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Supporting information for

^{13}C pNMR shifts of MOFs based on Cu(II)-paddlewheel dimers - DFT predictions for spin-½ defects

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Thermodynamics of proton defects

To assess the thermodynamic accessibility of the proton defect, we use the following reaction between the activated (L = vacant) or hydrated (L = H_2O) non-defective paddlewheel reacting and a benzoic acid dimer to form the $Cu(H)_2$ defect (**1a**), activated and hydrated respectively:

$$L_2Cu_2(O_2CPh)_4 + 2(PhCO_2H)_2 \rightarrow 2LCu(O_2CPh)_2(PhCO_2H)_2 \quad \text{Eq 1}$$

where L = none or water. The electronic energy indicates that formation of this kind of defect could be viable, with ΔE = 5.2 and –1.2 kcal/mol at the CAM-B3LYP-D3/PCM(water)//xTB and CAM-B3LYP-D3/PCM(water)//PBE0-D3 level, respectively, for the hydrated species (L = H_2O in eq 1; for activated and other solvent models see Table S4). Due to the entropic penalty arising from the change in particle numbers, computed free energies are notably endergonic, *e.g.,* ΔG = +14.0 kcal/mol at CAM-B3LYP-D3/PCM(water)//PBE0-D3 (hydrated model, see Table S4). Clearly, the paddlewheel dimer is favoured thermodynamically, in agreement with the frequent observation of this motif in Cu(II) carboxylate structures in general. If defect formation is reversible (*i.e.,* under thermodynamic control) during MOF synthesis, a free energy difference on the order of $\Delta G \approx 1$ kcal/mol between the non-defective dimer and the defective dimer would be inferred from a 10% occurrence of the latter. In that case, the protonated model discussed so far (**1a**) would not be a promising candidate because its formation is computed to be too endergonic (according to eq 1 - even when allowing for the usual overestimation of entropic contributions due to change in particle numbers from the standard thermodynamic correction expressions). Note, however, that there is an expected gain of entropy due to static disorder of the defect sites in the periodic crystal, which is not accounted for in these molecular models. It is also possible that MOF formation is kinetically controlled, and/or that the driving force for forming the extended network outweighs the energy penalty for formation of individual defects. In that case motifs such as **1a** could well be formed and incorporated into the bulk material. Deeper analysis of such thermodynamic and kinetic factors is beyond the scope of the present study, however.

Model 1b

As discussed in the main text, the coordination geometry proposed for model **1a** is not the only possible for such defect. We propose an alternative coordination environment (see Figure S1) where the Cu lies inside the cube formed by the eight oxygen atoms and the protons reside above and below the metal centre.

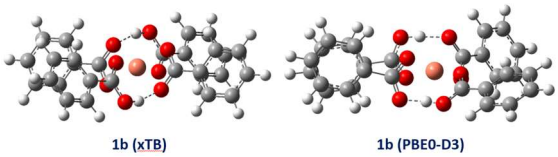

Figure S1. Molecular models representing an alternative coordination environment for the $Cu(H)_2$ defect.

In terms of magnetic properties **1b** shows a strong dependence on the optimisation method used. Although, both PBE0-D3 and xTB optimisation afford true minima in the potential energy surface, the resulting structures are different when it comes to the phenyl ring stacking. PBE0-D3 predicts a stronger pi stacking interaction resulting in a closer, parallel orientation of the aromatic rings, whereas in the xTB minimum energy structure the rings are oriented more perpendicular to each other. Such an arrangement is possible due to the hydrogen bonding interaction between the carboxylate and the carboxylic acid moieties. It is likely that the predicted structural difference arises from the dispersion corrections. The PBE0-D3 minimum of **1b** affords a computed pNMR spectrum closely related to that of the PBE0-D3 minimum **1a**, whereas the xTB minimum for **1a** shows a completely altered pNMR spectrum, where the shieldings of C1 and C3 are reversed, that is, C1 is the most deshielded resonance in **1a**, but much more shielded in **1b**, compared to the PBE0-D3 structure (see Table S1).

Table S1. ^{13}C and ^{1}H chemical shifts of the $Cu(H)_2$ defect model **1b** (in ppm).

Site	1b (PBE0)	1b (xTB)
C1	633	60
C2	–86	–122
C3	193	284
H	14.6	12.1

The abovementioned spectral change is reflected in the electron spin density. The xTB optimised structure of **1b** shows no delocalisation onto the phenyl groups bearing the carboxylic acid or on C1. In contrast, the PBE0-D3 structure does show spin delocalisation over all the aromatic rings and on C2, which explains why the predicted pNMR properties are significantly different.

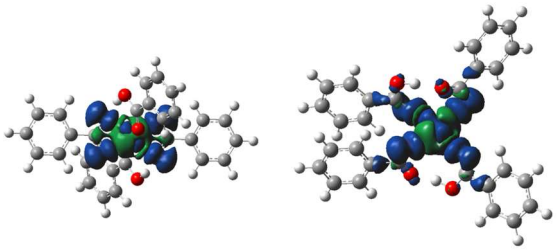

Figure S2. Spin density for the model **1b** optimised at the xTB (left) and DFT (right) level.

However, it is surprising how the sign of the spin density on C1 is the same for xTB and PBE0-D3 structures and yet the pNMR shift is more shielded for one and less shielded for the other. Based on this, spin density cannot be the sole reason for the differences in the spectra. A closer look to the paramagnetic shielding reveals how the sign of the hyperfine tensor is opposed for the models and it is intimately connected to the degree of shielding (see Table S6).

Looking at the relative energies (CAM-B3LYP-D3 single points), using the PBE0-D3 optimised structures, **1a** and **1b** are almost degenerate, whereas for the xTB structures **1b** is predicted to be disfavoured by *ca*. 8 kcal/mol (see Table S5). Note, however, that **1b** does not have a free coordination site, so that formation from a hydrated dimer would be entropically favoured due to the release of water:

$$L_2Cu_2(O_2CPh)_4 + 2(PhCO_2H)_2 \rightarrow 2\ \mathbf{1b} + 2\ L\ \ (L = H_2O) \qquad \text{Eq 2}$$

However, the distortions imposed to mimic a good fit into the MOF framework serve to disfavour **1b** significantly (by up to ca. 50 kcal/mol at the PBE0-D3 level with respect to the fully optimised structure, see Table S8). Therefore, this model does not seem to be a viable candidate for the defects.

Tables

Table S2. ^{13}C and ^{1}H chemical shifts of the $Cu(H)_2$ defect (in ppm).

Site	Model	PBE0-D3	xTB	Exp	Pristine[a]
C1 (avg)	Activated (**1a**)	646	548	786	778
C2 (avg)	Activated (**1a**)	−28	−23	−86	−110
C3 (avg)	Activated (**1a**)	148	155	228	186
C3' (avg)	Activated (**1a**)	208	206		
H (avg)	Activated (**1a**)	13.3	10.4	-	-
C1 (avg)	Activated (**1b**)	633	60	786	778
C2 (avg)	Activated (**1b**)	−86	−122	−86	−110
C3 (avg)	Activated (**1b**)	193	284	228	186
H (avg)	Activated (**1b**)	14.6	12.1	-	-
C1 (avg)	Hydrated (**1a**)	564	549	853	842
C2 (avg)	Hydrated (**1a**)	−16	−40	−50	−85
C3 (avg)	Hydrated (**1a**)	147	148	228	181
C3' (avg)	Hydrated (**1a**)	208	215		
H (avg)	Hydrated (**1a**)	13.3	10.9	-	-

[a]CAM-B3LYP/IGLO-II level, using the Boltzmann equilibrium between S = 0 and 1, with singlet-triplet gap fitted to match the experimental NMR data obtained at T = 298 K.

Table S3. Predicted temperature dependence of the three δ (^{13}C) and δ(^{1}H) resonances in the activated and hydrated Cu(H)$_2$, using xTB and PBE0-D3 geometries.

Site	250 K	270 K	290 K	310 K	330 K	350 K	Model	Method
C1 (avg)	743	698	660	626	597	571	Activated (**1a**)	PBE0-D3
C2 (avg)	-69	-50	-34	-19	-6	5	Activated (**1a**)	PBE0-D3
C3 (avg)	148	148	148	147	147	147	Activated (**1a**)	PBE0-D3
C3′ (avg)	221	215	210	206	202	199	Activated (**1a**)	PBE0-D3
H (avg)	12.4	12.8	13.2	13.5	13.8	14.0	Activated (**1a**)	PBE0-D3
C1 (avg)	727	684	646	614	585	560	Activated (**1b**)	PBE0-D3
C2 (avg)	−139	−115	−94	−76	−60	−45	Activated (**1b**)	PBE0-D3
C3 (avg)	203	198	194	191	188	186	Activated (**1b**)	PBE0-D3
H (avg)	14.1	14.4	14.5	14.7	14.8	15.0	Activated (**1b**)	PBE0-D3
C1 (avg)	626	590	559	532	509	488	Activated (**1a**)	xTB
C2 (avg)	-63	-45	-29	-15	-3	8	Activated (**1a**)	xTB
C3 (avg)	157	156	155	154	153	152	Activated (**1a**)	xTB
C3′ (avg)	219	213	208	204	200	197	Activated (**1a**)	xTB
H (avg)	9.2	9.8	10.2	10.7	11.0	11.3	Activated (**1a**)	xTB
C1 (avg)	44	51	57	63	67	71	Activated (**1b**)	xTB
C2 (avg)	−182	−154	−131	−111	−93	−77	Activated (**1b**)	xTB
C3 (avg)	311	298	288	278	270	262	Activated (**1b**)	xTB
H (avg)	12.2	12.1	12.1	12.0	12.0	12.0	Activated (**1b**)	xTB
C1 (avg)	644	607	575	547	523	501	Hydrated (**1a**)	PBE0-D3
C2 (avg)	-56	-38	-22	-8	3	14	Hydrated (**1a**)	PBE0-D3
C3 (avg)	148	147	147	147	146	146	Hydrated (**1a**)	PBE0-D3
C3′ (avg)	221	215	210	206	202	199	Hydrated (**1a**)	PBE0-D3
H (avg)	12.4	12.8	13.2	13.5	13.7	13.9	Hydrated (**1a**)	PBE0-D3
C1 (avg)	627	591	560	533	510	489	Hydrated (**1a**)	xTB
C2 (avg)	-83	-63	-46	-31	-18	-6	Hydrated (**1a**)	xTB
C3 (avg)	150	149	148	148	147	147	Hydrated (**1a**)	xTB
C3′ (avg)	229	223	217	212	208	204	Hydrated (**1a**)	xTB
H (avg)	9.8	10.3	10.8	11.2	11.5	11.8	Hydrated (**1a**)	xTB

Table S4. Electronic and Gibbs energy formation for the Cu(H)$_2$ defect in the gas phase, water, methanol and DCM.

$L_2Cu_2(O_2CPh)_4$ + $2(PhCO_2H)_2$ → $2L_2Cu_2(O_2CPh)_2(PhCO_2H)_2$

Model	Method	Solvent	ΔE (kcal/mol)	ΔG (kcal/mol)
Activated (**1a**)	xTB	Gas Phase	5.57	22.22
Activated (**1a**)	PBE0-D3	Gas Phase	−0.95	10.39
Activated (**1b**)	xTB	Gas Phase	21.90	37.43
Activated (**1b**)	PBE0-D3	Gas Phase	0.41	9.94
Hydrated	xTB	Gas Phase	4.35	20.12
Hydrated	PBE0-D3	Gas Phase	−2.99	12.39
Activated (**1a**)	xTB	Water	8.36	25.01
Activated (**1a**)	PBE0-D3	Water	−0.22	11.13
Hydrated	xTB	Water	5.18	20.94
Hydrated	PBE0-D3	Water	−1.43	13.95
Activated (**1a**)	xTB	Methanol	8.29	24.94
Activated (**1a**)	PBE0-D3	Methanol	−0.20	11.14
Hydrated	xTB	Methanol	5.20	20.97
Hydrated	PBE0-D3	Methanol	−1.44	13.94
Activated (**1a**)	xTB	DCM	7.97	24.62
Activated (**1a**)	PBE0-D3	DCM	−0.19	11.16
Hydrated	xTB	DCM	5.26	21.03
Hydrated	PBE0-D3	DCM	−1.56	13.82

Table S5. Relative energies between **1a** and **1b**.

Model	Method	ΔE (kcal/mol)[a]	ΔG (kcal/mol)[a]
Activated (**1a**)	PBE0-D3	0.00	0.00
Activated (**1b**)	PBE0-D3	0.68	–0.23
Activated (**1a**)	xTB	0.00	0.00
Activated (**1b**)	xTB	8.17	7.60

[a]The energies are calculated relative to the **1a** model

Table S6. Sign of the hyperfine coupling and relative chemical shift.

Atom[a]	Ax	Ay	Az	δ (ppm)
C3 (**1a**)	+	+	+	562
C17 (**1a**)	+	+	+	521
C35 (**1a**)	+	+	+	776
C46 (**1a**)	+	+	+	673
C3 (**1b**)	–	–	–	–17
C17 (**1b**)	–	+	–	137
C35 (**1b**)	–	+	–	136
C46 (**1b**)	–	–	–	–17

[a] C1 is averaged over the four C centres indicated.

Table S7. ^{13}C and ^{1}H chemical shifts of the $Cu(H)_2$ defect with and without constraints (in ppm), together with the deviation between the two.

xTB	**1a**	**1a** (constrained)	**1b**	**1b** (constrained)	**1a** H_2O	**1a** H_2O (constrained)
C1	548	862	60	740	549	840
C2	–23	–228	–122	–306	–40	–140
C3	155	153	284	155	148	145
C3’	206	225	-	-	215	221
H	10.4	11.0	12.1	15.7	10.9	12.9
PBE0-D3	**1a**	**1a** (constrained)	**1b**	**1b** (constrained)	**1a** H_2O	**1a** H_2O (constrained)
C1	646	882	633	708	564	853
C2	–28	–240	–86	–342	–16	–149
C3	148	158	193	141	147	153
C3’	208	229	-	-	208	227
H	13.3	10.3	14.6	11.2	13.3	12.2
	1a[a]	**1b**[a]	**1a** H_2O[a]	**1a**[b]	**1b**[b]	**1a** H_2O[b]
ΔC1	314	680	291	236	75	290
ΔC2	205	184	100	212	256	132
ΔC3	71	129	3	10	52	6
ΔC3’	53	-	6	21	-	18
ΔH	0.6	3.6	2.0	3.0	3.4	1.1
<ΔC>	161	331	100	120	128	112

[a]xTB optimised geometry. [b] PBE0-D3 optimised geometry.

Table S8. Relative energies between constrained and unconstrained models.

Model	Method	ΔE (kcal/mol)[a]
1a	xTB	0.00
1a (constrained)	xTB	7.03
1b	xTB	0.00
1b (constrained)	xTB	18.53
1a H_2O	xTB	0.00
1a H_2O (constrained)	xTB	10.14
1a	PBE0-D3	0.00
1a (constrained)	PBE0-D3	14.19
1b	PBE0-D3	0.00
1b (constrained)	PBE0-D3	50.51
1a H_2O	PBE0-D3	0.00
1a H_2O (constrained)	PBE0-D3	17.77

[a]The energies are calculated relative to the unconstrained model

Table S9. ^{13}C chemical shifts of the unconstrained Cu(I)Cu(II) defect (in ppm)

Site	Model	PBE0-D3	xTB	Exp	Pristine[a]
C1 (avg)	Activated	933	1605	786	778
C2 (avg)	Activated	–78	–235	–86	–110
C3 (avg)	Activated	180	46	228	186
C1 (avg)	Activated (TS)	1521	-	786	778
C2 (avg)	Activated (TS)	–265	-	–86	–110
C3 (avg)	Activated (TS)	47	-	228	186
C1 (avg)	Hydrated	944	1560	853	842
C2 (avg)	Hydrated	–15	–170	–50	–85
C3 (avg)	Hydrated	184	56	228	181

[a]CAM-B3LYP/IGLO-II level, using the Boltzmann equilibrium between S = 0 and 1, with singlet-triplet gap fitted to the experimental data obtained at T = 298 K.

Table S10. Predicted temperature dependence of the three $\delta(^{13}C)$ and δ (^{1}H) resonances in the activated and hydrated Cu(I)Cu(II) model, using xTB and PBE0-D3 geometries.

Site	250 K	270 K	290 K	310 K	330 K	350 K	Model	Method
C1 (avg)	1884	1756	1645	1548	1463	1388	Activated	xTB
C2 (avg)	–314	–278	–247	–219	–196	–174	Activated	xTB
C3 (avg)	28	36	44	50	55	60	Activated	xTB
C1 (avg)	1083	1014	955	903	857	817	Activated	PBE0-D3
C2 (avg)	–128	–105	–86	–68	–53	–40	Activated	PBE0-D3
C3 (avg)	188	184	181	179	177	175	Activated	PBE0-D3
C1 (avg)	1784	1663	1559	1468	1388	1317	Activated (TS)	PBE0-D3
C2 (avg)	–351	–311	–278	–248	–222	–199	Activated (TS)	PBE0-D3
C3 (avg)	29	37	45	51	56	61	Activated (TS)	PBE0-D3
C1 (avg)	1831	1707	1599	1506	1424	1351	Hydrated	xTB
C2 (avg)	–237	–206	–180	–157	–137	–119	Hydrated	xTB
C3 (avg)	40	47	54	59	64	69	Hydrated	xTB
C1 (avg)	1096	1026	965	913	866	826	Hydrated	PBE0-D3
C2 (avg)	–53	–36	–21	–8	4	14	Hydrated	PBE0-D3
C3 (avg)	193	189	186	183	180	178	Hydrated	PBE0-D3

Table S11. ^{13}C and ^{1}H chemical shifts of the Cu(I)Cu(II)defect with and without constraints (in ppm), together with the deviation between the two.

xTB	activated	activated (constrained)	hydrated	hydrated (constrained)
C1	1605	1785	1560	1767
C2	–235	–271	–170	–176
C3	46	18	56	44
PBE0-D3	activated	activated (constrained)	hydrated	hydrated (constrained)
C1	933	967	944	1001
C2	–78	–218	–15	–124
C3	180	129	184	150
	activated[a]	activated[b]	hydrated[a]	hydrated[b]
ΔC1	180	34	206	57
ΔC2	36	140	5	108
ΔC3	28	51	12	35
<ΔC>	81	75	75	67

[a]xTB optimised geometry. [b] PBE0-D3 optimised geometry.

Optimised coordinates (xyz in Å)

1a-activated (xTB opt)

Cu	-0.00000417172150	-0.00055367766139	-1.37430690771615
O	-1.62360899361001	0.91449407804167	-1.63304103936244
O	1.62359725476946	-0.91586387932759	-1.63214673222549
C	-2.24152374313177	1.09843179791649	-0.53967206328207
O	-1.16951159969282	-1.55913635411455	-0.73054663620236
O	1.16949134938070	1.55865580271755	-0.73206343609051
C	-1.51237104668139	-1.62398203944170	0.45957690324296
C	-2.93858654263345	-1.78534695589377	0.81030050866582
C	-3.34970549395064	-1.80408670807742	2.14095273372939
C	-4.69853447443481	-1.85046005905939	2.43821743685008
C	-5.63749017084030	-1.87750973408605	1.41854075666529
C	-5.23003064117884	-1.86523307237202	0.09364882091307
C	-3.88446136967947	-1.81912005266022	-0.21327222694285
O	1.70136768647009	-0.98069668530979	0.57583427838505
C	2.24150347405205	-1.09873352390145	-0.53859393423250
O	-1.70139759131211	0.98149496556815	0.57487597635224
O	0.68434575301303	1.57221861776049	1.45527852078151
C	1.51234673286241	1.62465498317571	0.45799880446586
O	-0.68437295278079	-1.57057833074047	1.45680856367376
H	-2.60792432875492	-1.76782957889032	2.92274008084108
H	-5.02162771851120	-1.85902545114807	3.46858213118664
H	-6.69051790446099	-1.90600559055000	1.65690913599386
H	-5.96326436275155	-1.88208650054095	-0.69843752435196
H	-3.54334937351653	-1.79727648041019	-1.23685576629108
H	-0.26002187337802	1.35229459464106	1.15657280718430
H	0.25999450630288	-1.35094421822224	1.15789208265989
C	3.69770626992886	-1.40180603016785	-0.61785723210520
C	4.42770234254455	-1.53956286839992	0.55793542217416
C	4.33790983917504	-1.48142863831354	-1.84965991231727
C	5.79203896383043	-1.74968912287593	0.50019737899597
H	3.91038637397600	-1.46901614890409	1.50253531925393
C	5.70254859990442	-1.69529084890119	-1.90055430666423
H	3.75351708655453	-1.36939718718528	-2.74987081681249
C	6.42976752928856	-1.82625556942945	-0.72783241252923
H	6.36062890968159	-1.85265012175231	1.41260828377475
H	6.20331247724663	-1.75746490983509	-2.85563922288380
H	7.49693774213279	-1.98919783120297	-0.77146442553611
C	2.93856097157924	1.78636389986262	0.80856715559714
C	3.88443654794387	1.81914194983028	-0.21503720202509
C	3.34967753529429	1.80640681937126	2.13920093927495
C	5.23000515909294	1.86556373960706	0.09184007969604
H	3.54332579489864	1.79629295685829	-1.23859932404343
C	4.69850593904241	1.85307886737375	2.43642161653499
H	2.60789536663977	1.77090987338685	2.92102226332992
C	5.63746254299646	1.87913752095893	1.41672003083285
H	5.96323975786094	1.88164433028891	-0.70026175774867
H	5.02159728491336	1.86265526305960	3.46677804984858
H	6.69048986419083	1.90787593653405	1.65506176917059
C	-3.69772972630753	1.40140995013712	-0.61924786306570
C	-4.33791377906615	1.47984978615890	-1.85113625474746
C	-4.42774758343703	1.54026663050842	0.55640146328005
C	-5.70255740624428	1.69362545762706	-1.90225592085382
H	-3.75350125814177	1.36698987398964	-2.75123131562466

C	-5.79208812571920	1.75030540775282	0.49844109470192
H	-3.91044711643391	1.47061602459329	1.50107664413310
C	-6.42979854446385	1.82568482569731	-0.72967096603086
H	-6.20330272130307	1.75490318732329	-2.85740913547640
H	-6.36069717882665	1.85410209144054	1.41074610083427
H	-7.49697252217115	1.98856158153515	-0.77347583502602

1a-activated (PBE0-D3 opt)

Cu	0.000044	-0.000774	-1.200289
O	-1.488773	1.158242	-1.498341
O	1.488718	-1.160294	-1.497202
C	-2.154590	1.382984	-0.428678
O	-1.331591	-1.421556	-0.755293
O	1.331899	1.419908	-0.755997
C	-1.604648	-1.768181	0.412030
C	-3.004016	-2.042767	0.787797
C	-3.325665	-2.538792	2.054415
C	-4.657746	-2.727896	2.399177
C	-5.666008	-2.409557	1.489711
C	-5.345371	-1.909913	0.229005
C	-4.014935	-1.733474	-0.126313
O	1.671932	-1.315095	0.726642
C	2.154652	-1.384148	-0.427441
O	-1.671763	1.314632	0.725387
O	0.728129	1.899939	1.356426
C	1.604698	1.768251	0.410844
O	-0.728220	-1.898890	1.357843
H	-2.529152	-2.762784	2.755970
H	-4.912830	-3.115431	3.381214
H	-6.707306	-2.547462	1.768372
H	-6.130665	-1.645155	-0.472482
H	-3.742718	-1.334252	-1.097073
H	-0.220304	1.655695	1.039220
H	0.220400	-1.655286	1.040431
C	3.605047	-1.679044	-0.585607
C	4.393288	-1.854887	0.553514
C	4.191298	-1.706870	-1.853191
C	5.762297	-2.054243	0.425841
H	3.914553	-1.812887	1.526205
C	5.560723	-1.910533	-1.978574
H	3.562426	-1.559629	-2.725173
C	6.346625	-2.081549	-0.839587
H	6.376704	-2.183684	1.312368
H	6.018017	-1.933308	-2.963879
H	7.417863	-2.236259	-0.939011
C	3.003908	2.043865	0.786402
C	4.015073	1.733450	-0.127061
C	3.325179	2.542055	2.052263
C	5.345386	1.910960	0.228173
H	3.743160	1.332551	-1.097214
C	4.657141	2.732214	2.396914
H	2.528481	2.766913	2.753329
C	5.665652	2.412778	1.488113
H	6.130887	1.645388	-0.472775
H	4.911936	3.121436	3.378357
H	6.706858	2.551529	1.766697

C	-3.604945	1.678000	-0.586931
C	-4.191377	1.704791	-1.854450
C	-4.392978	1.855030	0.552148
C	-5.560788	1.908571	-1.979812
H	-3.562672	1.556658	-2.726403
C	-5.761965	2.054541	0.424500
H	-3.914119	1.813795	1.524813
C	-6.346485	2.080783	-0.840865
H	-6.018224	1.930508	-2.965071
H	-6.376208	2.184925	1.311001
H	-7.417710	2.235592	-0.940266

1a-activated-constrained (xTB)

Cu	-0.25831280440607	-0.04573819531008	1.11021921372256
O	-0.19861591689553	1.98808477387496	0.99310455725062
O	-0.43034376685904	-1.97313425164900	1.13657016516687
C	0.21541373221422	2.59632828424867	0.00039736231033
O	1.56863974535496	-0.11890539537507	1.73973629855564
O	-2.16943322288098	0.17098729905364	0.44643838450398
C	2.40361261836505	-0.10302989235647	0.78549841807508
C	3.83828993603316	-0.23476436266142	1.17665727954214
C	4.84010460097682	-0.26714416212017	0.21205103950799
H	4.56116511113247	-0.22233559075095	-0.82988358403311
C	6.16499419499738	-0.35909956459837	0.59907337517005
H	6.94400652671330	-0.38741984645553	-0.14858857662922
C	6.49109386910211	-0.41344243854296	1.94468220961057
H	7.52649356650121	-0.48329401258160	2.24567877821425
C	5.49252821788012	-0.37850764978503	2.90570588726888
H	5.75211927857931	-0.42118647072687	3.95356833068955
C	4.16730259603354	-0.29033620450900	2.52631788634511
H	3.37522384754743	-0.26396586919438	3.25817330177139
O	-0.02398318397507	-1.85428620713464	-1.04252057464672
C	-0.22059112417891	-2.49882444834580	0.00224103098292
O	0.70671256129100	2.03929407300734	-1.05975834462743
O	-1.63781865483627	-0.06586048463817	-1.72053869791630
C	-2.46823490089611	0.15523668025327	-0.75270284624644
O	2.09428518968961	0.05622970765269	-0.40813750239539
C	-0.27771637211071	-3.99033891224094	-0.04123206863489
C	-0.60791515734148	-4.68957404921816	1.11417857715110
C	-0.04160163602574	-4.67542014286737	-1.22855984145804
C	-0.69971659240874	-6.06743066493182	1.07879944826926
H	-0.78734448305799	-4.13885863100468	2.02425722800589
C	-0.13228728568076	-6.05538843101465	-1.25597422963575
H	0.21278709395991	-4.11156668364234	-2.11328362246087
C	-0.46223407828083	-6.75078305656866	-0.10377172894623
H	-0.95663098124314	-6.61425641862563	1.97443946553919
H	0.05338791077921	-6.58942062653899	-2.17631545471497
H	-0.53456904909978	-7.82863124954238	-0.12718001969624
C	-3.88149855496269	0.32407399292569	-1.16423004180546
C	-4.88372613233716	0.39743739998779	-0.19807188852807
C	-4.21453188622159	0.32484757472624	-2.51677629673653
C	-6.20825234901316	0.47211006466629	-0.58553332127601
H	-4.60298006208362	0.38733012957867	0.84378621451806
C	-5.54092932872273	0.40558156081378	-2.89444924953763
H	-3.43039447429486	0.26059784727981	-3.25431110305418
C	-6.53700296225463	0.47719079225592	-1.93247793017387

H	-6.98606812167836	0.52407949808788	0.16129976900288
H	-5.80264055442414	0.40762490409026	-3.94198166010755
H	-7.57267818698485	0.53390239564685	-2.23347033856933
C	0.24171327851213	4.07783739036772	-0.00182779106042
C	-0.09553084894337	4.78255967350903	1.15275281243570
C	0.68385747394368	4.76103144706146	-1.13228453282717
C	0.00909458712811	6.16056184969329	1.17272121138962
H	-0.42807286458423	4.23192024448426	2.01914685635843
C	0.77974441407061	6.13886639880418	-1.10461611291321
H	0.94798785263230	4.20414046145425	-2.01715790285106
C	0.44549408243943	6.83863729839252	0.04487014627060
H	-0.24696281887372	6.70746843884199	2.06757551026869
H	1.12096108912523	6.67184179234558	-1.97945188360078
H	0.52831158960413	7.91532441180643	0.06261972868799
H	-0.81089232294593	-0.63844620419448	-1.44474952021990
H	1.11394429207031	1.09637635367139	-0.89266127968819

1a-activated-constrained (PBE0-D3 opt)

O	-1.513225	1.294509	1.256272
O	1.466668	-1.211710	1.178615
C	-1.791364	1.793843	0.090056
O	1.513518	1.292794	1.268582
O	-1.471388	-1.207871	1.189977
C	1.782275	1.802108	0.104328
C	2.832057	2.854139	0.101276
C	3.325006	3.344338	-1.110314
H	2.927999	2.948818	-2.039936
C	4.306339	4.327988	-1.111257
H	4.692142	4.706050	-2.053645
C	4.797043	4.823771	0.095379
H	5.564819	5.592891	0.092860
C	4.306067	4.335497	1.304962
H	4.689464	4.721690	2.245023
C	3.324742	3.351842	1.309915
H	2.935972	2.957903	2.242893
Cu	-0.000171	-0.093940	-0.994180
O	1.354080	-1.437778	-1.049876
C	1.790649	-1.771327	0.104216
O	-1.334412	1.364557	-0.985554
O	-1.338511	-1.455874	-1.035424
C	-1.782740	-1.780055	0.118299
O	1.319187	1.380648	-0.971572
C	2.843085	-2.820703	0.107242
C	3.336967	-3.309989	1.318822
C	3.337480	-3.316676	-1.101410
C	4.320978	-4.290962	1.319741
H	2.936596	-2.908019	2.244320
C	4.321511	-4.297622	-1.096480
H	2.935006	-2.929806	-2.031350
C	4.813456	-4.784948	0.113091
H	4.704487	-4.674259	2.261550
H	4.707364	-4.684123	-2.036023
H	5.582331	-5.553434	0.115651
C	-2.831643	-2.832953	0.123518
C	-3.323918	-3.321554	1.336032
C	-3.324188	-3.333060	-1.084180

C	-4.304442	-4.306015	1.338812
H	-2.925323	-2.916180	2.260810
C	-4.304721	-4.317485	-1.077391
H	-2.922785	-2.946816	-2.014845
C	-4.795023	-4.804172	0.133105
H	-4.686622	-4.688847	2.281350
H	-4.689210	-4.707110	-2.016203
H	-5.561145	-5.575396	0.137126
C	-2.843473	2.843541	0.084853
C	-3.337268	3.342399	1.292558
C	-3.337651	3.330241	-1.127650
C	-4.320981	4.323648	1.285786
H	-2.947342	2.951168	2.226189
C	-4.321380	4.311500	-1.130415
H	-2.939846	2.933835	-2.056555
C	-4.813243	4.808376	0.075298
H	-4.705326	4.710644	2.225129
H	-4.708067	4.686918	-2.073496
H	-5.582900	5.575607	0.071350
H	1.306519	0.267643	1.217731
H	-1.310221	0.266623	1.213962

1a-hydrated (xTB opt)

Cu	-0.09117812894022	-0.11310915276338	-1.55527549574730
O	-1.74113539058108	0.81894413989608	-1.66904424466429
O	1.60484660834431	-1.03974714585944	-1.64324211530959
C	-2.32119826586743	1.04300268184022	-0.56791236585275
O	-1.20840272714553	-1.60278243430674	-0.68988121913669
O	1.15157554537010	1.51783567357894	-0.85710525390363
C	-1.54215051939900	-1.59470474682832	0.50397010923460
C	-2.96685317434429	-1.73266988083959	0.87467527561733
C	-3.37141578995674	-1.63386857910505	2.20343521563534
C	-4.71840643051975	-1.66208938257331	2.51114198721419
C	-5.66194695392385	-1.78934593300164	1.50352612931441
C	-5.26083242670895	-1.89509684150142	0.18100634738996
C	-3.91717761815380	-1.86519327264878	-0.13633111278152
O	1.68263330217746	-1.04875118753243	0.57541659980489
C	2.21002818942467	-1.18329173063990	-0.53840379754876
O	-1.76196031079075	1.01294652026964	0.54172234244946
O	0.65165620497246	1.54136152834343	1.32320164992871
C	1.48607330007081	1.57632315154902	0.33303085211641
O	-0.70600668987042	-1.48885423618279	1.48878630891335
H	-2.62588540229256	-1.52022298807080	2.97415159736829
H	-5.03660723373062	-1.57805399101299	3.53969879946857
H	-6.71364698071881	-1.80342080705068	1.74915743522586
H	-5.99783549912834	-1.98987830648738	-0.60209030130290
H	-3.58080401382999	-1.93222335321715	-1.15958771607556
H	-0.30280733008711	1.33865540576586	1.02431631683836
H	0.24070093012660	-1.30542830881511	1.16254945730759
C	3.67804543980730	-1.46719654924182	-0.60921746751870
C	4.40610106875502	-1.54895695018861	0.57250597404066
C	4.32538554642649	-1.59296505003809	-1.83273727224126
C	5.77330398804996	-1.74301218771056	0.52874603218305
H	3.88386333797815	-1.44861877608896	1.51154391416108
C	5.69312215154578	-1.78975104835309	-1.87112880291823
H	3.74647752747350	-1.53868985629504	-2.74234811663620

C	6.41798345025184	-1.86007788506553	-0.69216263430600
H	6.33850525482423	-1.80193095472402	1.44710764488817
H	6.19715426958428	-1.88754147478218	-2.82163035204424
H	7.48741334068782	-2.00953979706185	-0.72575223911374
C	2.91369209009420	1.70821302140348	0.70436969319279
C	3.87607726000941	1.76846072362232	-0.30109906251887
C	3.30649337270132	1.68378126813899	2.03977162313583
C	5.21734372191974	1.80188006425212	0.02555451752892
H	3.55428632152307	1.78022431588270	-1.33131194191296
C	4.65080461125254	1.71682301836710	2.35905282312443
H	2.55249005242897	1.62490509578547	2.80832502264691
C	5.60538921717365	1.77305969479093	1.35566403966022
H	5.96218563367708	1.84110470596440	-0.75505768583980
H	4.95800059749366	1.69226656292007	3.39404059108030
H	6.65489520212103	1.79178814254157	1.60988595137101
C	-3.79333234142141	1.30111835827117	-0.62382133064305
C	-4.47682495710299	1.22654460725055	-1.83190730604069
C	-4.48582696954322	1.54858690550312	0.55589013725636
C	-5.84875976822596	1.39386347443922	-1.85461394120606
H	-3.91917141691301	1.03117947988618	-2.73493784436698
C	-5.85753461132842	1.71256894835278	0.52669562427634
H	-3.93466039319028	1.59779549191152	1.48249948097526
C	-6.53935037289621	1.63332798367719	-0.67703382831853
H	-6.38368646080473	1.33468242232343	-2.79129912294003
H	-6.39742984140551	1.90044236295657	1.44311359286602
H	-7.61228163001264	1.75935420967403	-0.69779322761353
O	0.60230468971765	0.65227806781574	-3.53319731293916
H	1.40503777037953	0.11786712318837	-3.50002446611705
H	0.82819753864303	1.53072307317372	-3.20615609714245

1a-hydrated (PBE0-D3 opt)

Cu	-0.083321	1.050777	-0.989948
O	-1.704649	1.838691	-0.296527
O	1.575389	0.538579	-1.783658
C	-2.353192	1.164378	0.586802
O	-1.172259	-0.525067	-1.519366
O	1.184991	1.432907	0.925928
C	-1.397113	-1.557550	-0.853170
C	-2.769241	-2.092282	-0.765741
C	-3.033413	-3.278091	-0.075039
C	-4.342824	-3.725047	0.046753
C	-5.386845	-2.987540	-0.510920
C	-5.123540	-1.804907	-1.199086
C	-3.815278	-1.359392	-1.332157
O	1.833602	-1.289792	-0.498136
C	2.270115	-0.396187	-1.256673
O	-1.856283	0.303877	1.336063
O	0.511554	-0.227125	2.256229
C	1.437870	0.529166	1.733560
O	-0.486142	-2.212632	-0.212228
H	-2.210408	-3.829822	0.366597
H	-4.552669	-4.645556	0.583792
H	-6.410988	-3.334894	-0.403861
H	-5.937726	-1.221585	-1.618329
H	-3.589138	-0.434416	-1.851288
H	-0.389851	0.028397	1.867338

H	0.445364	-1.775208	-0.347573
C	3.734288	-0.371136	-1.541147
C	4.558676	-1.332586	-0.953346
C	4.290519	0.634082	-2.335010
C	5.932156	-1.288537	-1.157485
H	4.103355	-2.090168	-0.324313
C	5.665162	0.675159	-2.539709
H	3.633617	1.374854	-2.779430
C	6.486518	-0.284774	-1.950322
H	6.573067	-2.032964	-0.693250
H	6.098388	1.456532	-3.158103
H	7.561263	-0.249793	-2.109011
C	2.819108	0.229641	2.164744
C	3.869267	0.969954	1.617900
C	3.085505	-0.808281	3.061334
C	5.181376	0.674401	1.962463
H	3.643916	1.755941	0.905326
C	4.399311	-1.099076	3.407030
H	2.260236	-1.382379	3.468509
C	5.446170	-0.360010	2.857369
H	5.997147	1.237070	1.518838
H	4.609672	-1.907268	4.101629
H	6.473011	-0.595740	3.123892
C	-3.823035	1.410848	0.655494
C	-4.444755	2.288861	-0.234773
C	-4.589241	0.695840	1.578340
C	-5.825383	2.450391	-0.201203
H	-3.834310	2.825659	-0.953495
C	-5.968593	0.857425	1.610128
H	-4.083542	0.005531	2.245284
C	-6.587740	1.733934	0.720158
H	-6.309307	3.131737	-0.895622
H	-6.564299	0.295986	2.324440
H	-7.667295	1.858013	0.743170
O	0.529778	3.053838	-1.081691
H	1.195813	2.937948	-0.379038
H	-0.251941	3.401276	-0.617681

1a-hydrated-constrained (xTB opt)

Cu	-0.36250340745284	-0.08019889877159	1.23313290508119
O	-0.15723285967942	2.00274909594701	1.07337526252842
O	-0.47217542160121	-2.00360430212580	1.09780762505171
C	0.18517085372457	2.57874731411636	0.03556012515526
O	1.54439813034431	-0.16346469409494	1.74719710161972
O	-2.19415561779335	0.20552731800787	0.43016573846928
C	2.37410848823764	-0.12073162215295	0.79017462316547
C	3.81305295384669	-0.25298800604862	1.18478934861640
C	4.81903021974320	-0.27783089316113	0.22466338280948
H	4.54320543630214	-0.22813724258632	-0.81787556499110
C	6.14309086401543	-0.36913956930482	0.61535424266555
H	6.92427815714308	-0.39240768837879	-0.13015320856083
C	6.46518240089779	-0.42926214984291	1.96145732667203
H	7.49953270222594	-0.49848491994910	2.26604387674736
C	5.46310851363959	-0.40129547350731	2.91864133276074
H	5.71870728779009	-0.44883527392241	3.96743366325355
C	4.13956573027317	-0.31472128077860	2.53406761955218

H	3.34810759112613	-0.29710173742931	3.26704544326107
O	-0.01747721028181	-1.87389108082884	-1.07626101830918
C	-0.23335964437281	-2.51501747706132	-0.03395005172622
O	0.60407851865523	1.99057306365974	-1.03576143188397
O	-1.64808910812183	-0.10652219043675	-1.72501972433952
C	-2.48086212307697	0.14499213276341	-0.76962762182257
O	2.07735078807650	0.06898016006245	-0.39884191736267
C	-0.28424482481083	-4.00933430295259	-0.08227596547893
C	-0.62163599607578	-4.71365876291618	1.06772250383628
C	-0.04149708625126	-4.68773135665448	-1.27132252992689
C	-0.71197000987785	-6.09139242649684	1.02579811991393
H	-0.80934262188257	-4.16648166548228	1.97832996353085
C	-0.13159693542880	-6.06753871909378	-1.30563877928746
H	0.21676962711155	-4.11939852106103	-2.15202134756269
C	-0.46709370073244	-6.76870722888308	-0.15863914884402
H	-0.97440209263343	-6.64262024833113	1.91720923436676
H	0.05859056895705	-6.59731011368325	-2.22762788892437
H	-0.53878780242388	-7.84653577733501	-0.18790987951611
C	-3.89365180203123	0.30703672216604	-1.19430870510265
C	-4.90099943115281	0.37397899850357	-0.23356010820974
C	-4.21908556492172	0.31253012060553	-2.54816945886995
C	-6.22362387083172	0.44766773890009	-0.62788680119484
H	-4.62509212109383	0.35887923031259	0.80963742306801
C	-5.54371608984367	0.39262141410914	-2.93305906531485
H	-3.43029809153415	0.25321292079094	-3.28126855128465
C	-6.54517553934983	0.45850371352540	-1.97644256066201
H	-7.00566665320780	0.49439775577066	0.11499438138854
H	-5.79955233760342	0.39882528097043	-3.98211046556656
H	-7.57931701945578	0.51512180982175	-2.28296250462983
C	0.21648571786007	4.06150173809610	0.00523886629987
C	-0.12523074969001	4.77346958012287	1.15307838516964
C	0.66641245218762	4.73856696613660	-1.12557802471166
C	-0.01808600355451	6.15034463660574	1.16774392161839
H	-0.47084531858088	4.23189818134574	2.01998296619274
C	0.76565207354331	6.11703231678429	-1.10453477808861
H	0.93472187219669	4.17486612915500	-2.00511393548846
C	0.42673527900152	6.82254316197112	0.03960907723396
H	-0.27983147696044	6.70272962922775	2.05777582394603
H	1.11304411289334	6.64442587850777	-1.98022413188657
H	0.51147078047814	7.89912104153254	0.05332673092857
H	-0.81056076304503	-0.67102937196266	-1.43707263334684
H	1.02793610127148	1.05221016939549	-0.85996843439394
O	-0.67826245932323	0.41081401257603	3.44134757004398
H	0.17999516000514	0.04498639949680	3.68201160037302
H	-0.55343818456952	1.35409384854026	3.29478447750610

1a-hydrated-constrained (PBE0-D3 opt)

O	-1.421731	-1.349256	-1.387520
O	1.448462	1.263119	-1.294930
C	-1.710364	-1.853635	-0.228879
O	1.595179	-1.229369	-1.370652
O	-1.490148	1.149125	-1.327981
C	1.861244	-1.746997	-0.211266
C	2.944478	-2.764732	-0.196899
C	3.442070	-3.237274	1.019641
H	3.024691	-2.851643	1.944430

C	4.454375	-4.188940	1.030901
H	4.844282	-4.552589	1.977332
C	4.971582	-4.670201	-0.170546
H	5.763937	-5.413992	-0.160126
C	4.476055	-4.199481	-1.385210
H	4.880495	-4.574511	-2.321071
C	3.463659	-3.247932	-1.400480
H	3.070935	-2.866738	-2.337220
Cu	0.033633	0.082872	0.984329
O	1.341142	1.473111	0.938212
C	1.754926	1.824668	-0.216547
O	-1.295774	-1.410924	0.858023
O	-1.364685	1.421053	0.895714
C	-1.816547	1.718475	-0.262509
O	1.371702	-1.366540	0.867163
C	2.773074	2.907510	-0.211701
C	3.261838	3.410855	-1.419672
C	3.240463	3.420625	1.000455
C	4.213800	4.422946	-1.413336
H	2.882830	2.994331	-2.347739
C	4.192449	4.432703	1.002781
H	2.844247	3.019306	1.926881
C	4.679302	4.934053	-0.203116
H	4.594040	4.816861	-2.352185
H	4.558041	4.832043	1.945139
H	5.423520	5.726529	-0.200110
C	-2.898668	2.737265	-0.278619
C	-3.395528	3.208205	-1.496313
C	-3.417889	3.222767	0.923779
C	-4.407143	4.160611	-1.509367
H	-2.975215	2.813843	-2.416129
C	-4.429448	4.175148	0.906717
H	-3.012839	2.855920	1.860037
C	-4.924268	4.644274	-0.308866
H	-4.792688	4.530381	-2.455726
H	-4.834603	4.554593	1.841089
H	-5.714391	5.390732	-0.320555
C	-2.728466	-2.936614	-0.231122
C	-3.195050	-3.452687	-1.442561
C	-3.217602	-3.437412	0.977525
C	-4.146775	-4.465026	-1.443007
H	-2.808444	-3.049989	-2.372772
C	-4.169178	-4.449863	0.973073
H	-2.838596	-3.032618	1.910085
C	-4.634009	-4.963813	-0.236212
H	-4.509890	-4.866014	-2.384934
H	-4.551064	-4.838050	1.913008
H	-5.378149	-5.755775	-0.237723
H	1.340811	-0.211232	-1.312759
H	-1.241396	-0.316811	-1.336282
O	-0.568147	0.107624	3.208487
H	-1.088713	0.906708	3.025707
H	-1.215455	-0.611110	3.162077

1b (xTB opt)

O	-0.89527230444271	1.36302538951643	-1.17273192822342

O	1.75720703986737	-0.47019234541892	-0.80824796776234
C	-1.83968671630375	1.36367655363029	-0.35178756855242
C	-3.01610608072850	2.22969262926039	-0.54505680065380
C	-4.05440982075132	2.21476887656178	0.38190785519467
H	-3.97845873928722	1.56489382309800	1.24053545861503
C	-5.15571082481308	3.02822811096998	0.19332627510480
H	-5.96307476805913	3.01885885370015	0.91063409547921
C	-5.22435508711654	3.85629363600978	-0.91641236642128
H	-6.08670638156725	4.49062955466072	-1.06170060869504
C	-4.19052257249825	3.87391695066697	-1.84021677376328
H	-4.24874959592349	4.52121093221260	-2.70279780285552
C	-3.08647745045449	3.06313224443082	-1.65762656605968
H	-2.26844686770009	3.05628174661575	-2.36161307180844
O	-1.08388707690961	-1.81077466697817	-0.93713305021994
O	2.53302653193011	2.10655247704879	-0.91045293247589
C	-1.88009231786006	-2.46533503552395	-0.27614766723376
C	-2.15935159460862	-3.88714709332926	-0.57756754904084
C	-3.13962136933256	-4.59467233358745	0.11459517854239
H	-3.70723752134818	-4.09699757038034	0.88492271834694
C	-3.37410286435417	-5.92162354645110	-0.19370818857306
H	-4.13459296567664	-6.47201532887268	0.34007468915448
C	-2.63538946797703	-6.54739399355845	-1.18598709038739
H	-2.82245586745863	-7.58453921663668	-1.42296515283024
C	-1.65722453501019	-5.84640554651124	-1.87477859355854
H	-1.08293192556702	-6.33766835488927	-2.64601637023465
C	-1.41830152686762	-4.51934218438394	-1.57428569655329
H	-0.66300221308769	-3.95077519934476	-2.09487131194281
Cu	-0.00758839809140	0.06146773502930	-0.07931712343832
O	0.88042886775210	-1.23825744758086	1.01478446150435
C	1.82816208961248	-1.23449767220430	0.19763008677972
O	-1.76969425030502	0.59679611179920	0.65226181985241
O	1.06739588163525	1.93775627090514	0.77214094995454
C	1.85206505661258	2.59638461142418	0.10144348876933
O	-2.56088355148107	-1.97582126927653	0.73598379105954
C	2.11562407839398	4.02392240617722	0.38932906491151
C	3.08470625719161	4.73700437152852	-0.31279696912031
H	3.65593750496824	4.23919248494927	-1.08035913967576
C	3.30360227723791	6.06962515011013	-0.01776663318572
H	4.05541124360942	6.62439615232160	-0.55925961313153
C	2.56034216038052	6.69548910252796	0.97105085253506
H	2.73510998979762	7.73711514661672	1.19752680422043
C	1.59331595116651	5.98890314452888	1.66977259046385
H	1.01541412359204	6.48022477420679	2.43827194932947
C	1.37004929099339	4.65618260831103	1.38260492384374
H	0.62355544959134	4.08317535225709	1.91097628780247
C	3.01006524721617	-2.09136399049081	0.39822120108293
C	4.05796154695215	-2.06155907114683	-0.51752921357885
H	3.98483274159635	-1.40805124259645	-1.37365205806909
C	5.16537513468504	-2.86479043038331	-0.32108945087961
H	5.98038462181902	-2.84341254849097	-1.02944684283988
C	5.23043272919768	-3.69776732712070	0.78518067064094
H	6.09760707207251	-4.32402783466641	0.93670203138603
C	4.18694135871375	-3.73047645122792	1.69764176155898
H	4.24240491526462	-4.38159991957096	2.55752656336735
C	3.07694810463555	-2.92961747109090	1.50739075187462
H	2.25156296362368	-2.93431504478085	2.20276113229799
H	-2.31924123091448	-1.02755017445181	0.88992493931807

H 2.29940025994697 1.15511653389659 -1.05672310970271

1b (PBE0-D3)

O	-1.767175	1.321774	0.743522
O	1.001971	-2.310701	1.008361
C	-1.744875	2.210605	-0.166664
C	-2.607202	3.407220	-0.000149
C	-2.619305	4.389024	-0.993181
H	-1.999000	4.246432	-1.872197
C	-3.417774	5.516491	-0.843530
H	-3.428713	6.280777	-1.615535
C	-4.204208	5.664848	0.297807
H	-4.827912	6.547159	0.414807
C	-4.194258	4.684953	1.289505
H	-4.808630	4.803444	2.177630
C	-3.397880	3.555753	1.142000
H	-3.373860	2.779890	1.900292
O	1.079103	1.020853	0.772531
O	-1.375001	-3.090702	0.898163
C	1.887410	1.637477	0.056320
C	3.332971	1.590346	0.334617
C	4.238729	2.317667	-0.442639
H	3.865746	2.970636	-1.224533
C	5.601928	2.184213	-0.212863
H	6.310257	2.745904	-0.814875
C	6.059141	1.323321	0.783774
H	7.126771	1.212166	0.953051
C	5.155469	0.600489	1.560533
H	5.514884	-0.079361	2.326686
C	3.792085	0.734493	1.339907
H	3.070541	0.164169	1.915185
Cu	-0.520195	0.003516	0.045003
O	0.798383	-1.083027	-0.849750
C	1.472013	-1.812360	-0.043459
O	-1.018561	2.089306	-1.195311
O	-2.031545	-1.236186	-0.202129
C	-2.233447	-2.383965	0.238888
O	1.536361	2.337198	-0.985836
C	-3.549756	-3.021031	0.021252
C	-3.787091	-4.328408	0.454552
H	-2.993464	-4.874295	0.953298
C	-5.030852	-4.909420	0.241008
H	-5.218165	-5.925575	0.575588
C	-6.035605	-4.188476	-0.402020
H	-7.007640	-4.645165	-0.567608
C	-5.799055	-2.884146	-0.833327
H	-6.584246	-2.324362	-1.332980
C	-4.557482	-2.298423	-0.623031
H	-4.350265	-1.283966	-0.947494
C	2.909978	-2.025799	-0.361025
C	3.682039	-2.845998	0.464444
H	3.195536	-3.358134	1.288361
C	5.045625	-2.977423	0.231793
H	5.647372	-3.614648	0.874050
C	5.641374	-2.285510	-0.821844
H	6.709834	-2.380474	-0.996933

C	4.871737	-1.470690	-1.650060
H	5.338692	-0.926588	-2.465899
C	3.506882	-1.343253	-1.423501
H	2.892219	-0.702961	-2.047720
H	0.527667	2.288438	-1.100490
H	-0.421802	-2.665550	0.951181

1b-constrained (xTB)

O	0.03776029671846	1.80645042849007	0.69781111391258
O	-0.20931681659064	-1.99095013061213	1.24440976152269
C	0.17661060133468	2.61074129839020	-0.21897812665867
O	1.71775519430432	-0.50141848835530	2.02256551881410
O	-2.08011726402042	-0.04969671023057	0.31285860068311
C	2.40353995051758	-0.20047652938770	0.95545156586164
C	3.85954540134180	-0.21281701964037	1.21714226705036
C	4.82980666867836	-0.26207618938562	0.21569643579184
H	4.51545316049666	-0.22698897331644	-0.81647629381483
C	6.16825741913263	-0.37081984686470	0.55408903572614
H	6.91650045851401	-0.41610567948759	-0.22230004249898
C	6.53882035263084	-0.42657280140392	1.88728113283123
H	7.58180640180249	-0.51589783790047	2.15312103523226
C	5.57366359512404	-0.37040025446619	2.88161527335749
H	5.87230409965821	-0.41244446308087	3.91874543121750
C	4.23938638831867	-0.26670806104326	2.55479542793601
H	3.49076623849030	-0.22557397582062	3.32771548737113
O	-0.07700022727775	-1.85773525624822	-0.94264676216595
C	-0.18950037588799	-2.52875092269135	0.11135375305171
O	0.15751837983241	2.30706421899791	-1.48680595187342
O	-1.55868982634773	0.43054201384545	-1.76477032685847
C	-2.40950134271576	0.21374997403033	-0.86767641990639
O	1.91847610348471	0.01489279584929	-0.15197454369076
C	-0.28077184207739	-4.00509375893403	0.02546531419975
C	-0.61343399565347	-4.69557512294153	1.18301245376897
C	-0.03471622377999	-4.69101119123978	-1.15926738879342
C	-0.70129019245793	-6.07264832823582	1.15294580122373
H	-0.80090028082930	-4.13785945615225	2.08710813769413
C	-0.11935376570234	-6.07141835923312	-1.17996269937845
H	0.21899860462005	-4.12885365082705	-2.04494628290153
C	-0.45303793487202	-6.76031035891738	-0.02488112598240
H	-0.96358647148768	-6.61761149128310	2.04831040724037
H	0.07266234258314	-6.61060930962590	-2.09592656725121
H	-0.52112456103869	-7.83864356422994	-0.04249044196255
C	-3.84591695729043	0.29350252761573	-1.22190215825888
C	-4.84069964174035	0.37127473247200	-0.25302820831597
C	-4.17379032105690	0.30113163105193	-2.57081683560222
C	-6.16550488664555	0.46316753546213	-0.63992608035378
H	-4.55778239532855	0.35952568917962	0.78844975495877
C	-5.49864667459152	0.38524882514483	-2.94868463038290
H	-3.38188022311588	0.23809524896291	-3.30051276284231
C	-6.49293160966868	0.46917251627471	-1.98633950350756
H	-6.94297976003730	0.52782658756384	0.10702290076680
H	-5.76324624387380	0.38706766827955	-3.99626446638883
H	-7.52838392152210	0.53829436648788	-2.28765790666770
C	0.31891335197457	4.06897870824343	-0.01204315616226
C	-0.04289563491218	4.72720893033441	1.16345488016818
C	0.75343839663861	4.80100538165818	-1.11267017014945

C	0.02165877162795	6.10909830271853	1.22976116796485
H	-0.38468145464248	4.14288327867118	2.00437355598773
C	0.81990628737789	6.17491715829187	-1.03503783920078
H	1.03697855197586	4.29145878821034	-2.01806525851188
C	0.45096959468318	6.83184971795594	0.12934074098677
H	-0.26734266402092	6.61704733393320	2.13703375447351
H	1.15696680306217	6.74674140717270	-1.88707832678936
H	0.49722764890573	7.90979725941485	0.17757109185237
H	-0.30924916274655	1.43854901394761	-1.70255471959772
H	0.80655820848464	-0.89312512614991	1.83710579672187
Cu	-0.12694683868574	-0.09182636719049	-0.05274851661516

1b-constrained (PBE0-D3)

O	-1.706948	1.315232	1.196520
O	1.073588	-1.485060	1.007015
C	-1.786244	1.799984	-0.031002
O	1.120739	1.348714	0.964718
O	-1.696904	-1.155859	1.098080
C	1.786392	1.799385	0.030602
C	2.839063	2.848542	0.045668
C	3.349044	3.342481	-1.157288
H	2.973873	2.951651	-2.094823
C	4.332853	4.323524	-1.141314
H	4.727202	4.707111	-2.077793
C	4.808690	4.813343	0.073686
H	5.578379	5.580503	0.085919
C	4.300451	4.321595	1.274699
H	4.676003	4.700960	2.220802
C	3.316774	3.340351	1.262736
H	2.905317	2.950214	2.189494
O	1.696447	-1.156338	-1.098322
C	1.786160	-1.773982	0.016561
O	-1.120802	1.347742	-0.964544
O	-1.073658	-1.486336	-1.006721
C	-1.787286	-1.773690	-0.016840
O	1.705029	1.314993	-1.197081
C	2.835688	-2.826281	0.029283
C	3.312348	-3.321438	1.245416
C	3.345050	-3.318568	-1.174602
C	4.293852	-4.304871	1.255504
H	2.895598	-2.935025	2.171044
C	4.326427	-4.302079	-1.160505
H	2.962500	-2.916750	-2.106480
C	4.801065	-4.795382	0.053553
H	4.667602	-4.689826	2.200547
H	4.719370	-4.688420	-2.096993
H	5.567894	-5.565756	0.063672
C	-2.838595	-2.824157	-0.029787
C	-3.348227	-3.316183	1.174165
C	-3.316292	-3.318269	-1.245864
C	-4.331079	-4.298223	1.160027
H	-2.964783	-2.915279	2.106071
C	-4.299329	-4.300165	-1.255994
H	-2.899204	-2.932224	-2.171495
C	-4.806850	-4.790382	-0.054048
H	-4.724255	-4.684373	2.096498

H	-4.673949	-4.684218	-2.201057
H	-5.574832	-5.559603	-0.064189
C	-2.835982	2.852413	-0.046162
C	-3.344558	3.347752	1.156914
C	-3.312590	3.345334	-1.263113
C	-4.325508	4.331657	1.140969
H	-2.970283	2.956004	2.094423
C	-4.293928	4.328915	-1.275054
H	-2.902317	2.954063	-2.189924
C	-4.800490	4.822334	-0.074015
H	-4.718544	4.716537	2.077468
H	-4.668792	4.708977	-2.221149
H	-5.568176	5.591500	-0.086217
H	-1.669681	0.274895	1.216786
H	1.665770	0.274909	-1.216989
Cu	-0.000896	-0.112558	0.001445

Cu(I)Cu(II)-activated (xTB opt)

Cu	-0.37337750484886	0.03806157263127	1.23111243319038
O	-0.09806372090125	2.14482898026852	0.79812563443547
O	-0.37919258848123	-2.07888950768400	0.76183610048956
C	0.26362869267633	2.59972865194172	-0.30456342129349
O	1.45999468171025	-0.08990326489566	1.92032800799161
O	-2.28360271601235	0.16894483598241	0.79919490229217
C	2.37024332696817	-0.14314117774293	1.05833246775477
C	3.77892610483970	-0.24158464985728	1.59582604154123
C	4.85273411636145	-0.30623291523368	0.71625611184356
H	4.64902651720679	-0.28407626934942	-0.34351005959387
C	6.14397216001946	-0.39642216291448	1.20306292980320
H	6.97931333926298	-0.44671096409693	0.51775849754199
C	6.37005144584551	-0.42252793478179	2.57001591094252
H	7.38060605934105	-0.49309631750091	2.95022135252452
C	5.30142567089075	-0.35822022987063	3.44986650747087
H	5.48019471814980	-0.37874543937888	4.51648863280493
C	4.00889943244335	-0.26798412771872	2.96573370715328
H	3.16070518492771	-0.21669086655460	3.63122631290605
Cu	0.36457871582392	0.01016698093178	-1.23950442010745
O	0.27291165574475	-1.94509631913636	-1.38496197329913
C	-0.07975575763731	-2.55878129270869	-0.34889393123223
O	0.53310560937082	1.96252533533679	-1.35135643171458
O	-1.79337185047433	0.15521346065034	-1.39428855388153
C	-2.57171482355568	0.19866924869743	-0.42167823851123
O	2.25302807453847	-0.12469103184609	-0.18247257533761
C	-0.14811042330374	-4.06348495528560	-0.46794014566605
C	-0.52857566387848	-4.82823085646164	0.62809607400730
C	0.16727068087125	-4.68927798453428	-1.66758656266291
C	-0.59272547924519	-6.20574367373964	0.52439555465873
H	-0.76880112710500	-4.31947318235991	1.54926326708367
C	0.10223885873080	-6.06722628093271	-1.76848606249236
H	0.46034588843729	-4.07653489185973	-2.50639385593178
C	-0.27753625326505	-6.82694028344010	-0.67357075104833
H	-0.88896044497172	-6.80034111320184	1.37801434318712
H	0.34782831784780	-6.55419651510534	-2.70262111362975
H	-0.32794598553038	-7.90478296325582	-0.75401317574271
C	-4.04380148842244	0.29953461234736	-0.74689335663140
C	-4.98717200577774	0.35297485331271	0.27164865929197

C	-4.45898594892638	0.33923919210149	-2.07238636397207
C	-6.33291778189563	0.44525046567168	-0.03429967669833
H	-4.64316786145961	0.32076837793348	1.29417923562788
C	-5.80512160147426	0.43152938686838	-2.37539195702372
H	-3.70762815657361	0.29633278243234	-2.84615157795453
C	-6.74361719778898	0.48464013826653	-1.35717830320892
H	-7.06719157909721	0.48682678766318	0.75890638045506
H	-6.12751948278347	0.46239801199571	-3.40741560244862
H	-7.79670728560057	0.55683808234642	-1.59497121690149
C	0.39537093833669	4.10203673162798	-0.39779588306691
C	0.11712693067151	4.89168710080710	0.71122079162950
C	0.79344991582767	4.70085599287092	-1.58656928983258
C	0.23614822530134	6.26712614595814	0.63114561881590
H	-0.19034177353405	4.40363626276690	1.62355899404344
C	0.91167658811471	6.07679375086959	-1.66382794423163
H	1.00463098925179	4.06904763821836	-2.43578402721434
C	0.63343763189365	6.86138608961397	-0.55602290799505
H	0.01937374817157	6.88111959452616	1.49485109035292
H	1.22163985596444	6.54276009212368	-2.58949560461076
H	0.72636438388726	7.93762184260553	-0.61797567622671

Cu(I)Cu(II)-activated (PBE0-D3 opt)

Cu	-0.001015	-0.000037	1.685067
O	2.353816	0.012962	0.878968
O	-2.354459	-0.013057	0.879408
C	2.678667	0.015318	-0.315393
O	0.010351	-1.936548	1.643707
O	-0.011143	1.936476	1.643679
C	0.014492	-2.512656	0.525826
C	0.023413	-4.013696	0.541816
C	0.028008	-4.731979	-0.654788
H	0.025025	-4.176915	-1.587113
C	0.036190	-6.122748	-0.635632
H	0.039751	-6.677772	-1.570677
C	0.039802	-6.804319	0.580046
H	0.046194	-7.891854	0.594915
C	0.035226	-6.089754	1.776815
H	0.038040	-6.619136	2.726672
C	0.027033	-4.699203	1.757544
H	0.023292	-4.117898	2.673814
Cu	-0.000013	-0.000007	-0.883627
O	-1.882374	-0.011619	-1.318619
C	-2.679010	-0.015341	-0.315056
O	1.882218	0.011614	-1.319133
O	-0.011877	1.971563	-0.617361
C	-0.014563	2.512618	0.525812
O	0.011967	-1.971579	-0.617338
C	-4.143604	-0.023125	-0.670364
C	-5.094286	-0.028490	0.350833
C	-4.563812	-0.024819	-2.001062
C	-6.451434	-0.035455	0.046506
H	-4.736236	-0.026982	1.375771
C	-5.921236	-0.031735	-2.307166
H	-3.807589	-0.020559	-2.779312
C	-6.867666	-0.037067	-1.284003
H	-7.187949	-0.039601	0.846764

H	-6.243637	-0.032967	-3.345953
H	-7.928816	-0.042468	-1.523252
C	-0.022799	4.013659	0.541839
C	-0.026588	4.699137	1.757583
C	-0.026591	4.731975	-0.654749
C	-0.034153	6.089691	1.776886
H	-0.023469	4.117808	2.673840
C	-0.034147	6.122747	-0.635560
H	-0.023482	4.176935	-1.587087
C	-0.037931	6.804288	0.580134
H	-0.037099	6.619050	2.726755
H	-0.037077	6.677796	-1.570593
H	-0.043831	7.891826	0.595028
C	4.143338	0.023174	-0.670391
C	5.093782	0.028501	0.351027
C	4.563855	0.024966	-2.000990
C	6.451002	0.035522	0.047017
H	4.735486	0.026918	1.375879
C	5.921351	0.031941	-2.306779
H	3.807811	0.020734	-2.779415
C	6.867543	0.037231	-1.283396
H	7.187331	0.039636	0.847447
H	6.243994	0.033250	-3.345490
H	7.928750	0.042675	-1.522396

Cu(I)Cu(II)-hydrated (xTB opt)

O	-0.80643601827829	-1.26879344174326	-2.00956777032171
O	-0.83519394662469	2.43624210438587	-0.38067121562181
C	-0.79960479646823	-2.26202086949692	-1.25217450298386
O	1.34578470759785	0.48297089525384	-0.83577901375637
O	-2.90366990018828	0.38468659532983	-0.73583416752237
C	1.85700376493920	0.00246957731617	0.19279522981080
C	3.36351541163896	-0.01358989310378	0.25544884700065
C	4.01866974110029	-0.39852717738706	1.41890292699952
H	3.43171840192194	-0.68479067255898	2.27817819516321
C	5.40099021494394	-0.40835464080793	1.46374783951726
H	5.90967484046417	-0.70781929250871	2.36960036918999
C	6.13528895081976	-0.03704915884364	0.34907752326408
H	7.21641422315553	-0.04718860472838	0.38561035912756
C	5.48469128370229	0.34697621514422	-0.81274780450157
H	6.05927508113098	0.63588627899473	-1.68215571102688
C	4.10295779545882	0.36034992643001	-0.86041737321540
H	3.57206841617782	0.65636703499682	-1.75235120413964
O	-1.90982830442238	1.87980908891279	-2.90642569426224
Cu	-0.72800990427373	-0.43755741986603	1.16868274865062
O	-0.70792718042896	1.62989029190128	1.71019720349728
C	-0.78162421716062	2.54416300315626	0.86643802271887
O	-0.75458198060847	-2.26570816037789	-0.00103451915459
O	-2.69113346530521	-0.51895219686038	1.30585782548205
C	-3.34751618431070	-0.09595418035267	0.32590518387075
O	1.26225201308289	-0.47759696752802	1.19155303777307
O	1.07362865399096	-3.22814334217371	1.94164757170523
H	-2.61152661670733	1.38257498961445	-2.46941482343587
H	-1.62103800855439	2.53034130264734	-2.25731394465526
H	0.32537331428587	-3.16709776560023	1.33248785849615
H	1.39267406045427	-2.31818443103214	1.96324064340585

C	-0.85027493176613	-3.61131714255582	-1.92654292187573
C	-0.87727460887107	-4.77804599181298	-1.17208421796103
C	-0.87173509997470	-3.68745958940627	-3.31436248886970
C	-0.92441544117786	-6.00841451984021	-1.80241321502727
H	-0.86007969137187	-4.70633365183799	-0.09548780816421
C	-0.91875608610393	-4.91921291394550	-3.94066614432845
H	-0.85070708367420	-2.76831166823059	-3.87984942067373
C	-0.94500704113111	-6.08114334141570	-3.18576676154006
H	-0.94400853696186	-6.91523945134365	-1.21400151728846
H	-0.93474270081854	-4.97709501712445	-5.02048918645669
H	-0.98132737730264	-7.04454262688193	-3.67661724561743
C	-4.84976229848825	-0.17614762189809	0.45907950425239
C	-5.42512567458437	-0.48496779821667	1.68557604132553
C	-5.66332503943216	0.05825333103843	-0.64253404565976
C	-6.80078299883181	-0.55408305484810	1.80839768477446
H	-4.77495242588498	-0.66768077173524	2.52745824731656
C	-7.03874563118277	-0.01610220408998	-0.51809884759395
H	-5.20044965229079	0.29314313778070	-1.58920545758269
C	-7.60910961403823	-0.32027985772726	0.70734492705753
H	-7.24756572022391	-0.79218147525408	2.76401061833997
H	-7.67020433777764	0.16339685506035	-1.37748076573835
H	-8.68507083422452	-0.37640950270783	0.80409043408230
C	-0.81772747674888	3.95332125568378	1.41031264877498
C	-0.62333447189511	5.03834893722298	0.56473518508180
C	-1.04483563602761	4.16718457061480	2.76430348195967
C	-0.65494389709360	6.32545610371389	1.07025673693844
H	-0.44404438311419	4.85411141627682	-0.48388415125072
C	-1.08187003613348	5.45533715901953	3.26583293867077
H	-1.18867001666712	3.30908710619767	3.40303910638102
C	-0.88628300652184	6.53560142011189	2.42007572943799
H	-0.49939760441936	7.16918310958821	0.41186947673835
H	-1.26214926120829	5.62138852928441	4.31911666863347
H	-0.91308726643123	7.54284716937244	2.81370869307115
Cu	-0.73669673505067	0.56617448885014	-1.24414231729465

Cu(I)Cu(II)-hydrated (PBE0 opt)

O	-1.675451	1.308972	0.256547
O	1.510545	-0.933479	0.452550
C	-2.117899	2.095349	-0.644528
O	1.083721	1.737726	0.342936
O	-1.283314	-1.345179	0.676454
C	2.132811	1.877046	-0.372121
C	3.202212	2.744045	0.235044
C	4.342803	3.051421	-0.507220
H	4.421265	2.648605	-1.511982
C	5.342622	3.845953	0.042493
H	6.227851	4.087363	-0.540967
C	5.209740	4.334495	1.341452
H	5.992358	4.954241	1.773319
C	4.073741	4.025961	2.087675
H	3.970627	4.400725	3.103428
C	3.070630	3.234737	1.535350
H	2.174295	2.982150	2.093771
O	0.243192	-0.733595	2.941748
Cu	-0.278553	-1.085305	-2.082795
O	1.372579	-2.141417	-1.444089

C	1.930107	-1.804174	-0.379925
O	-1.727659	2.201119	-1.820664
O	-1.848140	-2.053949	-1.377693
C	-1.987720	-2.022150	-0.134792
O	2.342798	1.384486	-1.495933
O	0.155866	0.672653	-2.821910
H	-0.472129	-1.167902	2.451203
H	0.994888	-0.874793	2.343162
H	-0.560544	1.254014	-2.441080
H	0.988841	0.972731	-2.356222
C	-3.263208	2.971638	-0.204023
C	-3.869543	3.820441	-1.129899
C	-3.725076	2.944360	1.113069
C	-4.930359	4.633752	-0.746314
H	-3.488311	3.820298	-2.146000
C	-4.785316	3.759502	1.498103
H	-3.237012	2.278585	1.817922
C	-5.390177	4.604689	0.569058
H	-5.400679	5.292066	-1.472858
H	-5.141544	3.736384	2.525343
H	-6.220052	5.239912	0.870649
C	-3.076866	-2.858663	0.464749
C	-3.786267	-3.750291	-0.342159
C	-3.392663	-2.754461	1.820919
C	-4.796167	-4.535164	0.202482
H	-3.527041	-3.808037	-1.394195
C	-4.406289	-3.536325	2.364175
H	-2.839143	-2.050813	2.434132
C	-5.108025	-4.429344	1.556798
H	-5.343204	-5.229868	-0.429824
H	-4.650134	-3.448521	3.419916
H	-5.899062	-5.041627	1.983150
C	3.221205	-2.474981	-0.016004
C	3.978845	-2.030898	1.068962
C	3.672246	-3.554314	-0.777764
C	5.174150	-2.664814	1.391521
H	3.622867	-1.179855	1.640517
C	4.863578	-4.191787	-0.450972
H	3.070233	-3.872912	-1.622598
C	5.616146	-3.748254	0.635189
H	5.763035	-2.311191	2.233931
H	5.208409	-5.035169	-1.044164
H	6.548774	-4.245691	0.890588
Cu	-0.092800	0.198891	0.233533

Cu(I)Cu(II)-activated-constrained (xTB opt)

Cu	-0.38199316809509	0.04272983610198	1.25312861392553
O	0.07505147019188	2.03139146059544	1.13278135612502
O	-0.70895060300609	-1.95162526567430	0.94422910434660
C	0.16748892495880	2.57065362005808	0.00849087061566
O	1.58042972636160	-0.36459699110591	1.62630657510003
O	-2.22476439544604	0.44328610293792	0.47873421210651
C	2.42836028334706	-0.14120848783625	0.73446027865887
C	3.85517517896202	-0.24263012859176	1.16616873580230
C	4.86811727834461	-0.28199499695686	0.21289563243068
H	4.59558330205608	-0.23596845179749	-0.82995023721774

C	6.18698929629708	-0.37576685289348	0.61680200542487
H	6.97917939293867	-0.40801159203047	-0.11919121423000
C	6.49835882677032	-0.43088668593567	1.96644068103348
H	7.53166094336634	-0.50446114426556	2.27919555514029
C	5.48961258202324	-0.39208773470604	2.91641282184964
H	5.73997543925787	-0.43414375846910	3.96798901342317
C	4.16825799832951	-0.29782034178794	2.52091268213571
H	3.36208853164742	-0.26712057058949	3.23717220498143
Cu	0.37156373972486	0.01404849514571	-1.26259144434757
O	0.43640356166302	-2.00692305801421	-1.00228211443016
C	-0.17158657689796	-2.51443260702940	-0.03442763606076
O	0.18672047152601	2.03925880482045	-1.12344562430549
O	-1.63566206913840	-0.12425243916059	-1.62643871280293
C	-2.44408754414427	0.19345188908305	-0.72696787055022
O	2.24991571760530	0.15520056880657	-0.46711934127977
C	-0.27024591433123	-4.00517755731940	-0.05016490765023
C	-0.60131463226952	-4.69146701616287	1.11419802467258
C	-0.03113956537020	-4.70438167041902	-1.22927409852018
C	-0.69110253920461	-6.07092934669114	1.09543207273632
H	-0.78368547808787	-4.12306934743115	2.01288615288611
C	-0.12456370360717	-6.08369128751991	-1.23990119381479
H	0.22604051118353	-4.14619432334067	-2.11597802185896
C	-0.45364977887325	-6.76698310245565	-0.07958280984206
H	-0.94564789076393	-6.61073500034950	1.99769973889173
H	0.05769950828386	-6.63319198692050	-2.15373409700031
H	-0.52534365715383	-7.84664125810891	-0.09104579045716
C	-3.87328109616643	0.28752531181600	-1.15242931793160
C	-4.87942663331018	0.36381959626735	-0.19418767472482
C	-4.19551265273224	0.29817597036671	-2.50609647366837
C	-6.20059982989974	0.45057251718105	-0.59205579404161
H	-4.59969469868448	0.35505608285917	0.84772708818593
C	-5.51920484579715	0.38464722893603	-2.89556255068595
H	-3.39469437326500	0.23601599114852	-3.22631591165379
C	-6.52111386354907	0.46092753821703	-1.94063842089912
H	-6.98767612363939	0.50892806386491	0.14780760095751
H	-5.77651184128174	0.39458213142269	-3.94625504006991
H	-7.55622303063332	0.52866982310824	-2.24869874631657
C	0.26994707985517	4.06121155590765	0.01889833469526
C	-0.06718001056334	4.77235419760110	1.16649665146627
C	0.70273251179797	4.73542665157446	-1.11886561385451
C	0.02903800044843	6.15149740355679	1.17200667808278
H	-0.39728608849719	4.22297785885529	2.03434588733710
C	0.79707291489138	6.11463846724607	-1.10474147230004
H	0.95508413378642	4.15824918275839	-1.99472988371809
C	0.46071114199497	6.82264776689007	0.03854443078254
H	-0.23341043428724	6.71051616124000	2.06019622310862
H	1.13474745312604	6.64475908990614	-1.98520980681937
H	0.53530710486994	7.90214357817453	0.04620214403428

Cu(I)Cu(II)- activated-constrained (PBE0 opt)

Cu	-0.000224	0.001033	1.445866
O	0.366030	-2.087542	0.773279
O	-0.365917	2.087628	0.773281
C	0.452335	-2.545243	-0.377678
O	-1.955976	-0.344316	1.400856
O	1.956235	0.343893	1.400759

C	-2.545185	-0.452360	0.295508
C	-4.028831	-0.715958	0.406288
C	-4.795848	-0.851565	-0.744440
H	-4.298885	-0.762515	-1.705675
C	-6.154142	-1.092910	-0.648526
H	-6.752699	-1.198600	-1.550739
C	-6.753756	-1.200146	0.596190
H	-7.822486	-1.390041	0.670636
C	-5.991716	-1.065433	1.745703
H	-6.461533	-1.149489	2.723158
C	-4.632964	-0.823989	1.652720
H	-4.009902	-0.713540	2.534027
Cu	0.000070	-0.000348	-1.099190
O	-0.338402	1.882233	-1.461868
C	-0.452335	2.545083	-0.377798
O	0.338188	-1.882682	-1.461955
O	2.022957	0.363848	-0.856677
C	2.545218	0.452196	0.295486
O	-2.023041	-0.363533	-0.856653
C	-0.716019	4.028728	-0.488628
C	-0.852921	4.795530	0.662101
C	-0.822826	4.633064	-1.735057
C	-1.094352	6.153808	0.566172
H	-0.763807	4.294121	1.620605
C	-1.064330	5.991805	-1.828055
H	-0.712396	4.013795	-2.619900
C	-1.200351	6.753627	-0.678551
H	-1.200924	6.750982	1.469056
H	-1.147691	6.463625	-2.804837
H	-1.390306	7.822303	-0.753675
C	4.028854	0.715801	0.406258
C	4.632983	0.823806	1.652698
C	4.795877	0.851407	-0.744461
C	5.991740	1.065222	1.745690
H	4.009909	0.713329	2.533987
C	6.154175	1.092725	-0.648538
H	4.298932	0.762379	-1.705709
C	6.753787	1.199937	0.596181
H	6.461556	1.149253	2.723149
H	6.752744	1.198407	-1.550746
H	7.822520	1.389807	0.670634
C	0.716065	-4.028886	-0.488455
C	0.853030	-4.795631	0.662307
C	0.822824	-4.633280	-1.734857
C	1.094479	-6.153910	0.566432
H	0.763960	-4.294158	1.620788
C	1.064342	-5.992023	-1.827801
H	0.712328	-4.014053	-2.619717
C	1.200431	-6.753787	-0.678267
H	1.201097	-6.751041	1.469339
H	1.147673	-6.463885	-2.804566
H	1.390398	-7.822464	-0.753346

Cu(I)Cu(II)-hydrated-constrained (xTB opt)

O	-1.14056981042100	-1.40815770151015	-1.81888090660409
O	-0.58127861737120	2.31269504129373	-0.23536745962709

C	-0.77526475951490	-2.33101922291916	-1.06693663546309
O	1.19649322567322	0.21093842861120	-1.09056813846491
O	-2.86499525565504	0.67396987808321	-0.73764619269291
C	1.76404912130671	0.01278485563657	0.00124057997729
C	3.26119917594974	0.05109425859982	-0.04344273293815
C	4.00574370287957	-0.44537723161237	1.02123710460962
H	3.48583181418467	-0.84813238004294	1.87798918459949
C	5.38706959461736	-0.40353962788415	0.97329464984003
H	5.96474838768334	-0.78465620006363	1.80584130169528
C	6.02756779943367	0.12799139434395	-0.13488774362169
H	7.10885919286901	0.15429825074630	-0.16059124080947
C	5.28636771556155	0.62296196250290	-1.19644025022419
H	5.79748987078382	1.03317782544586	-2.05560019478923
C	3.90475896643594	0.58865993183383	-1.15332323761920
H	3.30225750454401	0.95996372358312	-1.96635173392569
O	-1.39231584209299	2.03869492236870	-2.96183485151603
Cu	-0.79913791698172	-0.50761933197569	1.26040001588829
O	-1.00669666606145	1.45096913597517	1.80521490044522
C	-0.77723258731572	2.36584534719281	0.99556069393238
O	-0.43648582896513	-2.29185492591395	0.13237941274623
O	-2.74908671887619	-0.77530561356498	0.98767378285951
C	-3.33512480700394	-0.06494004580497	0.14985349515396
O	1.25658993499188	-0.22038413631382	1.12138923968182
O	-0.04965023247897	-1.95232515243304	3.04109357005589
H	-2.23824764344787	1.75969436485110	-2.59725880897925
H	-0.97189206526926	2.55970799409640	-2.26899652757671
H	-0.19660940927686	-2.52948335955574	2.28434715761216
H	0.70471278008516	-1.40266895361674	2.80454157388797
C	-0.74959605132546	-3.72502717874251	-1.72091137209161
C	-0.49906177863832	-4.85570521410333	-0.94372319323278
C	-0.97665881567632	-3.85688296182360	-3.09141240937206
C	-0.47661566928721	-6.11864144561532	-1.53614169737274
H	-0.33427935677265	-4.73434142041965	0.11626763451971
C	-0.95373320420958	-5.11950102562141	-3.68370208574111
H	-1.16315124704784	-2.96728204326931	-3.67053829952079
C	-0.70408389140059	-6.25052222538926	-2.90596424319423
H	-0.29253940321439	-6.99347386010450	-0.92728144212116
H	-1.12432893292964	-5.22829126436674	-4.74441234392490
H	-0.68807046818190	-7.23346234729150	-3.35609641459621
C	-4.87221285660786	-0.12628715182145	0.22194281768781
C	-5.49489374288891	-0.81142933092251	1.26504896705393
C	-5.64213554592793	0.50341389128331	-0.75678706379956
C	-6.88742791089211	-0.86627748503566	1.33071240365550
H	-4.87802235233688	-1.28743961092579	2.00946797509589
C	-7.03432711692602	0.44813512500625	-0.69133567764237
H	-5.14139637803216	1.02053990206120	-1.56147496639491
C	-7.65705040691125	-0.23642287225423	0.35269782085221
H	-7.37644620140725	-1.39256162342503	2.13668603786230
H	-7.62627315196829	0.92902839042992	-1.45855470852909
H	-8.73682597984095	-0.27672685472225	0.39172205552602
C	-0.73341187295530	3.77752483918137	1.60943426715382
C	-0.61797757075769	4.89462128133249	0.78239605452404
C	-0.80882104638579	3.93900371955964	2.99343374856184
C	-0.57908784293975	6.17353563844469	1.33857685667389
H	-0.55151130141590	4.75020765513562	-0.28542643729814
C	-0.76945714076958	5.21761444388311	3.54943924958637
H	-0.90677725049114	3.06009852247582	3.60951267872730

C	-0.65497738860969	6.33500556024195	2.72194822977439
H	-0.48575063611578	7.03645646627810	0.69326635627716
H	-0.83615709045464	5.34991358907157	4.61902744253329
H	-0.62686437048690	7.32982873469008	3.14437079476352
Cu	-0.81233007624649	0.47526464808108	-1.23510851497147

Cu(I)Cu(II)-hydrated-constrained (PBE0 opt)

O	-1.790662	0.940587	1.374138
O	1.853938	-0.882747	1.300147
C	-2.328364	1.209237	0.276804
O	1.006968	1.929015	0.934651
O	-0.961952	-1.845841	0.841949
C	1.238026	2.358563	-0.205427
C	1.934457	3.693823	-0.283893
C	2.313245	4.222306	-1.512084
H	2.102212	3.652450	-2.411541
C	2.951852	5.447734	-1.570758
H	3.250270	5.859112	-2.532480
C	3.213386	6.151739	-0.406488
H	3.715037	7.115758	-0.455455
C	2.836618	5.627308	0.819731
H	3.041609	6.179145	1.734160
C	2.200043	4.401554	0.882359
H	1.894088	3.961505	1.826016
O	0.196126	-1.718539	3.371729
Cu	0.054700	0.031232	-1.148275
O	1.852063	-0.923484	-0.951756
C	2.350810	-1.175078	0.183148
O	-1.835159	0.992798	-0.874323
O	-0.852841	-1.661703	-1.391621
C	-1.175206	-2.254101	-0.315191
O	0.950015	1.776140	-1.305666
O	-0.670996	0.958499	-3.325897
H	-0.407763	-2.002894	2.662979
H	1.033446	-1.649356	2.881496
H	-1.456677	1.061420	-2.759347
H	-0.082825	1.654595	-2.986985
C	-3.689989	1.852563	0.376647
C	-4.404614	2.176754	-0.770202
C	-4.234428	2.121886	1.627045
C	-5.651848	2.765507	-0.664737
H	-3.963917	1.956003	-1.737322
C	-5.481352	2.710628	1.728260
H	-3.653638	1.855610	2.503928
C	-6.191585	3.033317	0.582797
H	-6.210600	3.017748	-1.563322
H	-5.904179	2.919763	2.708236
H	-7.172890	3.496111	0.662339
C	-1.882266	-3.581443	-0.454299
C	-1.981731	-4.190898	-1.699037
C	-2.436053	-4.199392	0.660083
C	-2.625283	-5.408323	-1.825579
H	-1.547825	-3.685746	-2.556354
C	-3.083165	-5.414764	0.530039
H	-2.347213	-3.705135	1.622350
C	-3.176930	-6.021494	-0.711990

H	-2.698698	-5.884786	-2.800624
H	-3.517951	-5.893175	1.404534
H	-3.684457	-6.978386	-0.813147
C	3.677553	-1.896635	0.227384
C	4.370539	-2.020887	1.425051
C	4.210135	-2.438329	-0.936030
C	5.585967	-2.680345	1.457390
H	3.935427	-1.588324	2.320197
C	5.422588	-3.102308	-0.899554
H	3.652054	-2.321680	-1.859876
C	6.112152	-3.223456	0.296421
H	6.127538	-2.772305	2.395983
H	5.835523	-3.529264	-1.810724
H	7.066932	-3.744113	0.323545
Cu	0.033823	0.089987	1.443008

Cu(I)Cu(II)- activated-TS (PBE0-D3)

Cu	0.000000	0.000000	1.259122
Cu	0.000000	0.000000	-1.259122
O	-1.388790	1.391150	-1.483517
C	-1.819383	1.818877	-0.374920
O	-1.454864	1.451955	0.769512
C	-2.882470	2.881422	-0.441490
C	-3.413999	3.410148	0.735447
C	-3.343904	3.345144	-1.674310
C	-4.397020	4.392651	0.680927
H	-3.037138	3.031518	1.680100
C	-4.327077	4.327791	-1.729812
H	-2.915245	2.918661	-2.575408
C	-4.855587	4.853500	-0.552068
H	-4.807714	4.801149	1.601326
H	-4.683159	4.685650	-2.693106
H	-5.624339	5.621847	-0.595082
O	1.388790	-1.391150	-1.483517
C	1.819383	-1.818877	-0.374920
O	1.454864	-1.451955	0.769512
C	2.882470	-2.881422	-0.441490
C	3.413999	-3.410148	0.735447
C	3.343904	-3.345144	-1.674310
C	4.397020	-4.392651	0.680927
H	3.037138	-3.031518	1.680100
C	4.327077	-4.327791	-1.729812
H	2.915245	-2.918661	-2.575408
C	4.855587	-4.853500	-0.552068
H	4.807714	-4.801149	1.601326
H	4.683159	-4.685650	-2.693106
H	5.624339	-5.621847	-0.595082
O	1.388790	1.391150	1.483517
C	1.819383	1.818877	0.374920
O	1.454864	1.451955	-0.769512
C	2.882470	2.881422	0.441490
C	3.413999	3.410148	-0.735447
C	3.343904	3.345144	1.674310
C	4.397020	4.392651	-0.680927
H	3.037138	3.031518	-1.680100
C	4.327077	4.327791	1.729812

H	2.915245	2.918661	2.575408
C	4.855587	4.853500	0.552068
H	4.807714	4.801149	-1.601326
H	4.683159	4.685650	2.693106
H	5.624339	5.621847	0.595082
O	-1.388790	-1.391150	1.483517
C	-1.819383	-1.818877	0.374920
O	-1.454864	-1.451955	-0.769512
C	-2.882470	-2.881422	0.441490
C	-3.413999	-3.410148	-0.735447
C	-3.343904	-3.345144	1.674310
C	-4.397020	-4.392651	-0.680927
H	-3.037138	-3.031518	-1.680100
C	-4.327077	-4.327791	1.729812
H	-2.915245	-2.918661	2.575408
C	-4.855587	-4.853500	0.552068
H	-4.807714	-4.801149	-1.601326
H	-4.683159	-4.685650	2.693106
H	-5.624339	-5.621847	0.595082

CuDimer-activated-nondefective (xTB opt)

Cu	-0.260651	0.236026	1.176657
O	-1.585984	-1.189053	1.056653
O	1.110539	1.619501	1.089417
C	-1.748581	-1.824601	-0.027936
O	-1.581831	1.512139	0.529177
O	1.100648	-1.076419	1.643067
C	-1.744030	1.682084	-0.716639
C	-2.767762	2.672338	-1.141127
C	-2.992728	2.904315	-2.500105
H	-2.410236	2.352015	-3.229805
C	-3.950318	3.830362	-2.895129
H	-4.125649	4.011148	-3.951836
C	-4.684378	4.525846	-1.935952
H	-5.433023	5.249809	-2.246410
C	-4.460868	4.295346	-0.579681
H	-5.033788	4.838219	0.166716
C	-3.504109	3.370081	-0.180813
H	-3.314063	3.175265	0.869294
Cu	0.260284	-0.236849	-1.176563
O	1.586165	1.185827	-1.070206
C	1.751076	1.821227	0.014374
O	-1.105684	-1.623099	-1.101869
O	1.581027	-1.509819	-0.515565
C	1.741073	-1.679731	0.730313
O	-1.106255	1.077851	-1.630336
C	2.781399	2.892264	0.026105
C	3.009784	3.627916	1.191395
C	3.520366	3.162366	-1.128116
C	3.973343	4.628945	1.200495
H	2.425173	3.402399	2.076927
C	4.483065	4.164184	-1.115181
H	3.327620	2.579613	-2.022569
C	4.709942	4.897479	0.048162
H	4.151355	5.201323	2.106447
H	5.058006	4.374648	-2.012511

H	5.463216	5.680729	0.056770
C	2.765206	-2.668674	1.156885
C	2.988419	-2.899872	2.516289
C	3.503708	-3.366010	0.197938
C	3.946424	-3.824741	2.913080
H	2.404271	-2.347956	3.244956
C	4.460843	-4.290117	0.598568
H	3.314978	-3.171753	-0.852510
C	4.682612	-4.519839	1.955258
H	4.120411	-4.004908	3.970116
H	5.035415	-4.832695	-0.146773
H	5.431563	-5.242890	2.267103
C	-2.778765	-2.895747	-0.041884
C	-3.520354	-3.165548	1.110720
C	-3.004428	-3.631773	-1.207472
C	-4.482963	-4.167422	1.095892
H	-3.329649	-2.582486	2.005407
C	-3.967883	-4.632889	-1.218455
H	-2.417843	-3.406524	-2.091766
C	-4.707110	-4.901108	-0.067733
H	-5.059957	-4.377632	1.991964
H	-4.143765	-5.205577	-2.124628
H	-5.460305	-5.684417	-0.077825

CuDimer-activated -nondefective (PBE0-D3 opt)

Cu	-0.260651	0.236026	1.176657
O	-1.585984	-1.189053	1.056653
O	1.110539	1.619501	1.089417
C	-1.748581	-1.824601	-0.027936
O	-1.581831	1.512139	0.529177
O	1.100648	-1.076419	1.643067
C	-1.744030	1.682084	-0.716639
C	-2.767762	2.672338	-1.141127
C	-2.992728	2.904315	-2.500105
H	-2.410236	2.352015	-3.229805
C	-3.950318	3.830362	-2.895129
H	-4.125649	4.011148	-3.951836
C	-4.684378	4.525846	-1.935952
H	-5.433023	5.249809	-2.246410
C	-4.460868	4.295346	-0.579681
H	-5.033788	4.838219	0.166716
C	-3.504109	3.370081	-0.180813
H	-3.314063	3.175265	0.869294
Cu	0.260284	-0.236849	-1.176563
O	1.586165	1.185827	-1.070206
C	1.751076	1.821227	0.014374
O	-1.105684	-1.623099	-1.101869
O	1.581027	-1.509819	-0.515565
C	1.741073	-1.679731	0.730313
O	-1.106255	1.077851	-1.630336
C	2.781399	2.892264	0.026105
C	3.009784	3.627916	1.191395
C	3.520366	3.162366	-1.128116
C	3.973343	4.628945	1.200495
H	2.425173	3.402399	2.076927
C	4.483065	4.164184	-1.115181

H	3.327620	2.579613	-2.022569
C	4.709942	4.897479	0.048162
H	4.151355	5.201323	2.106447
H	5.058006	4.374648	-2.012511
H	5.463216	5.680729	0.056770
C	2.765206	-2.668674	1.156885
C	2.988419	-2.899872	2.516289
C	3.503708	-3.366010	0.197938
C	3.946424	-3.824741	2.913080
H	2.404271	-2.347956	3.244956
C	4.460843	-4.290117	0.598568
H	3.314978	-3.171753	-0.852510
C	4.682612	-4.519839	1.955258
H	4.120411	-4.004908	3.970116
H	5.035415	-4.832695	-0.146773
H	5.431563	-5.242890	2.267103
C	-2.778765	-2.895747	-0.041884
C	-3.520354	-3.165548	1.110720
C	-3.004428	-3.631773	-1.207472
C	-4.482963	-4.167422	1.095892
H	-3.329649	-2.582486	2.005407
C	-3.967883	-4.632889	-1.218455
H	-2.417843	-3.406524	-2.091766
C	-4.707110	-4.901108	-0.067733
H	-5.059957	-4.377632	1.991964
H	-4.143765	-5.205577	-2.124628
H	-5.460305	-5.684417	-0.077825

CuDimer-activated -nondefective-trimmed (Reference [10])

Cu	0.72067075253163	-1.30435164432969	-0.34033155026716
O	0.73750955066525	-0.58475759475468	-2.20553481523349
O	0.72202954441765	-1.67417328675044	1.62404766259122
C	0.80061637868890	0.64499983202791	-2.43819730754894
O	-1.23962412293510	-1.01072093009920	-0.26434809262883
O	2.71103793804544	-1.25264823399976	-0.31721807315488
C	-1.73444419094761	0.10154718194363	0.05037114757651
C	-3.22523636079155	0.19259309934734	0.07226722424523
C	-3.84255313982973	1.39241289772546	0.41342520729969
H	-3.22744912704750	2.24415991279757	0.65859329662767
C	-5.22266155862894	1.47215698954946	0.43249344730989
H	-5.70437963905455	2.40176271087172	0.69682380522321
C	-5.98767480748039	0.36113678545779	0.11294525229004
H	-7.06573923505231	0.42695225065709	0.12867457396487
C	-5.37309445642248	-0.83407233747142	-0.22691285693842
H	-5.97176714693050	-1.69777277520589	-0.47533901810757
C	-3.99356666971701	-0.92270013945020	-0.24844407308472
H	-3.49398674764301	-1.84250740967485	-0.50982158626856
Cu	0.88422978109278	1.19591855196755	0.37140996801484
O	0.86203350342400	0.47758907985593	2.23632631647699
C	0.78153155287544	-0.75101786132512	2.46945452531876
O	0.87879597260960	1.56678407648647	-1.59285114105953
O	2.85203371531729	0.89887565936396	0.29569933929629
C	3.34138506801191	-0.21044575930652	-0.02167884330038
O	-1.09892096044257	1.14472465246011	0.34849957033330
C	0.73675812465618	-1.16358680347170	3.92797573718573
H	1.19788858304955	-2.13913428790815	4.04637667103183

H	1.23452887969436	-0.41495054682762	4.53609140941760
H	-0.30748557004670	-1.22863060129859	4.22706426211170
C	4.85435914808387	-0.29653147473645	-0.06810656153706
H	5.17038778682849	-1.30979694486489	0.15917682569772
H	5.17547973668807	-0.04401561320840	-1.07664974543730
H	5.28327828396883	0.41677379749958	0.62857592716291
C	0.76476158595512	1.06239500743532	-3.89564362515461
H	-0.27585791157975	1.21086594486171	-4.17707126007055
H	1.30171535033995	1.99719956382609	-4.02231102717655
H	1.18871525530774	0.27621056813637	-4.51240966293350

CuDimer-hydrated -nondefective (xTB opt)

Cu	-0.80821103370409	0.52856345358283	-1.23547771397450
O	-0.82948646662150	-1.34696251569533	-1.84524781954256
O	-0.84637130582472	2.28866302716140	-0.22198224165044
C	-0.77215197736076	-2.32987247195171	-1.06971804330803
O	1.17578133054003	0.49139947732641	-1.05076899252713
O	-2.83627031623445	0.41040782100834	-0.89796061662095
C	1.78756162003247	0.03638767956876	-0.05658135797014
C	3.28396208185619	0.08519586134935	-0.11694352183473
C	4.03714234000404	-0.10305731490761	1.03681029546362
H	3.52849319854996	-0.27639481965326	1.97280770350450
C	5.41759224726212	-0.05488966630585	0.97293304536959
H	6.00355449399030	-0.19672964666867	1.86910766255356
C	6.04886232502887	0.17571996574968	-0.23906725263974
H	7.12752339535414	0.21064073045692	-0.28643321865507
C	5.29909018210178	0.36363503058485	-1.38957024554842
H	5.79351970326724	0.54398518378446	-2.33265080509196
C	3.91826111312633	0.32199579988020	-1.33189289837759
H	3.31411677849488	0.46835438392074	-2.21383835705959
O	-1.49342923420546	1.83936205101153	-2.94754693597677
Cu	-0.72908000879675	-0.54582132741147	1.26188164658394
O	-0.70958079876347	1.36688573688511	1.81985700204453
C	-0.77117998997177	2.33772721537384	1.03021529776869
O	-0.69974549107751	-2.29938849388119	0.18267311745921
O	-2.69768613820327	-0.53319846530059	1.13348554862467
C	-3.32582366767495	-0.08485662600389	0.14594609142530
O	1.28121000459766	-0.45867417976380	0.98001174355392
O	-0.13265650542763	-1.94217071730662	2.93923831834139
H	-2.41299531071535	1.58618688878132	-2.80940866123660
H	-1.34629255152262	2.64020232186238	-2.43223272978134
H	-0.30913946858211	-2.71701152307182	2.39402647056685
H	0.80017605326404	-1.72951943023918	2.82439890898919
C	-4.82105005819781	-0.14477898942001	0.22806114697160
C	-5.59341446866769	0.06209722998989	-0.90968301030570
C	-5.43518946976549	-0.41042853202237	1.44745305451172
C	-6.97238199044555	0.00403431696839	-0.82561605383539
H	-5.10067442065577	0.25812093131134	-1.84968068320204
C	-6.81463714382779	-0.46267808511920	1.52544602687562
H	-4.81655878235184	-0.57069385473398	2.31684832923046
C	-7.58338561758890	-0.25583982830922	0.39082941892918
H	-7.57302012585275	0.16096525342852	-1.70948484938135
H	-7.29317914625230	-0.66596626968104	2.47205618076184
H	-8.66094692950302	-0.29875223403477	0.45403057307750
C	-0.75865260769695	3.70158930855713	1.65069565662794
C	-0.97258015340018	3.83975322892242	3.01808180269895

C	-0.53192941697307	4.82595017944486	0.86434984261473
C	-0.96466984813845	5.09796894421418	3.59127546035802
H	-1.14348737495955	2.95363277130085	3.60953327218596
C	-0.52067221624560	6.08090381451190	1.44482467984667
H	-0.35857084264358	4.69989981116202	-0.19342586069056
C	-0.73904748495414	6.21795012729767	2.80650149954380
H	-1.13358288161442	5.20746097513272	4.65234671582493
H	-0.34086415244849	6.95453583363787	0.83569682888169
H	-0.73161088585322	7.19975957272533	3.25702285551666
C	-0.78736505254518	-3.68341722751201	-1.71288111409939
C	-0.57927509905529	-3.79833893108801	-3.08334515147346
C	-1.01063942786133	-4.82111066995058	-0.94503638326910
C	-0.58973413888483	-5.04651193790061	-3.67799124872759
H	-0.41089945691644	-2.90221676144282	-3.66028338426903
C	-1.02431307409345	-6.06599789325946	-1.54678633698354
H	-1.17938633620071	-4.71343042650412	0.11550518467846
C	-0.81192118216725	-6.17977980045782	-2.91153846709987
H	-0.42535752442704	-5.13773828443576	-4.74150606187025
H	-1.20133874381210	-6.94994995070724	-0.95188625098227
H	-0.82121628244012	-7.15375301511106	-3.37872607382613

CuDimer-hydrated -nondefective (PBE0-D3 opt)

Cu	0.015854	-0.005864	1.269185
O	1.257687	1.498808	1.160414
O	-1.257947	-1.523483	1.094215
C	1.790129	1.800803	0.054691
O	1.512467	-1.261795	1.126559
O	-1.515913	1.259168	1.060091
C	1.807143	-1.794231	0.019645
C	2.871659	-2.834680	0.027165
C	3.186605	-3.528759	-1.143040
H	2.638994	-3.303135	-2.051966
C	4.180659	-4.499657	-1.129616
H	4.421569	-5.041750	-2.039736
C	4.866211	-4.777342	0.051615
H	5.644758	-5.535459	0.061056
C	4.553936	-4.085970	1.220769
H	5.088550	-4.303314	2.141136
C	3.556834	-3.118097	1.210970
H	3.295432	-2.569450	2.109654
O	-0.770414	-0.039181	3.384488
Cu	-0.016049	-0.005442	-1.269564
O	-1.502848	-1.272934	-1.126377
C	-1.793753	-1.807516	-0.019502
O	1.505672	1.271383	-1.061231
O	-1.269442	1.489509	-1.161418
C	-1.803875	1.787329	-0.055500
O	1.269459	-1.513676	-1.094035
O	0.772313	-0.036168	-3.384433
H	-1.384865	0.685172	3.182600
H	-1.287910	-0.838438	3.192794
H	1.380610	0.693535	-3.183190
H	1.295554	-0.830728	-3.188657
C	-2.854710	2.841190	-0.071081
C	-3.424188	3.286647	1.123574
C	-3.272195	3.387150	-1.287208

C	-4.404300	4.271350	1.102794
H	-3.087216	2.855139	2.059938
C	-4.254241	4.370127	-1.305955
H	-2.817240	3.028150	-2.204280
C	-4.820484	4.813027	-0.111980
H	-4.844481	4.618271	2.033426
H	-4.579526	4.792598	-2.252438
H	-5.587663	5.582534	-0.127856
C	-2.851239	-2.855114	-0.027038
C	-3.534368	-3.143280	-1.210883
C	-3.161845	-3.550939	1.143287
C	-4.525191	-4.117580	-1.220567
H	-3.276426	-2.593136	-2.109649
C	-4.149624	-4.528220	1.129987
H	-2.615858	-3.321486	2.052229
C	-4.833199	-4.810624	-0.051270
H	-5.058248	-4.338623	-2.140956
H	-4.387186	-5.071594	2.040221
H	-5.606866	-5.573720	-0.060629
C	2.834024	2.861514	0.070842
C	3.248342	3.409096	1.287326
C	3.400433	3.311485	-1.123579
C	4.224294	4.398111	1.306667
H	2.795870	3.046476	2.204204
C	4.374428	4.302227	-1.102198
H	3.065971	2.878622	-2.060218
C	4.787533	4.845464	0.112931
H	4.547179	4.821804	2.253424
H	4.812253	4.652623	-2.032640
H	5.549969	5.619661	0.129271

Benzoic acid dimer (xTB opt)

C	-4.23946390319319	-0.42980872578550	-0.81963247376152
O	-3.87136379984082	0.22679837799735	-1.78364864345092
C	-5.66744494862360	-0.74171930508470	-0.57965833512357
C	-6.62015281252160	-0.28039997308111	-1.48534781789848
C	-6.06482316502061	-1.48318090570905	0.53027189352853
C	-7.95768490336775	-0.55926934508508	-1.28187768406608
H	-6.29103734764596	0.29258173635727	-2.33897253652706
C	-7.40488289152954	-1.75780061268684	0.72712225887790
H	-5.31942663730165	-1.83561378376144	1.22594211364464
C	-8.35037464528174	-1.29763664380807	-0.17626598185367
H	-8.69645316868093	-0.20213198507804	-1.98376516652588
H	-7.71544589474954	-2.33227297838557	1.58718210646532
H	-9.39651928211845	-1.51502898535156	-0.01790473435794
O	-3.41626559891692	-0.91157367750822	0.07912317668397
H	-2.45710889085504	-0.67627455299705	-0.12000452964163
C	-0.56652298929928	0.43396180155119	-1.51032699606116
O	-0.93405962257269	-0.22779778382728	-0.54961157949703
C	0.86072601555401	0.75224044242390	-1.74624892389472
C	1.81423432362443	0.28440391092768	-0.84475916334518
C	1.25657166236028	1.50651458333022	-2.84806561520479
C	3.15104825300822	0.56923102241539	-1.04453822415617
H	1.48632365904073	-0.29843342612140	0.00263011247940
C	2.59589429467148	1.78726520116114	-3.04110400290386
H	0.51057263946088	1.86399080487300	-3.54050837737636

C	3.54220813023657	1.32036226210029	-2.14205739642218
H	3.89044449538315	0.20699245600873	-0.34592824492369
H	2.90522235755031	2.37190412076053	-3.89473313941804
H	4.58778213495427	1.54277032404947	-2.29728852174722
O	-1.38986660579050	0.91706368252125	-2.40824860885663
H	-2.34859738678902	0.67836702450879	-2.21134332389211

Benzoic acid dimer (PBE0-D3 opt)

C	-1.909658	-0.011484	-0.000949
O	-1.265831	1.038092	-0.001903
C	-3.390454	-0.015013	-0.000115
C	-4.061110	1.210045	-0.000360
C	-4.113165	-1.210687	0.000922
C	-5.449328	1.239460	0.000447
H	-3.476002	2.124045	-0.001168
C	-5.502286	-1.176594	0.001739
H	-3.579143	-2.154857	0.001089
C	-6.169948	0.046413	0.001496
H	-5.971807	2.191711	0.000267
H	-6.066279	-2.104880	0.002560
H	-7.256354	0.069957	0.002124
O	-1.364838	-1.206343	-0.000913
H	-0.362598	-1.125251	-0.001749
C	1.909649	0.011481	-0.000977
O	1.265838	-1.038103	-0.002129
C	3.390451	0.015014	-0.000123
C	4.061107	-1.210045	-0.000251
C	4.113168	1.210686	0.000799
C	5.449325	-1.239464	0.000567
H	3.475996	-2.124043	-0.000984
C	5.502288	1.176589	0.001611
H	3.579147	2.154855	0.000867
C	6.169948	-0.046420	0.001498
H	5.971802	-2.191716	0.000475
H	6.066285	2.104873	0.002333
H	7.256354	-0.069969	0.002140
O	1.364844	1.206351	-0.000599
H	0.362582	1.125412	-0.001419

Mulliken charges and spin density

Table S12: Mulliken charges and atomic spin densities for all Cu complexes of this study (triplet states, CAM-B3LYP/IGLO-II level, atomic sequence identical to that of the atomic coordinates above).

1a (xTB-opt)
Cu 0.391650 0.710565
O -0.498145 0.093503
O -0.498145 0.093501
C 0.743441 -0.005408
O -0.491718 0.038486
O -0.491719 0.038486
C 0.650341 0.004158
C -0.117569 0.002651
C -0.040587 0.001572
C -0.089721 -0.000669
C -0.062369 0.001454

C -0.070310 -0.000873
C -0.045292 0.001248
O -0.580964 0.000847
C 0.743444 -0.005408
O -0.580962 0.000847
O -0.412575 0.003201
C 0.650343 0.004158
O -0.412576 0.003201
H 0.111441 -0.000066
H 0.088115 0.000092
H 0.088750 -0.000067
H 0.088801 0.000039
H 0.128036 -0.000299
H 0.322037 -0.000176
H 0.322037 -0.000176
C -0.169464 0.005271
C -0.026834 -0.000364
C -0.045053 -0.000295
C -0.084692 0.000612
H 0.113329 0.000019
C -0.091884 0.000362
H 0.112608 -0.000043
C -0.069326 -0.000630
H 0.082473 0.000066
H 0.085273 -0.000001
H 0.086030 0.000026
C -0.117569 0.002652
C -0.045291 0.001247
C -0.040586 0.001571
C -0.070311 -0.000872
H 0.128036 -0.000299
C -0.089721 -0.000668
H 0.111441 -0.000066
C -0.062368 0.001453
H 0.088800 0.000039
H 0.088115 0.000092
H 0.088750 -0.000067
C -0.169467 0.005271
C -0.045051 -0.000295
C -0.026833 -0.000364
C -0.091884 0.000362
H 0.112608 -0.000043
C -0.084692 0.000612
H 0.113331 0.000019
C -0.069326 -0.000629
H 0.085273 -0.000001
H 0.082472 0.000066
H 0.086029 0.000026

1a (PBE0-D3 opt)

Cu 0.384566 0.690769
O -0.501411 0.094522
O -0.501399 0.094539
C 0.703609 -0.004570
O -0.493672 0.048437
O -0.493717 0.048431

C 0.664433 0.001496
C -0.150013 0.004334
C -0.033726 0.000942
C -0.089269 -0.000226
C -0.061596 0.000804
C -0.090048 -0.000475
C -0.021983 0.000596
O -0.553365 0.001560
C 0.703564 -0.004571
O -0.553418 0.001556
O -0.406344 0.002050
C 0.664459 0.001487
O -0.406349 0.002061
H 0.115870 -0.000029
H 0.090379 0.000087
H 0.091299 -0.000042
H 0.091360 0.000029
H 0.134851 -0.000286
H 0.317197 -0.000100
H 0.317182 -0.000101
C -0.160026 0.005747
C -0.036537 -0.000320
C -0.043446 -0.000313
C -0.086863 0.000558
H 0.114683 0.000011
C -0.093730 0.000299
H 0.116672 -0.000082
C -0.070179 -0.000512
H 0.085614 0.000071
H 0.086786 0.000002
H 0.087221 0.000021
C -0.150093 0.004340
C -0.021902 0.000591
C -0.033698 0.000938
C -0.090100 -0.000471
H 0.134856 -0.000286
C -0.089268 -0.000223
H 0.115871 -0.000029
C -0.061589 0.000799
H 0.091367 0.000029
H 0.090386 0.000087
H 0.091307 -0.000042
C -0.160024 0.005739
C -0.043453 -0.000307
C -0.036520 -0.000314
C -0.093727 0.000296
H 0.116664 -0.000082
C -0.086856 0.000553
H 0.114683 0.000011
C -0.070178 -0.000508
H 0.086787 0.000002
H 0.085612 0.000071
H 0.087221 0.000021

1a hydrated (xTB opt)

Cu 0.387605 0.720259

O -0.497201 0.094491
O -0.538055 0.081583
C 0.708660 -0.004209
O -0.493276 0.038557
O -0.511284 0.016481
C 0.643617 0.004032
C -0.122372 0.001867
C -0.037546 0.001827
C -0.089191 -0.000819
C -0.060843 0.001611
C -0.068685 -0.001007
C -0.044858 0.001499
O -0.569799 0.000664
C 0.715543 -0.003604
O -0.571996 0.001207
O -0.418085 0.001473
C 0.632676 0.000937
O -0.412360 0.003719
H 0.109647 -0.000075
H 0.086269 0.000097
H 0.086879 -0.000071
H 0.087089 0.000040
H 0.128241 -0.000123
H 0.319627 -0.000037
H 0.318942 -0.000248
C -0.156837 0.006022
C -0.027953 -0.000317
C -0.050121 -0.000565
C -0.082568 0.000691
H 0.115900 0.000032
C -0.093127 0.000415
H 0.093603 0.000010
C -0.069989 -0.000706
H 0.082143 0.000082
H 0.083803 -0.000006
H 0.085805 0.000026
C -0.110350 0.001285
C -0.040027 0.000549
C -0.039813 0.000672
C -0.068521 -0.000356
H 0.094039 -0.000192
C -0.088192 -0.000300
H 0.112190 -0.000031
C -0.064191 0.000595
H 0.085994 0.000019
H 0.087760 0.000042
H 0.087796 -0.000027
C -0.170265 0.006997
C -0.044284 -0.000416
C -0.026887 -0.000071
C -0.092834 0.000226
H 0.116480 -0.000198
C -0.083604 0.000557
H 0.111158 0.000028
C -0.069537 -0.000340
H 0.083163 0.000006
H 0.080683 0.000099

H 0.083921 0.000008
O -0.461844 0.025894
H 0.321057 -0.000770
H 0.326205 -0.000111

1a hydrated (PBE0-D3 opt)

Cu 0.447883 0.706088
O -0.556370 0.081647
O -0.512713 0.086544
C 0.688935 -0.002390
O -0.505581 0.052585
O -0.541452 0.004117
C 0.656793 0.001709
C -0.141519 0.003136
C -0.037655 0.001571
C -0.089762 -0.000615
C -0.063633 0.001423
C -0.086659 -0.000912
C -0.030421 0.001237
O -0.553737 0.001249
C 0.702508 -0.003571
O -0.551718 0.001928
O -0.415894 0.000471
C 0.609391 -0.000327
O -0.407821 0.003131
H 0.115092 -0.000055
H 0.089102 0.000102
H 0.090054 -0.000065
H 0.090526 0.000042
H 0.132451 -0.000024
H 0.320407 -0.000009
H 0.311348 -0.000252
C -0.169764 0.007248
C -0.028377 -0.000468
C -0.047789 -0.000900
C -0.088795 0.000820
H 0.115179 0.000034
C -0.093457 0.000531
H 0.120466 -0.000002
C -0.070915 -0.000853
H 0.082791 0.000091
H 0.084895 -0.000009
H 0.085490 0.000032
C -0.119166 0.000429
C -0.028406 0.000199
C -0.039246 0.000155
C -0.084567 -0.000097
H 0.104864 -0.000084
C -0.090186 -0.000080
H 0.114472 -0.000008
C -0.065170 0.000167
H 0.090054 0.000008
H 0.088894 0.000010
H 0.089262 -0.000008
C -0.161377 0.005297
C -0.044001 -0.000286

C -0.033822 0.000217
C -0.093113 0.000026
H 0.107200 -0.000055
C -0.087196 0.000309
H 0.113675 0.000000
C -0.071041 -0.000038
H 0.085634 0.000009
H 0.085188 0.000090
H 0.086857 -0.000003
O -0.454007 0.050032
H 0.331045 -0.000526
H 0.324874 -0.001048

1b (xTB-opt)

O -0.472998 0.085934
O -0.574839 0.071609
C 0.884199 -0.005404
C -0.173415 0.001155
C -0.041048 0.000371
H 0.110361 0.000013
C -0.091664 0.000882
H 0.088581 -0.000017
C -0.064125 -0.001137
H 0.090224 0.000043
C -0.089624 0.000810
H 0.089218 -0.000029
C -0.044829 0.000413
H 0.118975 0.000080
O -0.463023 0.000493
O -0.429535 -0.000178
C 0.609149 -0.000230
C -0.159672 0.000115
C -0.028268 -0.000127
H 0.110294 0.000005
C -0.090707 0.000079
H 0.088293 -0.000004
C -0.061549 -0.000118
H 0.090079 0.000005
C -0.091344 0.000074
H 0.089621 -0.000003
C -0.035023 -0.000128
H 0.126327 0.000018
Cu 0.156256 0.690667
O -0.473021 0.086093
C 0.884276 -0.005386
O -0.574633 0.071600
O -0.463111 0.000491
C 0.609172 -0.000238
O -0.429628 -0.000178
C -0.159203 0.000119
C -0.028353 -0.000131
H 0.110263 0.000005
C -0.090692 0.000083
H 0.088279 -0.000005
C -0.061586 -0.000123
H 0.090054 0.000005

C -0.091286 0.000077
H 0.089596 -0.000003
C -0.035089 -0.000132
H 0.126241 0.000018
C -0.172851 0.001151
C -0.040729 0.000376
H 0.110122 0.000014
C -0.091737 0.000885
H 0.088572 -0.000017
C -0.064111 -0.001140
H 0.090219 0.000043
C -0.089619 0.000811
H 0.089204 -0.000029
C -0.044794 0.000413
H 0.118925 0.000080
H 0.337827 -0.000135
H 0.337777 -0.000141

1b (PBE0-D3 opt)

O -0.479927 0.096449
O -0.528480 0.003480
C 0.765925 -0.004989
C -0.170077 0.005065
C -0.043415 -0.000586
H 0.113895 -0.000036
C -0.090977 0.000877
H 0.086262 0.000056
C -0.066180 -0.001016
H 0.087837 0.000043
C -0.092456 0.000626
H 0.086780 -0.000022
C -0.044441 -0.000531
H 0.118473 -0.000045
O -0.475575 0.048548
O -0.418332 -0.000142
C 0.675122 0.000661
C -0.172215 0.003243
C -0.032822 0.001314
H 0.112601 -0.000058
C -0.090570 -0.000515
H 0.090375 0.000089
C -0.056108 0.001251
H 0.091047 -0.000057
C -0.081609 -0.000757
H 0.090440 0.000036
C -0.021151 0.000991
H 0.135834 -0.000189
Cu 0.328543 0.693779
O -0.516752 0.083594
C 0.683681 -0.003609
O -0.575362 0.002134
O -0.484663 0.059585
C 0.672832 -0.002434
O -0.408844 0.002018
C -0.176387 0.006975
C -0.026401 -0.000758

H 0.116141 0.000049
C -0.090656 0.000940
H 0.091617 0.000076
C -0.059526 -0.001183
H 0.092958 0.000045
C -0.095142 0.000774
H 0.092835 -0.000023
C -0.021127 -0.001405
H 0.132309 -0.000072
C -0.156865 0.005670
C -0.050357 0.000140
H 0.111925 -0.000019
C -0.090628 0.000281
H 0.084648 0.000078
C -0.064007 -0.000003
H 0.084844 0.000000
C -0.081961 -0.000003
H 0.083923 0.000013
C -0.039973 -0.000062
H 0.122654 -0.000057
H 0.332601 -0.000226
H 0.316885 -0.000086

1a-constrained (xTB opt)

Cu 0.367510 0.656992
O -0.466002 0.053054
O -0.502158 0.112387
C 0.673395 -0.003727
O -0.501671 0.112924
O -0.465043 0.054069
C 0.705549 -0.004601
C -0.168697 0.009570
C -0.041044 -0.000703
H 0.110939 0.000037
C -0.089592 0.000985
H 0.083636 0.000102
C -0.065501 -0.001089
H 0.084789 0.000043
C -0.093693 0.000686
H 0.083089 -0.000005
C -0.036632 -0.000892
H 0.119099 -0.000352
O -0.541640 0.000009
C 0.702847 -0.004564
O -0.426857 0.000429
O -0.428281 0.000457
C 0.676340 -0.003891
O -0.542628 0.000074
C -0.168701 0.009793
C -0.036215 -0.000956
C -0.040818 -0.000707
C -0.093684 0.000696
H 0.119073 -0.000350
C -0.089690 0.001001
H 0.110697 0.000039
C -0.065544 -0.001102

H 0.083039 -0.000005
H 0.083456 0.000106
H 0.084670 0.000042
C -0.168452 0.006123
C -0.030993 -0.001063
C -0.025409 -0.000694
C -0.090804 0.000652
H 0.124826 -0.000120
C -0.089769 0.000793
H 0.120513 0.000038
C -0.058094 -0.001012
H 0.093026 -0.000017
H 0.092609 0.000059
H 0.094255 0.000039
C -0.167939 0.006100
C -0.030919 -0.001057
C -0.025132 -0.000668
C -0.090784 0.000635
H 0.124829 -0.000116
C -0.089807 0.000775
H 0.120448 0.000038
C -0.058047 -0.000983
H 0.093045 -0.000016
H 0.092632 0.000059
H 0.094267 0.000037
H 0.325588 -0.000072
H 0.326074 -0.000084

1a-constrained (PBE0-D3 opt)

O -0.425279 0.000455
O -0.533162 -0.000345
C 0.684430 -0.004202
O -0.424104 0.000439
O -0.532288 -0.000380
C 0.681728 -0.004099
C -0.164147 0.006383
C -0.032103 -0.001162
H 0.125144 -0.000113
C -0.091103 0.000728
H 0.093485 -0.000020
C -0.059173 -0.001120
H 0.094766 0.000043
C -0.089428 0.000885
H 0.093509 0.000055
C -0.030151 -0.000808
H 0.123003 0.000045
Cu 0.318704 0.650357
O -0.499020 0.111513
C 0.696974 -0.004628
O -0.457718 0.059812
O -0.499304 0.110929
C 0.694185 -0.004573
O -0.458270 0.059251
C -0.167428 0.009167
C -0.042510 -0.000748
C -0.035127 -0.001089

C -0.090239 0.001046
H 0.113929 0.000034
C -0.093904 0.000782
H 0.118939 -0.000277
C -0.066545 -0.001222
H 0.083937 0.000101
H 0.083728 -0.000015
H 0.085141 0.000049
C -0.166543 0.009259
C -0.042507 -0.000758
C -0.035083 -0.001129
C -0.090242 0.001061
H 0.113866 0.000035
C -0.093939 0.000795
H 0.119044 -0.000277
C -0.066536 -0.001237
H 0.083933 0.000102
H 0.083723 -0.000016
H 0.085126 0.000050
C -0.164835 0.006369
C -0.030200 -0.000827
C -0.032175 -0.001163
C -0.089429 0.000896
H 0.123128 0.000045
C -0.091092 0.000741
H 0.125023 -0.000115
C -0.059190 -0.001141
H 0.093507 0.000054
H 0.093479 -0.000020
H 0.094771 0.000044
H 0.322935 -0.000022
H 0.322636 -0.000016

1a hydrated-constrained (xTB opt)
Cu 0.354298 0.695239
O -0.492637 0.042630
O -0.509207 0.106995
C 0.666551 -0.003152
O -0.532627 0.094987
O -0.474264 0.049239
C 0.683662 -0.003736
C -0.157280 0.009029
C -0.043172 -0.000616
H 0.111171 0.000041
C -0.088489 0.000890
H 0.083982 0.000098
C -0.066192 -0.000975
H 0.084655 0.000036
C -0.095833 0.000619
H 0.081421 -0.000004
C -0.032247 -0.000856
H 0.096657 -0.000321
O -0.535022 -0.000144
C 0.697522 -0.004649
O -0.424373 0.000227
O -0.428225 0.000352
C 0.670789 -0.002742

O -0.536207 0.000050
C -0.171732 0.010244
C -0.035555 -0.001118
C -0.041703 -0.000748
C -0.094806 0.000722
H 0.120206 -0.000340
C -0.089727 0.001019
H 0.110243 0.000044
C -0.066312 -0.001125
H 0.081715 -0.000004
H 0.082282 0.000115
H 0.083381 0.000042
C -0.169867 0.005914
C -0.031829 -0.000946
C -0.026965 -0.000501
C -0.092058 0.000504
H 0.128765 -0.000114
C -0.089894 0.000644
H 0.119282 0.000033
C -0.058970 -0.000764
H 0.091718 -0.000011
H 0.091191 0.000061
H 0.092730 0.000027
C -0.163417 0.005173
C -0.026645 -0.000848
C -0.029061 -0.000592
C -0.093781 0.000536
H 0.106451 -0.000162
C -0.088466 0.000651
H 0.121280 0.000032
C -0.058414 -0.000823
H 0.091863 -0.000014
H 0.093322 0.000047
H 0.094469 0.000031
H 0.322164 -0.000170
H 0.321078 -0.000143
O -0.476324 -0.000509
H 0.324592 -0.000081
H 0.313860 -0.000063

1a hydrated-constrained (PBE0-D3 opt)

O -0.420954 0.000175
O -0.529278 -0.000475
C 0.674569 -0.003324
O -0.424429 0.000332
O -0.526886 -0.000444
C 0.679654 -0.003473
C -0.167474 0.006343
C -0.032483 -0.001152
H 0.128969 -0.000101
C -0.092085 0.000661
H 0.092251 -0.000018
C -0.060239 -0.001003
H 0.093136 0.000038
C -0.089741 0.000818
H 0.091851 0.000060

C -0.032353 -0.000723
H 0.121488 0.000041
Cu 0.307027 0.687485
O -0.503419 0.106452
C 0.691811 -0.004542
O -0.483247 0.050454
O -0.541309 0.091016
C 0.678417 -0.003355
O -0.462841 0.056613
C -0.172141 0.009287
C -0.044031 -0.000777
C -0.035368 -0.001200
C -0.090302 0.001047
H 0.112826 0.000035
C -0.094988 0.000794
H 0.122820 -0.000282
C -0.067301 -0.001226
H 0.082528 0.000107
H 0.082641 -0.000015
H 0.083769 0.000049
C -0.155411 0.008195
C -0.044179 -0.000637
C -0.027258 -0.000961
C -0.089184 0.000909
H 0.115146 0.000035
C -0.098341 0.000684
H 0.095697 -0.000260
C -0.066303 -0.001059
H 0.085167 0.000092
H 0.083329 -0.000013
H 0.086043 0.000041
C -0.159265 0.005720
C -0.032623 -0.000761
C -0.026035 -0.001049
C -0.088463 0.000807
H 0.124213 0.000042
C -0.094282 0.000679
H 0.106014 -0.000151
C -0.059067 -0.001036
H 0.094413 0.000049
H 0.092983 -0.000019
H 0.095446 0.000040
H 0.320328 -0.000149
H 0.316299 -0.000137
O -0.468567 -0.000577
H 0.318057 -0.000088
H 0.302958 -0.000092

1b-constrained (xTB opt)

O -0.440630 0.054568
O -0.563301 0.000317
C 0.702840 -0.004437
O -0.420135 0.000617
O -0.463835 0.105828
C 0.710329 -0.004325
C -0.166454 0.005248

C -0.040794 -0.000987
H 0.119634 0.000198
C -0.088633 0.000546
H 0.094576 -0.000009
C -0.057877 -0.000846
H 0.094841 0.000034
C -0.093048 0.000689
H 0.092430 0.000067
C -0.023994 -0.000684
H 0.123589 0.000034
O -0.466033 0.108744
C 0.775841 -0.005976
O -0.418817 0.000619
O -0.564508 0.000756
C 0.768719 -0.005849
O -0.443682 0.054000
C -0.175717 0.007073
C -0.041589 -0.000882
C -0.042838 -0.000593
C -0.093367 0.000934
H 0.116279 0.000037
C -0.091876 0.000677
H 0.113212 0.000147
C -0.067152 -0.001141
H 0.082634 0.000077
H 0.083661 -0.000010
H 0.084428 0.000052
C -0.170517 0.007139
C -0.044298 -0.000644
C -0.043206 -0.000902
C -0.091966 0.000712
H 0.112649 0.000135
C -0.093551 0.000956
H 0.116924 0.000049
C -0.067253 -0.001169
H 0.083567 -0.000010
H 0.082650 0.000076
H 0.084359 0.000052
C -0.158824 0.005253
C -0.042794 -0.000953
C -0.025545 -0.000631
C -0.088630 0.000515
H 0.120037 0.000201
C -0.093666 0.000663
H 0.123040 0.000037
C -0.058124 -0.000789
H 0.094634 -0.000008
H 0.092368 0.000068
H 0.094782 0.000031
H 0.353818 -0.000175
H 0.353303 -0.000164
Cu 0.067507 0.674037

1b-constrained (PBE0-D3 opt)

O -0.449548 0.001237
O -0.444594 0.102352

C 0.709171 -0.004745
O -0.412708 0.056939
O -0.555324 0.000748
C 0.708894 -0.004734
C -0.163731 0.004930
C -0.023652 -0.000912
H 0.128155 0.000045
C -0.092933 0.000753
H 0.093538 0.000039
C -0.059986 -0.000961
H 0.094446 0.000041
C -0.090350 0.000605
H 0.093143 -0.000007
C -0.048848 -0.000803
H 0.121925 0.000203
O -0.554776 0.000687
C 0.744832 -0.006685
O -0.412294 0.057018
O -0.444287 0.101685
C 0.745154 -0.006666
O -0.449018 0.001243
C -0.159898 0.006970
C -0.054240 -0.000724
C -0.038960 -0.001054
C -0.092089 0.000732
H 0.114453 0.000204
C -0.093412 0.000991
H 0.119085 0.000060
C -0.067330 -0.001181
H 0.084891 -0.000007
H 0.085304 0.000057
H 0.086212 0.000051
C -0.160048 0.006959
C -0.039020 -0.001060
C -0.054228 -0.000730
C -0.093419 0.000990
H 0.119130 0.000060
C -0.092076 0.000735
H 0.114469 0.000204
C -0.067315 -0.001183
H 0.085319 0.000057
H 0.084911 -0.000006
H 0.086231 0.000051
C -0.163693 0.004925
C -0.023674 -0.000913
C -0.048905 -0.000804
C -0.092929 0.000754
H 0.128184 0.000045
C -0.090345 0.000607
H 0.121939 0.000204
C -0.059979 -0.000963
H 0.093560 0.000039
H 0.093166 -0.000007
H 0.094465 0.000041
H 0.344475 -0.000315
H 0.344457 -0.000310
Cu 0.054102 0.681514

Cu(I)Cu(II)-activated (xTB opt)

Cu 0.330045 0.351914
O -0.521231 0.027297
O -0.521232 0.027297
C 0.751558 -0.006132
O -0.526336 0.042373
O -0.526337 0.042373
C 0.751556 -0.006131
C -0.177481 0.012401
C -0.043028 -0.001542
H 0.115691 0.000078
C -0.094873 0.001012
H 0.062538 0.000063
C -0.076436 -0.001327
H 0.060384 0.000049
C -0.094550 0.000910
H 0.061927 0.000074
C -0.045492 -0.001299
H 0.112304 0.000069
Cu 0.330055 0.351959
O -0.526336 0.042378
C 0.751559 -0.006132
O -0.526336 0.042378
O -0.521232 0.027301
C 0.751554 -0.006132
O -0.521233 0.027301
C -0.177481 0.012401
C -0.043028 -0.001542
C -0.045492 -0.001299
C -0.094873 0.001012
H 0.115693 0.000078
C -0.094550 0.000910
H 0.112303 0.000069
C -0.076436 -0.001327
H 0.062539 0.000063
H 0.061927 0.000074
H 0.060384 0.000049
C -0.177481 0.012401
C -0.045492 -0.001299
C -0.043028 -0.001542
C -0.094550 0.000910
H 0.112305 0.000069
C -0.094872 0.001012
H 0.115691 0.000077
C -0.076436 -0.001326
H 0.061927 0.000074
H 0.062538 0.000063
H 0.060384 0.000049
C -0.177481 0.012401
C -0.043028 -0.001542
C -0.045492 -0.001299
C -0.094872 0.001012
H 0.115693 0.000078
C -0.094550 0.000910
H 0.112303 0.000069

C -0.076436 -0.001327
H 0.062539 0.000063
H 0.061927 0.000074
H 0.060384 0.000049

Cu(I)Cu(II)-activated (PBE0-D3 opt)

Cu 0.263440 -0.000447
O -0.496148 0.000008
O -0.496200 0.000010
C 0.724120 -0.004875
O -0.526956 -0.001654
O -0.526959 -0.001654
C 0.774244 -0.001669
C -0.178133 0.007526
C -0.039958 -0.001110
H 0.121055 -0.000146
C -0.095913 0.000574
H 0.065176 -0.000014
C -0.075248 -0.000891
H 0.062787 0.000033
C -0.095118 0.000779
H 0.064451 0.000090
C -0.043827 -0.000670
H 0.115965 0.000067
Cu 0.360579 0.687715
O -0.536846 0.089234
C 0.724200 -0.004877
O -0.536866 0.089269
O -0.525755 0.062849
C 0.774242 -0.001669
O -0.525758 0.062847
C -0.163414 0.006785
C -0.053226 -0.000727
C -0.049492 -0.000405
C -0.093729 0.000732
H 0.111902 0.000043
C -0.095359 0.000487
H 0.111948 0.000012
C -0.078760 -0.000838
H 0.062159 0.000082
H 0.061843 0.000007
H 0.060253 0.000040
C -0.178133 0.007526
C -0.043826 -0.000670
C -0.039959 -0.001110
C -0.095118 0.000779
H 0.115966 0.000067
C -0.095913 0.000574
H 0.121055 -0.000146
C -0.075248 -0.000891
H 0.064452 0.000090
H 0.065176 -0.000014
H 0.062788 0.000033
C -0.163403 0.006781
C -0.053241 -0.000724

C -0.049514 -0.000401
C -0.093728 0.000729
H 0.111901 0.000043
C -0.095359 0.000484
H 0.111935 0.000012
C -0.078765 -0.000835
H 0.062153 0.000082
H 0.061835 0.000007
H 0.060246 0.000039

Cu(I)Cu(II)-hydrated (xTB opt)

O -0.521419 0.034532
O -0.564239 0.030602
C 0.737897 -0.006128
O -0.515399 0.019471
O -0.556896 0.013571
C 0.752261 -0.006056
C -0.167574 0.011667
C -0.039576 -0.001442
H 0.108775 0.000029
C -0.096210 0.000967
H 0.066972 0.000051
C -0.074492 -0.001414
H 0.063747 0.000054
C -0.094249 0.001088
H 0.065532 0.000067
C -0.045155 -0.001545
H 0.119046 0.000112
O -0.494019 0.002375
Cu 0.351958 0.430925
O -0.519422 0.038008
C 0.720117 -0.006244
O -0.577301 0.033740
O -0.521025 0.055017
C 0.745083 -0.005704
O -0.573125 0.050564
O -0.555268 -0.000051
H 0.310435 0.000129
H 0.304728 -0.000236
H 0.290827 0.000123
H 0.280296 -0.000136
C -0.172074 0.013461
C -0.027016 -0.001589
C -0.048008 -0.001475
C -0.101661 0.001056
H 0.109821 -0.000003
C -0.094772 0.001039
H 0.121719 0.000016
C -0.074178 -0.001420
H 0.067520 0.000072
H 0.064573 0.000082
H 0.062904 0.000049
C -0.164668 0.011225
C -0.048427 -0.001422
C -0.038025 -0.001449
C -0.094257 0.000929

H 0.116833 0.000010
C -0.098556 0.001089
H 0.105317 0.000104
C -0.074486 -0.001374
H 0.065917 0.000040
H 0.066466 0.000072
H 0.064214 0.000052
C -0.162424 0.013726
C -0.047305 -0.001845
C -0.046773 -0.001992
C -0.095917 0.001330
H 0.107326 0.000124
C -0.094734 0.001305
H 0.117786 0.000081
C -0.075129 -0.001789
H 0.065637 0.000074
H 0.065639 0.000049
H 0.063707 0.000065
Cu 0.290725 0.274171

Cu(I)Cu(II)-hydrated (PBE0-D3 opt)

O -0.535551 0.081258
O -0.578098 0.067872
C 0.667457 -0.002645
O -0.531690 0.088479
O -0.573475 0.062987
C 0.664865 -0.002971
C -0.158749 0.007691
C -0.054261 -0.000047
H 0.106292 0.000022
C -0.091878 0.000536
H 0.063743 0.000118
C -0.077047 -0.000365
H 0.062637 0.000009
C -0.099542 0.000255
H 0.067249 0.000008
C -0.043152 -0.000625
H 0.131104 -0.000050
O -0.516930 -0.000422
Cu 0.227205 -0.000816
O -0.519553 -0.000749
C 0.745537 -0.002369
O -0.545566 -0.000563
O -0.528742 0.000451
C 0.777094 -0.002536
O -0.543198 0.000769
O -0.531961 -0.000468
H 0.287034 -0.000011
H 0.291251 -0.000055
H 0.341403 0.000084
H 0.337302 0.000070
C -0.158542 0.008311
C -0.048885 -0.000499
C -0.032771 -0.001067
C -0.092049 0.000779
H 0.104123 0.000044

C -0.099123 0.000514
H 0.127664 -0.000020
C -0.076285 -0.000794
H 0.063506 0.000117
H 0.066145 -0.000003
H 0.062482 0.000028
C -0.163054 0.006187
C -0.053676 -0.000351
C -0.031563 -0.000761
C -0.092749 0.000570
H 0.113328 0.000038
C -0.100809 0.000382
H 0.115393 -0.000091
C -0.073709 -0.000540
H 0.068588 0.000081
H 0.072364 0.000003
H 0.067844 0.000018
C -0.159801 0.006993
C -0.037108 -0.000817
C -0.053378 -0.000448
C -0.097824 0.000469
H 0.119936 -0.000089
C -0.093245 0.000677
H 0.112195 0.000054
C -0.074656 -0.000710
H 0.071206 -0.000003
H 0.066377 0.000099
H 0.065865 0.000025
Cu 0.401432 0.684886
Atom Charge Spin
O -0.535551 0.081258
O -0.578098 0.067872
C 0.667457 -0.002645
O -0.531690 0.088479
O -0.573475 0.062987
C 0.664865 -0.002971
C -0.158749 0.007691
C -0.054261 -0.000047
H 0.106292 0.000022
C -0.091878 0.000536
H 0.063743 0.000118
C -0.077047 -0.000365
H 0.062637 0.000009
C -0.099542 0.000255
H 0.067249 0.000008
C -0.043152 -0.000625
H 0.131104 -0.000050
O -0.516930 -0.000422
Cu 0.227205 -0.000816
O -0.519553 -0.000749
C 0.745537 -0.002369
O -0.545566 -0.000563
O -0.528742 0.000451
C 0.777094 -0.002536
O -0.543198 0.000769
O -0.531961 -0.000468
H 0.287034 -0.000011

H 0.291251 -0.000055
H 0.341403 0.000084
H 0.337302 0.000070
C -0.158542 0.008311
C -0.048885 -0.000499
C -0.032771 -0.001067
C -0.092049 0.000779
H 0.104123 0.000044
C -0.099123 0.000514
H 0.127664 -0.000020
C -0.076285 -0.000794
H 0.063506 0.000117
H 0.066145 -0.000003
H 0.062482 0.000028
C -0.163054 0.006187
C -0.053676 -0.000351
C -0.031563 -0.000761
C -0.092749 0.000570
H 0.113328 0.000038
C -0.100809 0.000382
H 0.115393 -0.000091
C -0.073709 -0.000540
H 0.068588 0.000081
H 0.072364 0.000003
H 0.067844 0.000018
C -0.159801 0.006993
C -0.037108 -0.000817
C -0.053378 -0.000448
C -0.097824 0.000469
H 0.119936 -0.000089
C -0.093245 0.000677
H 0.112195 0.000054
C -0.074656 -0.000710
H 0.071206 -0.000003
H 0.066377 0.000099
H 0.065865 0.000025
Cu 0.401432 0.684886

Cu(I)Cu(II)-TS (PBE0-D3 opt)

Cu 0.311571 0.355121
Cu 0.311571 0.355121
O -0.523137 0.039475
C 0.757736 -0.006246
O -0.524173 0.029964
C -0.173539 0.011188
C -0.044123 -0.001600
C -0.049789 -0.001225
C -0.095856 0.001022
H 0.118804 0.000055
C -0.094652 0.000898
H 0.112769 0.000090
C -0.077055 -0.001350
H 0.063429 0.000043
H 0.062623 0.000072
H 0.061177 0.000053
O -0.523137 0.039475

C 0.757736 -0.006246
O -0.524173 0.029964
C -0.173539 0.011188
C -0.044123 -0.001600
C -0.049789 -0.001225
C -0.095856 0.001022
H 0.118804 0.000055
C -0.094652 0.000898
H 0.112769 0.000090
C -0.077055 -0.001350
H 0.063429 0.000043
H 0.062623 0.000072
H 0.061177 0.000053
O -0.523137 0.039475
C 0.757736 -0.006246
O -0.524173 0.029964
C -0.173539 0.011188
C -0.044123 -0.001600
C -0.049789 -0.001225
C -0.095856 0.001022
H 0.118804 0.000055
C -0.094652 0.000898
H 0.112769 0.000090
C -0.077055 -0.001350
H 0.063429 0.000043
H 0.062623 0.000072
H 0.061177 0.000053
O -0.523137 0.039475
C 0.757736 -0.006246
O -0.524173 0.029964
C -0.173539 0.011188
C -0.044123 -0.001600
C -0.049789 -0.001225
C -0.095856 0.001022
H 0.118804 0.000055
C -0.094652 0.000898
H 0.112769 0.000090
C -0.077055 -0.001350
H 0.063429 0.000043
H 0.062623 0.000072
H 0.061177 0.000053

Cu(I)Cu(II)-activated-constrained (xTB opt)

Cu 0.324336 0.337834
O -0.522284 0.039965
O -0.521654 0.040012
C 0.754815 -0.009080
O -0.524110 0.040256
O -0.523973 0.040231
C 0.759160 -0.009058
C -0.182672 0.015028
C -0.041761 -0.003002
H 0.115000 0.000100
C -0.096586 0.002047
H 0.061173 0.000031
C -0.076254 -0.002998

H 0.059451 0.000119
C -0.096590 0.002044
H 0.061142 0.000031
C -0.041821 -0.003000
H 0.115000 0.000099
Cu 0.323949 0.336423
O -0.521841 0.040190
C 0.752878 -0.009077
O -0.522427 0.040141
O -0.523839 0.039726
C 0.759115 -0.009057
O -0.523759 0.039698
C -0.175012 0.015286
C -0.043653 -0.003256
C -0.043685 -0.003250
C -0.096775 0.002242
H 0.114887 0.000115
C -0.096747 0.002241
H 0.114840 0.000114
C -0.076475 -0.003278
H 0.061180 0.000022
H 0.061169 0.000023
H 0.059393 0.000130
C -0.182533 0.015032
C -0.041859 -0.003002
C -0.041781 -0.003007
C -0.096580 0.002048
H 0.114957 0.000098
C -0.096602 0.002050
H 0.115036 0.000101
C -0.076258 -0.003002
H 0.061158 0.000031
H 0.061164 0.000031
H 0.059454 0.000119
C -0.177055 0.015212
C -0.043125 -0.003191
C -0.043185 -0.003184
C -0.096734 0.002190
H 0.114892 0.000110
C -0.096710 0.002190
H 0.114830 0.000110
C -0.076416 -0.003206
H 0.061186 0.000024
H 0.061171 0.000025
H 0.059419 0.000127

Cu(I)Cu(II)-activated-constrained (PBE0-D3 opt)

Cu 0.260057 0.004823
O -0.501563 0.000911
O -0.501760 0.000916
C 0.762199 -0.004832
O -0.525063 -0.000007
O -0.525019 -0.000007
C 0.734923 -0.003005
C -0.171569 0.008832
C -0.048083 -0.000967

H 0.115914 -0.000156
C -0.093244 0.000558
H 0.062376 0.000006
C -0.075025 -0.000870
H 0.060507 0.000031
C -0.094649 0.000768
H 0.062687 0.000097
C -0.040675 -0.000781
H 0.117840 0.000089
Cu 0.340320 0.682825
O -0.523580 0.083444
C 0.762358 -0.004834
O -0.523692 0.083502
O -0.526347 0.065843
C 0.734967 -0.003004
O -0.526298 0.065837
C -0.171352 0.006665
C -0.043579 -0.000765
C -0.051879 -0.000328
C -0.094343 0.000685
H 0.118485 0.000073
C -0.092918 0.000435
H 0.110245 0.000079
C -0.076137 -0.000787
H 0.062874 0.000072
H 0.061506 0.000020
H 0.060338 0.000035
C -0.171596 0.008833
C -0.040679 -0.000781
C -0.048082 -0.000967
C -0.094650 0.000768
H 0.117834 0.000089
C -0.093244 0.000558
H 0.115906 -0.000156
C -0.075028 -0.000870
H 0.062683 0.000097
H 0.062371 0.000006
H 0.060504 0.000031
C -0.171353 0.006669
C -0.043609 -0.000768
C -0.051874 -0.000331
C -0.094335 0.000689
H 0.118475 0.000073
C -0.092925 0.000439
H 0.110240 0.000079
C -0.076144 -0.000790
H 0.062864 0.000072
H 0.061495 0.000019
H 0.060329 0.000035

Cu(I)Cu(II)-hydrated-constrained (xTB opt)

O -0.522570 0.042306
O -0.556147 0.033623
C 0.758626 -0.011287
O -0.521515 0.033230
O -0.548378 0.030102

C 0.743823 -0.006757
C -0.170838 0.013417
C -0.036171 -0.002127
H 0.098210 0.000036
C -0.101003 0.001503
H 0.063349 0.000053
C -0.074831 -0.002118
H 0.061960 0.000079
C -0.096786 0.001507
H 0.064543 0.000048
C -0.040959 -0.002200
H 0.121723 0.000051
O -0.481375 -0.000358
Cu 0.256156 0.363333
O -0.520656 0.036480
C 0.743762 -0.007791
O -0.552454 0.032525
O -0.523261 0.043985
C 0.767105 -0.011598
O -0.555062 0.035846
O -0.480806 -0.000271
H 0.305428 0.000022
H 0.310261 -0.000040
H 0.306846 0.000050
H 0.307940 -0.000055
C -0.171133 0.015786
C -0.041152 -0.002993
C -0.047013 -0.003016
C -0.100907 0.002075
H 0.098645 0.000130
C -0.097023 0.002030
H 0.118749 0.000095
C -0.078284 -0.002906
H 0.063349 0.000044
H 0.064574 0.000034
H 0.061926 0.000113
C -0.173604 0.015603
C -0.046403 -0.003198
C -0.042199 -0.003101
C -0.097117 0.002121
H 0.119003 0.000098
C -0.100417 0.002175
H 0.098640 0.000139
C -0.078280 -0.003064
H 0.064681 0.000021
H 0.063369 0.000039
H 0.061983 0.000121
C -0.165940 0.015318
C -0.039945 -0.001981
C -0.045438 -0.002041
C -0.101438 0.001398
H 0.098193 0.000099
C -0.096954 0.001391
H 0.118959 0.000086
C -0.077949 -0.001855
H 0.063859 0.000080
H 0.065032 0.000069

H 0.062399 0.000066
Cu 0.250912 0.341431

Cu(I)Cu(II)-hydrated-constrained (PBE0-D3 opt)

O -0.517414 0.001537
O -0.564944 0.001283
C 0.714280 -0.002864
O -0.501320 0.000062
O -0.553734 -0.000195
C 0.748827 -0.003979
C -0.170085 0.006791
C -0.047507 -0.000496
H 0.104840 0.000077
C -0.095593 0.000434
H 0.065108 0.000015
C -0.074335 -0.000735
H 0.063720 0.000030
C -0.094021 0.000668
H 0.066537 0.000084
C -0.043297 -0.000655
H 0.122898 0.000079
O -0.515137 0.000055
Cu 0.357451 0.693516
O -0.518906 0.067909
C 0.716445 -0.003836
O -0.580239 0.049345
O -0.512983 0.088509
C 0.748560 -0.004849
O -0.571657 0.075220
O -0.492499 0.003834
H 0.299384 0.000019
H 0.291911 -0.000042
H 0.307998 0.000393
H 0.296550 -0.000462
C -0.167206 0.007159
C -0.036307 -0.000767
C -0.044796 -0.000646
C -0.099432 0.000452
H 0.101091 -0.000077
C -0.094767 0.000601
H 0.125826 0.000072
C -0.073464 -0.000691
H 0.064374 0.000013
H 0.065753 0.000075
H 0.062843 0.000025
C -0.167488 0.007946
C -0.053053 -0.000698
C -0.037595 -0.000789
C -0.093354 0.000544
H 0.120820 -0.000087
C -0.098342 0.000802
H 0.113609 0.000078
C -0.074128 -0.000870
H 0.064840 0.000011
H 0.066782 0.000092
H 0.063052 0.000035

C -0.162516 0.008989
C -0.043322 -0.000843
C -0.048875 -0.001114
C -0.095492 0.000833
H 0.115220 0.000096
C -0.093503 0.000615
H 0.120351 -0.000025
C -0.073921 -0.000941
H 0.066440 0.000098
H 0.065138 0.000007
H 0.063285 0.000034
Cu 0.227297 0.007226

CuDimer-activated -nondefective (xTB opt)

Cu 0.399770 0.641226
O -0.468743 0.085718
O -0.468515 0.085878
C 0.677766 -0.006060
O -0.498528 0.081866
O -0.468443 0.085151
C 0.772945 -0.006548
C -0.189176 0.016875
C -0.033233 -0.001884
H 0.120931 -0.000100
C -0.092729 0.001616
H 0.087498 0.000079
C -0.063001 -0.002142
H 0.088967 0.000076
C -0.092734 0.001616
H 0.087494 0.000079
C -0.033244 -0.001884
H 0.120935 -0.000099
Cu 0.399213 0.641107
O -0.468794 0.086017
C 0.678666 -0.006108
O -0.468688 0.085728
O -0.468570 0.085146
C 0.680825 -0.006092
O -0.498474 0.081866
C -0.244203 0.016075
H 0.100352 0.000870
H 0.100355 0.001049
H 0.109325 -0.000953
C -0.244046 0.015797
H 0.101183 0.000950
H 0.107713 -0.000914
H 0.101190 0.001001
C -0.244158 0.016036
H 0.109626 -0.000945
H 0.100268 0.000954
H 0.100259 0.000952

CuDimer-hydrated -nondefective (xTB opt)

Cu 0.371973 0.692096
O -0.476209 0.080922

O -0.501270 0.072194
C 0.667376 -0.005062
O -0.504338 0.071554
O -0.502613 0.064581
C 0.753894 -0.005329
C -0.173018 0.014805
C -0.041031 -0.001187
H 0.104511 -0.000045
C -0.094366 0.001101
H 0.085500 0.000087
C -0.064681 -0.001269
H 0.087803 0.000039
C -0.093810 0.001107
H 0.086929 0.000077
C -0.038745 -0.001310
H 0.124799 -0.000054
O -0.473861 -0.000286
Cu 0.368806 0.691767
O -0.477942 0.076610
C 0.668601 -0.005207
O -0.506206 0.062909
O -0.475735 0.079243
C 0.670532 -0.005042
O -0.523308 0.070374
O -0.473585 0.000093
C -0.248349 0.014630
H 0.090774 0.000598
H 0.100896 0.000989
H 0.105327 -0.000775
C -0.249225 0.014191
H 0.093235 0.000373
H 0.101410 -0.000616
H 0.101177 0.001063
C -0.249073 0.014341
H 0.103782 -0.000658
H 0.092538 0.000390
H 0.099543 0.001010
H 0.323640 -0.000031
H 0.321710 -0.000122
H 0.324124 -0.000004
H 0.318485 -0.000145
