500	7.96756200
C	6.12814600	9.16921300	9.36190800
C	0.02521900	5.16913000	10.20219900
C	-1.30588500	4.77229100	10.23821700
C	-1.98689200	4.63512300	9.02774500
C	-1.30932700	4.90263100	7.84050800
C	0.03024300	5.30833900	7.87192300
C	0.79178900	5.59891400	6.60176300
C	1.93582400	4.60753000	6.29601600
C	3.65731200	4.88356500	11.59143300
C	4.05325400	3.99271600	12.58024400
C	4.02365000	2.62904200	12.28833200
C	3.60562200	2.22395100	11.02372000
C	3.21510500	3.17447900	10.07308000
C	2.78861100	2.74055100	8.68968000
C	3.62459900	3.36613900	7.55606300
C	1.02104200	8.56409500	11.24425000
C	0.34744900	8.58352500	12.46095300
C	1.09903400	8.67717400	13.63324900
C	2.48942800	8.74385400	13.54278700
C	3.10433600	8.72331900	12.28697400
C	4.60529500	8.80494400	12.13480400

C	5.08899600	10.06401200	11.39308700
C	1.50104500	10.35959900	7.15170800
C	0.87997300	11.35460600	6.40556800
C	1.21133700	12.68453500	6.66279100
C	2.14916700	12.96622800	7.65512300
C	2.73487500	11.91991100	8.37184700
C	3.74818700	12.18807400	9.46065000
C	5.04025500	11.36393400	9.33315900
H	4.19015300	5.27359400	5.36620100
H	5.20839000	4.98523200	6.76189000
H	4.50643700	7.33758700	4.52440400
H	6.02525700	9.27598100	4.65699200
H	6.82593100	10.07136500	6.86042700
H	6.32459100	8.36407200	10.06944800
H	7.01591500	9.81340500	9.32798900
H	0.60127400	5.27576800	11.11556300
H	-1.78902400	4.57129500	11.18844000
H	-3.02660800	4.32246300	9.00866900
H	-1.81104800	4.80039800	6.88370600
H	1.18019400	6.61965900	6.66110000
H	0.09263800	5.55232100	5.76019500
H	1.54420700	3.59054000	6.39267900
H	2.21515500	4.72485600	5.24065400
H	3.66582400	5.95309200	11.77102000
H	4.37693300	4.35945800	13.54837000
H	4.32593900	1.89494000	13.02906500
H	3.58168000	1.17088100	10.76332800
H	1.72352200	2.95265200	8.54163800

H	2.89220700	1.65303300	8.62818300
H	4.65982700	3.44634000	7.89641300
H	3.62348900	2.68772600	6.69006800
H	0.49366200	8.48637200	10.29889300
H	-0.73595100	8.53411600	12.48415100
H	0.61162500	8.70114000	14.60336600
H	3.09832300	8.81763000	14.43820500
H	5.06295600	8.80489400	13.12881200
H	4.96936300	7.90923900	11.61728800
H	6.14108800	10.25522600	11.64651700
H	4.51848600	10.92853500	11.74164000
H	0.74973400	13.49088700	6.10078800
H	2.42801800	13.99102800	7.87824000
H	4.01930400	13.24773600	9.42990500
H	5.86893700	11.89751600	9.81987500
H	3.32057000	7.41185900	7.08694300
H	0.15477000	11.08885500	5.64392700
H	1.28979700	9.30417400	7.01769100
H	3.28133200	12.03011800	10.44235600
H	5.29250300	11.26874100	8.27479400

3 (open-shell singlet)

Cu	2.22105600	5.95591000	8.66099900
Cu	3.13612600	8.61951600	10.02152200
O	3.67867500	7.31672200	8.62520300
O	1.77959400	7.17369100	10.16485900
N	2.75159200	5.21916800	6.70768200
N	0.36049100	5.10662000	8.66933800
N	3.33437100	4.33157500	9.77084700

N	5.12211200	9.43628100	10.16995000
N	2.47901100	9.55301900	11.72680800
N	2.37472100	10.18999000	8.57144400
C	3.39560100	6.37577200	5.97122600
C	4.70871500	6.85702600	6.53310500
C	5.86373500	6.87278200	5.74463500
C	7.06588400	7.37645300	6.24025500
C	7.11821100	7.86273400	7.54593700
C	5.98818300	7.84189600	8.37032600
C	4.77602400	7.33818300	7.85624000
C	6.07021100	8.31594000	9.79845100
C	-0.12871500	4.61199500	9.82425700
C	-1.40186500	4.06389300	9.91234300
C	-2.19275800	4.03275300	8.76268900
C	-1.68038200	4.54254100	7.57057600
C	-0.39037300	5.07655600	7.54845800
C	0.25512000	5.58867500	6.28324300
C	1.53475200	4.80521800	5.93703100
C	3.67013300	4.57186500	11.05004600
C	4.44854400	3.70186100	11.80642800
C	4.90466800	2.53098300	11.20101400
C	4.55779500	2.27828700	9.87532900
C	3.76412700	3.19780100	9.18317900
C	3.34430800	2.94660300	7.75075100
C	3.71390500	4.06947100	6.76443000
C	1.23442000	10.06567900	11.78678600
C	0.70522700	10.59646700	12.95614800
C	1.49770300	10.58970300	14.10504000

C	2.78800700	10.06727100	14.03663200
C	3.26080700	9.55388700	12.82689100
C	4.67360100	9.04923900	12.65698100
C	5.42926700	9.84850300	11.57836600
C	1.30603000	9.90823800	7.80502700
C	0.81517800	10.77546600	6.83530700
C	1.47396300	11.99058600	6.64616100
C	2.58600600	12.28341900	7.43256300
C	3.01470700	11.36332200	8.39582000
C	4.20818400	11.66244900	9.28060700
C	5.32518000	10.60154500	9.25013300
H	0.85677200	7.36445100	10.38698500
H	2.65940100	7.18819000	5.96749300
H	3.54978900	6.06918700	4.92746700
H	5.81849200	6.49799000	4.72435800
H	7.95290400	7.39085000	5.61518700
H	8.05515600	8.25451100	7.93607200
H	5.85889800	7.49281100	10.49085100
H	7.09388400	8.65610100	9.99830500
H	0.53217600	4.66712300	10.68177600
H	-1.75951200	3.67125700	10.85804000
H	-3.19343700	3.61192100	8.79284300
H	-2.26989800	4.52344400	6.66137200
H	0.47551100	6.66202800	6.37234000
H	-0.44809400	5.48639900	5.45118100
H	1.35468100	3.74475700	6.12183900
H	1.74952500	4.90615700	4.86489400
H	3.27782100	5.49725700	11.46623700

H	4.68728600	3.93353500	12.83904600
H	5.51897700	1.82464000	11.75133500
H	4.89658000	1.37301700	9.37943500
H	2.26621500	2.74305700	7.72365700
H	3.82890300	2.03027000	7.39898400
H	4.69240000	4.47468200	7.02632100
H	3.80019400	3.65076700	5.75115600
H	0.66729600	10.05378300	10.86171600
H	-0.29885100	11.00611100	12.96216300
H	1.11909000	10.99440300	15.03952500
H	3.43127900	10.06140400	14.91010000
H	5.21126100	9.14983800	13.60529000
H	4.67372700	7.97768900	12.41310000
H	6.51186700	9.76050700	11.74057400
H	5.18040000	10.90648400	11.69052000
H	1.12879400	12.69821600	5.89863500
H	3.11996500	13.21977000	7.30543400
H	4.64959000	12.60975200	8.95684200
H	6.28448400	11.07548800	9.50633700
H	5.42469300	10.20524400	8.23714700
H	3.86203300	11.83266700	10.30924600
H	0.83169700	8.94693900	7.99582300
H	-0.05667200	10.51057600	6.2**4861500**

TS4 (open-shell triplet)

Cu	2.58294000	5.79302300	8.93688100
Cu	3.28297700	8.65406700	9.93083100
O	3.91263500	7.51029900	8.08909000
O	2.26691000	7.10112600	10.26174400

N	3.53802800	4.54853100	7.28191600
N	0.74862800	5.97001900	7.89856100
N	2.69390700	4.19529200	10.34805100
N	4.82459600	10.05565900	9.38157700
N	3.54695000	8.99600900	12.07034700
N	1.71880800	9.96987500	9.16041100
C	4.94879000	4.97935900	7.02342200
C	5.25848100	6.45386900	6.63028400
C	6.28068100	6.64459800	5.64414600
C	7.18801300	7.67579100	5.77888700
C	7.14897000	8.52345000	6.91083500
C	6.15857100	8.44126900	7.89437600
C	5.18320400	7.46949000	7.65421500
C	6.12372400	9.35947100	9.09822100
C	-0.34692700	6.03593100	8.67853500
C	-1.63733100	6.02338200	8.15886500
C	-1.79483200	5.94843500	6.77497900
C	-0.65957200	5.88859700	5.96767600
C	0.60660200	5.89852800	6.55903800
C	1.86780900	5.81768300	5.73227600
C	2.73028500	4.57073900	6.01187200
C	2.80364500	4.51170000	11.65027700
C	2.72161200	3.55841600	12.65983300
C	2.50611200	2.22775300	12.30339400
C	2.38979200	1.90100500	10.95241900
C	2.49022600	2.90937300	9.99111600
C	2.40880300	2.60705200	8.51281100
C	3.63542300	3.11784700	7.73878100

C	2.60323300	8.39272400	12.82047300
C	2.49959500	8.57630500	14.19422900
C	3.41206200	9.42247400	14.82334200
C	4.38662200	10.04791700	14.04998500
C	4.43344300	9.81654400	12.67070400
C	5.50765700	10.47184200	11.83267400
C	5.05064500	11.04225000	10.48344700
C	0.48712400	9.51507000	9.47742300
C	-0.67111700	10.23979500	9.23083400
C	-0.55558100	11.48934400	8.61911200
C	0.71067400	11.95490200	8.28424000
C	1.83866800	11.17588200	8.57374300
C	3.20885000	11.73367000	8.24296100
C	4.39451600	10.77239700	8.13621800
H	5.36729900	4.35304300	6.22382500
H	5.51525700	4.76181300	7.93258400
H	6.39139900	5.92327200	4.83864400
H	7.96838900	7.81933100	5.04013400
H	7.89921400	9.30600400	6.99494800
H	6.37916900	8.77051400	9.98268200
H	6.91464400	10.11437200	8.97566600
H	-0.15519500	6.10985500	9.74441900
H	-2.49242800	6.06880400	8.82440100
H	-2.78468800	5.93662800	6.32977800
H	-0.75089700	5.83376600	4.88810300
H	2.43953400	6.74697100	5.85109200
H	1.59370400	5.78054800	4.67350700
H	2.05649100	3.71139700	6.03296300

H	3.40934700	4.40815500	5.16414900
H	2.94274600	5.56902300	11.84838700
H	2.82150000	3.85503800	13.69803900
H	2.43256500	1.45450300	13.06200800
H	2.22455200	0.87430200	10.64234800
H	1.48666400	3.02885200	8.09408200
H	2.33968900	1.52452100	8.37516300
H	4.51348000	3.02926400	8.38273600
H	3.81994900	2.48186700	6.86246400
H	1.93300100	7.74154200	12.26734900
H	1.71861600	8.07130300	14.75207700
H	3.36475000	9.59667200	15.89394200
H	5.11150200	10.71387100	14.50693600
H	5.91591100	11.31230000	12.40201700
H	6.34901600	9.77909600	11.71326400
H	5.79662300	11.77664000	10.14322500
H	4.11266000	11.57554400	10.64271600
H	-1.43516800	12.08872600	8.40632400
H	0.83571100	12.92070100	7.80531000
H	3.14089400	12.22066800	7.26324100
H	5.24999400	11.35450600	7.76140700
H	3.95135100	6.92543700	6.87693800
H	-1.63719100	9.83588100	9.51336500
H	0.47910400	8.53317300	9.93949500
H	3.43185400	12.55300100	8.93640000
H	4.16671900	10.00800700	7.39115500

5 (open-shell triplet)

Cu	2.21263400	5.87128700	8.80131300

Cu	3.25839700	8.38929800	10.24460200
O	3.55505800	7.94060000	8.27695100
O	1.91189200	7.08833300	10.23300400
N	2.91881400	5.10092000	6.87931500
N	0.16339200	5.81286300	8.31720100
N	3.30913700	4.51838400	10.00726100
N	4.94949900	9.78666300	9.97712700
N	2.82375500	8.95017300	12.15757400
N	2.29418900	10.01481700	7.57050200
C	3.51829000	6.20658500	6.03903200
C	4.79314400	6.82373200	6.57187500
C	6.01386800	6.58209500	5.93154900
C	7.19730600	7.13323100	6.41818700
C	7.17217900	7.90461300	7.57532000
C	5.97327100	8.16252100	8.25420600
C	4.78599800	7.65520900	7.70620700
C	6.06710000	8.86442700	9.59850000
C	-0.63722900	5.97074700	9.39084800
C	-2.01534200	5.80269100	9.32541700
C	-2.58646400	5.46228900	8.10085100
C	-1.75931100	5.31076400	6.99028400
C	-0.38010500	5.49461400	7.12401600
C	0.53198800	5.37782400	5.92403100
C	1.78004300	4.50275300	6.10995500
C	3.43762200	4.84132200	11.31125200
C	4.14296900	4.05191400	12.21011200
C	4.73835300	2.88062600	11.74597300
C	4.58010900	2.53375300	10.40665600

C	3.84750400	3.36464100	9.55539800
C	3.60065900	2.96267800	8.11945300
C	3.94944000	4.03031800	7.07232100
C	1.53883900	8.81275000	12.53993800
C	1.09069600	9.22903100	13.78820400
C	2.01005700	9.79689200	14.67108000
C	3.34104800	9.92135100	14.27656600
C	3.72774400	9.48778300	13.00625900
C	5.15544400	9.59855500	12.53002800
C	5.31614200	10.45752000	11.26409600
C	1.27003300	9.68931800	6.75572600
C	0.30487100	10.59843300	6.35710600
C	0.40157900	11.90581900	6.83709800
C	1.45373700	12.23896600	7.68295500
C	2.39711800	11.27184600	8.04766700
C	3.53034000	11.67221800	8.97552300
C	4.82125000	10.84154400	8.92118400
H	2.74994000	6.97404700	5.92577400
H	3.71970100	5.80011500	5.03670200
H	6.03562600	5.95491300	5.04381300
H	8.13652400	6.95080500	5.90609300
H	8.10209900	8.30953000	7.96780500
H	6.13964300	8.10394600	10.38615200
H	7.01468000	9.42394900	9.62588400
H	-0.12304300	6.25056600	10.30440000
H	-2.62298400	5.93093700	10.21482000
H	-3.65914000	5.31646400	8.01157400
H	-2.17588800	5.05055900	6.02215600

H	0.80761800	6.38141200	5.57455700
H	-0.03922900	4.93736800	5.10010800
H	1.48216300	3.58222600	6.61721400
H	2.15441800	4.21286000	5.11676600
H	2.93042100	5.75788300	11.59314300
H	4.21288200	4.34791500	13.25122400
H	5.30634200	2.24030000	12.41406100
H	5.01302500	1.61794800	10.01820500
H	2.55953900	2.62977900	8.01737500
H	4.21086700	2.08105300	7.89990200
H	4.88433600	4.51551900	7.36019900
H	4.12485300	3.53907500	6.10289400
H	0.89717500	8.32968100	11.81015400
H	0.04824800	9.10509700	14.06075000
H	1.70035500	10.12996900	15.65722100
H	4.07902300	10.34920400	14.94788500
H	5.75778900	10.05769700	13.32124400
H	5.57635400	8.59605800	12.37814600
H	6.35656300	10.80456200	11.18914300
H	4.69194900	11.34822500	11.36965800
H	-0.32776000	12.65566300	6.54966400
H	1.55783800	13.24808300	8.06104100
H	3.78548900	12.70963000	8.73165900
H	5.68438400	11.51507100	9.01137600
H	3.07489200	8.89682100	7.91011100
H	-0.49619500	10.29313300	5.69164200
H	1.24186500	8.65349700	6.42980800
H	3.13834200	11.71047800	10.00138100

H	4.91342800	10.35840600	7.94703500

TS6 (open-shell singlet)

Cu	2.08723600	5.67157700	8.77610700
Cu	3.21753900	8.99454900	9.96700000
O	4.44874300	6.91851600	8.95671400
O	2.11315100	7.46730000	9.49524600
N	3.07588200	4.75470600	7.20495200
N	0.21433400	5.72387200	7.89043500
N	2.88555900	4.55775000	10.30545000
N	5.14615900	9.94082300	9.87486900
N	3.07704500	8.82161300	12.01143900
N	2.30001000	10.26287000	8.60247600
C	3.46118600	5.84326000	6.23652400
C	4.58842800	6.83699600	6.52843400
C	5.24397100	7.33748600	5.38984000
C	6.17129100	8.37346800	5.46448800
C	6.45844100	8.95058200	6.70118900
C	5.83485700	8.48067300	7.85979400
C	4.92283700	7.40498000	7.77555100
C	6.18225800	9.03203700	9.22252000
C	-0.71657500	6.35365500	8.64106000
C	-2.07465000	6.28597600	8.36272400
C	-2.48881500	5.53401600	7.26194500
C	-1.52769300	4.89915100	6.48006200
C	-0.17151500	5.01276300	6.80822000
C	0.87149600	4.40016300	5.89634200
C	2.13813600	3.80494100	6.52529900
C	2.55290600	4.97602200	11.54551800

C	2.98391200	4.32969600	12.69571700
C	3.81030500	3.21395400	12.55878100
C	4.16670300	2.79569700	11.28009500
C	3.68621700	3.47959500	10.15741000
C	4.03362800	2.97259700	8.77257300
C	4.28692700	4.02136000	7.68253900
C	1.82403800	8.65829200	12.48393700
C	1.53188800	8.67007300	13.84217400
C	2.58138200	8.85247700	14.74474700
C	3.87593500	9.00946100	14.25345900
C	4.10204800	8.98962200	12.87352200
C	5.48671700	9.14429200	12.29556900
C	5.62710300	10.26907500	11.25518900
C	1.26896500	9.78687500	7.87795200
C	0.51658700	10.59876600	7.03725700
C	0.84204800	11.95195400	6.94775000
C	1.91113500	12.43934200	7.69769100
C	2.63010100	11.57115900	8.52224100
C	3.81070100	12.04794200	9.33352400
C	5.07717100	11.21306100	9.08777100
H	2.54813800	6.42168000	6.05966100
H	3.70841100	5.35212300	5.28430300
H	5.01670000	6.90612900	4.41775000
H	6.66773500	8.72415900	4.56569500
H	7.18642600	9.75551500	6.76761400
H	6.35024700	8.20267100	9.90964000
H	7.11254000	9.61240100	9.15689900
H	-0.32229600	6.92999600	9.47116700

H	-2.78661200	6.80417200	8.99607400
H	-3.54232900	5.44583100	7.01423300
H	-1.81969600	4.31833100	5.61095300
H	1.13370700	5.13562800	5.12541400
H	0.39784300	3.57785700	5.34933900
H	1.84186900	3.05234900	7.25922000
H	2.69137500	3.28583000	5.72833500
H	1.93466100	5.86467100	11.58566200
H	2.67986100	4.69601400	13.67025500
H	4.17462000	2.68052400	13.43157300
H	4.81234400	1.93442200	11.14207800
H	3.26941200	2.25000800	8.45850200
H	4.95424900	2.38545500	8.85528800
H	4.98658700	4.76858000	8.05535600
H	4.74887300	3.52051400	6.81917900
H	1.05756800	8.50609000	11.73169600
H	0.50840800	8.54649200	14.17967700
H	2.39476500	8.87390600	15.81428500
H	4.71188600	9.14944500	14.93104400
H	6.18300900	9.36320500	13.11089800
H	5.80896300	8.18467700	11.87292900
H	6.68539300	10.55685300	11.18634900
H	5.08041100	11.14969300	11.60395600
H	0.27647400	12.61841700	6.30344900
H	2.19207600	13.48625800	7.64778000
H	4.02670800	13.08620400	9.06436500
H	5.96854600	11.81214000	9.32040200
H	3.40123800	7.14767300	9.13781400

H	-0.30683300	10.17773500	6.47024500
H	1.07567100	8.72905100	8.01947900
H	3.55214800	12.06323900	10.40113200
H	5.12972900	10.94847900	8.02981700

TS5 (open-shell singlet)

Cu	2.26529200	6.04293300	8.60339100
Cu	3.09668800	8.68738600	9.95753800
O	3.65494500	7.64971100	8.17453800
O	1.82027900	7.30202300	9.93758500
N	3.07869000	4.98860600	6.81894200
N	0.23582100	5.68992700	8.13806800
N	3.16957300	4.61075500	10.00522900
N	4.97640800	9.80639900	9.79629900
N	2.83491700	8.97400900	12.01014600
N	1.97275200	10.23807000	8.79744100
C	3.77846700	5.94180000	5.89015400
C	5.01848900	6.62333600	6.42128900
C	6.25040700	6.50481600	5.78848800
C	7.36673300	7.20312100	6.26457600
C	7.27839000	8.01425200	7.40292200
C	6.07942400	8.15764200	8.09552700
C	4.91158100	7.53724100	7.53066100
C	6.07562200	8.84814000	9.44478500
C	-0.60844900	5.78244300	9.18439300
C	-1.96386400	5.48889400	9.07814900
C	-2.46437500	5.09157100	7.83867100
C	-1.59170200	5.00982900	6.75426100
C	-0.24024300	5.31690000	6.93228400
C	0.73680000	5.25673800	5.78201100
C	1.96305100	4.36344300	6.03595400
C	3.16338800	5.01731500	11.29017000
C	3.65042000	4.23047200	12.32909100
C	4.16937500	2.97219600	12.02595000
C	4.16925700	2.54921500	10.69829000
C	3.65308200	3.38823200	9.70542100
C	3.58076000	2.91817200	8.27045400
C	4.05484800	3.91945400	7.20798100
C	1.57023500	8.81301100	12.44865800
C	1.20154100	9.05931800	13.76655600
C	2.18124100	9.47948100	14.66559600

C	3.49124400	9.63043700	14.21298800
C	3.79336800	9.36894300	12.87405100
C	5.20216700	9.50195800	12.34700700
C	5.33756800	10.41629000	11.11835800
C	0.73711100	9.84136900	8.43823600
C	-0.12256700	10.64134200	7.69131600
C	0.32307800	11.90069400	7.28971900
C	1.60451600	12.30910800	7.65554700
C	2.40737800	11.45602100	8.42068100
C	3.77510900	11.90957300	8.88718600
C	4.92608400	10.89697100	8.76853800
H	3.05002200	6.70575500	5.60103000
H	4.05537800	5.39892100	4.97503600
H	6.34909600	5.86205200	4.91839800
H	8.31844700	7.10549800	5.75164100
H	8.17119000	8.51128100	7.77179900
H	6.05870000	8.05419100	10.20114600
H	7.04113800	9.36437500	9.55196700
H	-0.15561000	6.12692100	10.10759700
H	-2.60667400	5.57101900	9.94809900
H	-3.51609900	4.85109600	7.71531900
H	-1.95187100	4.71189200	5.77476600
H	1.03965000	6.27594100	5.50877900
H	0.21993600	4.85756000	4.90379400
H	1.63404000	3.47281900	6.57294800
H	2.36763300	4.02168100	5.07144800
H	2.72793100	6.00135400	11.43825400
H	3.61530000	4.59566100	13.35029100
H	4.56208600	2.32777100	12.80690300
H	4.55699100	1.57168900	10.42927900
H	2.55894300	2.57692100	8.06222300
H	4.20672300	2.02586600	8.16748100
H	4.95785700	4.41736200	7.57158200
H	4.33502000	3.36334100	6.29966100
H	0.86958300	8.45146000	11.70485800
H	0.17082000	8.92253400	14.07562700
H	1.93263000	9.68411000	15.70262700
H	4.27812300	9.94703100	14.89009200
H	5.83132300	9.92738500	13.13505100
H	5.61418100	8.50395700	12.14936800
H	6.37167400	10.78727500	11.05628200
H	4.69637400	11.28518700	11.26929900

H	-0.31432800	12.55574300	6.70320800
H	1.97901800	13.28423700	7.35979400
H	4.06994000	12.78079200	8.29250500
H	5.87875900	11.44749400	8.80789000
H	4.20822200	8.40272500	7.10308500
H	-1.11494400	10.28526400	7.43479000
H	0.46781300	8.84581500	8.78114200
H	3.69067600	12.28471600	9.91474200
H	4.88000800	10.42546100	7.78289200

1^{D1} (open-shell triplet)

Cu	3.81584600	8.12187900	10.69502300
O	3.86986800	6.41874200	9.62032600
O	2.69329700	6.45446600	10.36836000
N	2.61590900	6.30261600	6.40957100
N	0.40130900	5.50462700	8.35626800
N	5.44928900	9.27786300	10.45961300
N	2.91796600	9.26845700	12.08023100
C	3.85143300	6.66857100	5.72307000
C	5.01870100	6.91438500	6.64317100
C	6.03709400	5.96366400	6.77393600
C	7.10226000	6.18832600	7.64802500
C	7.14136400	7.35157100	8.41602100
C	6.12681100	8.31092800	8.29823000
C	5.08476100	8.09722100	7.39082700
C	6.13117900	9.52970200	9.19022700
C	-0.02500200	4.81305500	9.43663000
C	-1.24558300	4.15207600	9.46008100
C	-2.05171300	4.20595500	8.32301200
C	-1.60802700	4.91788900	7.20875800
C	-0.37192000	5.56499700	7.24473600
C	0.13347500	6.36450500	6.06620000
C	1.51668500	5.95142500	5.52415200
C	1.57352200	9.38870000	12.12497100
C	0.93014000	10.21591100	13.03479200
C	1.70835300	10.94766200	13.93216600
C	3.09599600	10.81928400	13.88800200
C	3.68581500	9.96801900	12.95233200
C	5.18342200	9.76607800	12.89570900
C	5.84350000	10.13545500	11.55906500
H	3.62576600	7.56551800	5.12052500
H	4.08063700	5.87865500	4.99072200

H	6.00806100	5.05131100	6.18460100
H	7.89760300	5.45520100	7.73274300
H	7.96928600	7.51677800	9.10003700
H	7.15362900	9.87764300	9.38755300
H	5.60758900	10.37254500	8.70721700
H	0.64250800	4.79833100	10.29230700
H	-1.54896600	3.60769100	10.34716300
H	-3.01162800	3.69967700	8.30138100
H	-2.21615200	4.97506500	6.31249300
H	0.15627300	7.43144800	6.32410100
H	-0.57932900	6.26684300	5.24334500
H	1.55307000	4.85786100	5.38421600
H	1.66954100	6.39926100	4.53450900
H	1.01190500	8.79374800	11.41244200
H	-0.15203400	10.27958600	13.03881300
H	1.24255600	11.60512200	14.65941400
H	3.72380400	11.36862200	14.58113500
H	5.65249600	10.36752100	13.67841700
H	5.42007300	8.72003700	13.13225400
H	6.93761200	10.08673400	11.66710900
H	5.62012800	11.18090600	11.28383000
H	4.31986400	8.86184600	7.25931700

$TS1^{D1}$ (open-shell singlet)

Cu	2.07092600	6.77248800	8.19253500
Cu	3.55550000	8.57126600	10.37197300
O	3.62451600	7.72604400	8.68919300
O	2.06324900	7.54239500	9.90769100
N	2.56734100	6.34182800	6.29183400
N	0.37872700	5.72786500	8.21823200
N	5.32820500	9.50577100	10.33201900
N	2.93099400	9.38291100	12.07998900
C	3.87787900	6.56558400	5.68984600
C	4.98374800	6.82013600	6.69028900
C	5.91455800	5.83371700	6.98856300
C	6.93179800	6.07637800	7.92389400
C	7.00435400	7.30018300	8.59855600
C	6.08454600	8.30752400	8.32303900
C	5.05771700	8.07417700	7.36461800
C	6.11091400	9.61022500	9.10100200
C	-0.01243000	5.20875000	9.40171600
C	-1.13121200	4.39400500	9.51441600
C	-1.86681400	4.10999400	8.36390800

C	-1.46061900	4.65395500	7.14526800
C	-0.32914300	5.46866100	7.09349300
C	0.12587900	6.11693900	5.80636400
C	1.57128600	5.80083500	5.38628200
C	1.59506100	9.49783600	12.24125600
C	1.03789800	10.13055100	13.34454200
C	1.89274600	10.66140500	14.30986500
C	3.27123200	10.53433900	14.14058600
C	3.77493500	9.88416900	13.01352800
C	5.25917700	9.68133000	12.81718500
C	5.83082800	10.20987300	11.49144300
H	3.76841700	7.42529700	5.00543800
H	4.12727100	5.70775200	5.04873600
H	5.87171300	4.87243100	6.48494600
H	7.66540100	5.30378800	8.13107400
H	7.79399700	7.46448900	9.32602900
H	7.14151500	9.90833800	9.32737800
H	5.66233900	10.42119200	8.50449600
H	0.59713400	5.47347300	10.25893600
H	-1.41431900	3.99529100	10.48195300
H	-2.74691400	3.47656500	8.41292000
H	-2.02043500	4.45627800	6.23755900
H	0.00902600	7.20578300	5.88408300
H	-0.53117800	5.79606400	4.99401500
H	1.72798800	4.70865400	5.34880500
H	1.75072800	6.17055200	4.36724800
H	0.98818100	9.05975100	11.45602400
H	-0.03960300	10.20300900	13.43865400
H	1.49426200	11.16480500	15.18499300
H	3.95781200	10.92996300	14.88111300
H	5.79567100	10.17910000	13.62888300
H	5.49574200	8.61251500	12.90172200
H	6.92777400	10.15750100	11.51301600
H	5.57951800	11.27852300	11.36309500
H	4.50842100	8.92084800	6.96524200

2^{D1} (open-shell singlet)

Cu	2.18515600	6.73531300	8.32841400
Cu	3.58545800	8.38062100	10.34066500
O	4.02580100	7.42078100	8.68004000
O	2.04205900	7.45157100	10.03017500
N	2.59121900	6.31685900	6.40887100
N	0.38655700	5.82389900	8.33243200

N	5.32308400	9.40317700	10.34446100
N	2.84253500	9.25177400	12.02514000
C	3.90477500	6.42256500	5.80249900
C	5.06750700	6.67183100	6.73326700
C	6.17462900	5.85742400	6.67793700
C	7.31247500	6.14150000	7.45579600
C	7.35922100	7.25850900	8.32299100
C	6.28221600	8.09564300	8.43556600
C	5.00781500	7.82737600	7.68966000
C	6.35245900	9.31198200	9.32725700
C	-0.03591300	5.29513200	9.49945000
C	-1.22022500	4.57472300	9.59438400
C	-1.98926300	4.40119300	8.44443500
C	-1.55197200	4.96024500	7.24342800
C	-0.35479700	5.67618400	7.21024700
C	0.13633500	6.34380700	5.94631000
C	1.54193600	5.92511900	5.48496400
C	1.50535600	9.17526800	12.19292300
C	0.86454200	9.74228400	13.28749000
C	1.63090600	10.41066400	14.23980200
C	3.01118300	10.48749200	14.06071100
C	3.60214300	9.89642300	12.94308400
C	5.09857500	9.94914800	12.74954800
C	5.55663900	10.41684700	11.35536600
H	3.86473300	7.25682100	5.07500000
H	4.09705100	5.52360100	5.19829400
H	6.18914300	4.99376300	6.01976400
H	8.17454900	5.48373600	7.39409000
H	8.26311500	7.43995300	8.89695300
H	7.34129100	9.37095800	9.80251600
H	6.27580300	10.22273700	8.69973100
H	0.60217400	5.48087000	10.35620900
H	-1.52700800	4.16295000	10.54915700
H	-2.91948000	3.84300100	8.48003900
H	-2.13722700	4.85054700	6.33677700
H	0.11628500	7.43353300	6.07825100
H	-0.55684900	6.12009300	5.13127400
H	1.59590500	4.82686700	5.38476300
H	1.74108700	6.33431200	4.48474600
H	0.97861600	8.63072700	11.41679600
H	-0.21209300	9.65812200	13.38250600
H	1.16549000	10.86701500	15.10776500

H	3.63529500	10.99947500	14.78523400
H	5.52420900	10.63926500	13.48253800
H	5.54062800	8.96646500	12.95874500
H	6.61543600	10.70045000	11.38561300
H	4.98879000	11.31597900	11.06217100
H	4.66450500	8.74220900	7.17659300