SUPPORTING INFORMATION FOR,

The Oxidation of Cu(I) Hexaaza Macrocyclic Dinuclear Complexes

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Table S1. xyz coordinates and figures of the calculated **1-8** structures.

1

Cu	-0.003683	0.046317	0.032315
Cu	-0.013203	0.074238	3.626695
N	1.928707	0.133382	-0.744996
N	-1.296275	1.315824	-0.807746
N	-0.946950	1.567599	4.514282
N	1.932745	-0.210590	4.355525
N	-0.372776	-1.111447	-1.548744
N	-0.528803	-1.040643	5.224730
O	0.172466	0.527395	1.824597
O	0.204119	-0.885565	1.846640
C	-1.297655	1.151582	5.859092
C	-1.636583	-0.310633	5.845397
H	-2.541358	-0.475649	5.235240
H	-1.839954	-0.672303	6.872079
C	1.906634	-1.246907	5.349652
C	0.627203	-1.178736	6.118639
H	1.971086	-2.209957	4.802773
H	0.514135	-2.056432	6.781579
C	-1.723853	-0.755682	-1.979066
C	-1.848854	0.741143	-2.023802
H	-2.912564	1.018420	-2.135319
H	-1.315412	1.160262	-2.898607
H	-2.427742	-1.167122	-1.235319
H	-1.971231	-1.191938	-2.966605
C	1.994159	-0.720863	-1.903290
C	0.657119	-0.818444	-2.545954
H	0.657064	-1.570633	-3.356901
H	2.754631	-0.388128	-2.637004
H	0.408908	0.156314	-2.999874
C	-0.151225	5.273241	1.587053
C	-0.296794	4.682182	2.825502
C	-0.509862	4.581028	0.448336
C	-0.997462	3.280565	0.542820
C	-0.790647	3.384179	2.932154
C	-1.004766	2.815401	4.237404
C	-1.401478	2.580875	-0.649421
H	0.216335	6.300656	1.510258
H	-0.042154	5.243283	3.731879
H	-0.425133	5.060885	-0.533408
H	-1.840941	3.192390	-1.460583
C	-1.169857	2.698704	1.788835
H	-1.259246	3.527179	5.045111
H	-0.336104	-2.109729	-1.282596
H	-0.848589	-1.973198	4.916664
H	-1.670635	1.732009	1.871117
H	-0.428174	1.342641	6.518449
H	-2.144978	1.738407	6.255448
H	2.771340	-1.205528	6.041311
H	0.652002	-0.284752	6.765821
H	2.315129	-1.718884	-1.538689
C	2.931960	0.575963	4.268696
C	2.857571	0.984606	-0.540738
C	3.954232	3.417752	2.065463
C	3.715802	2.680533	3.209110
C	3.645412	2.889307	0.826860
C	3.095313	1.439868	3.122633
C	3.032239	1.645425	0.729229
C	2.737155	0.931253	1.882263
H	4.442970	4.393609	2.136571
H	4.035819	3.064995	4.184245
H	3.910243	3.440143	-0.082761
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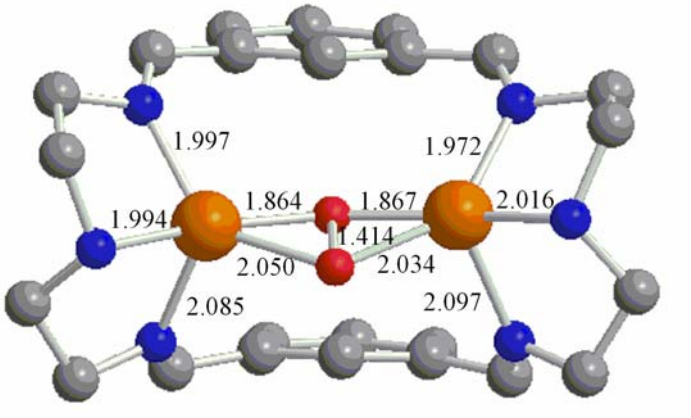

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N	-2.307985	1.556552	1.150913
N	3.106052	1.151799	0.747810
N	2.952271	-1.972666	0.799978
N	-2.448469	-0.382794	3.461297
N	3.226660	-0.385618	3.398772
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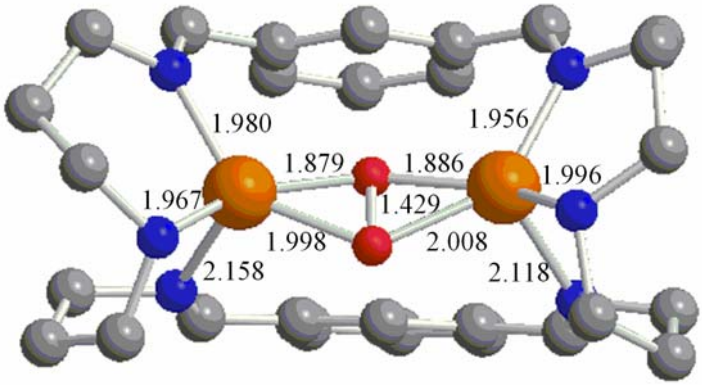
O	0.345008	-0.384574	1.157375
C	4.509963	0.989035	1.034157
C	4.874235	1.263749	2.461169
C	3.825461	0.953109	3.493366
H	5.100857	2.338679	2.584653
H	5.821155	0.742152	2.692950
H	2.988554	1.668249	3.391113
H	4.264353	1.089753	4.502747
C	3.990338	-2.755228	1.442023
C	4.846571	-2.041986	2.433357
C	4.138992	-1.508159	3.646423
H	3.461114	-3.581578	1.960792
H	5.582012	-2.783737	2.796795
H	4.885307	-1.201675	4.407745
H	3.541408	-2.324433	4.094139
C	-2.574164	0.974323	4.005466
C	-3.612602	1.631382	1.752233
C	-3.573037	1.822833	3.252283
H	-3.342179	2.878125	3.483257
H	-4.596988	1.657090	3.633182
H	-1.569119	1.427645	3.935892
H	-2.857817	0.939333	5.076436
C	-3.680638	-2.024599	1.114305
C	-3.649469	-2.354997	2.586729
C	-3.680744	-1.166661	3.509114
H	-3.993859	-2.915142	0.539261
H	-4.535392	-2.975437	2.810024
H	-3.880235	-1.491004	4.550126
H	-4.438541	-1.237193	0.926768
H	-2.772878	-2.996411	2.802788
H	-4.517328	-0.502565	3.225648
C	0.226922	2.928666	-2.681260
C	1.438369	2.603633	-2.110894
C	-0.923545	2.804294	-1.932773
C	-0.868716	2.340959	-0.619604
C	1.509103	2.136447	-0.799579
C	2.821297	1.853987	-0.280180
C	-2.102030	2.281185	0.120860
H	0.182450	3.316576	-3.703059
H	2.364629	2.733856	-2.682863
H	-1.890305	3.095447	-2.359954
H	-2.923186	2.918301	-0.263827
C	0.352173	2.020617	-0.042219
H	3.652994	2.295347	-0.866006
H	-1.733066	-0.878101	4.021978
H	2.494032	-0.421284	4.126951
H	0.407983	1.775985	1.024819
H	-4.122612	0.674172	1.523394
H	-4.230352	2.430232	1.296075
H	4.746979	-0.062708	0.779303
H	5.134813	1.612412	0.362845
H	4.625055	-3.230787	0.667494
H	5.455537	-1.261194	1.947979
C	2.750094	-2.146570	-0.451423
C	-2.113332	-1.784058	-0.615958
C	0.506433	-0.475292	-2.935779
C	1.657101	-0.930498	-2.321043
C	-0.732047	-0.744970	-2.386243
C	1.573167	-1.642604	-1.132407
C	-0.825106	-1.467963	-1.203704
C	0.327499	-1.942485	-0.596782
H	0.573710	0.087661	-3.871668
H	2.636435	-0.726525	-2.769422
H	-1.641759	-0.390582	-2.884825
H	0.255216	-2.580701	0.288107
H	3.465262	-2.759473	-1.034663
H	-2.866179	-2.272283	-1.264629



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Cu	-1.768339	-0.736914	0.780042
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N	-3.012620	0.374439	-0.349649
N	2.826842	0.623036	-0.288622
N	2.764739	-2.478543	0.482179
N	-3.201550	-0.169241	2.384689
N	3.045203	-0.319330	2.292412
O	-0.027890	0.055409	0.797930
O	-0.016070	-1.237721	1.419215
C	2.985598	1.610238	0.784460
C	3.664662	0.962183	1.962645
H	3.579697	2.482175	0.439422
H	1.974924	1.972881	1.052102
H	3.663160	1.660695	2.818023
H	4.730629	0.787446	1.720066
C	3.283326	-2.702347	1.835448
C	3.944342	-1.464114	2.339545
H	2.416795	-2.965599	2.471681
H	3.992412	-3.553747	1.865402
H	4.816584	-1.235489	1.697184
H	4.358423	-1.649884	3.349039
C	-4.101514	0.800348	1.766388
C	-3.474645	1.428300	0.554351
H	-4.419616	1.587541	2.473853
H	-5.028246	0.274681	1.463331
H	-4.203808	2.095371	0.049350
H	-2.595208	2.038787	0.834499
C	-4.045533	-2.286412	1.529745
C	-3.846498	-1.424249	2.745185
H	-4.525240	-3.244668	1.809848
H	-3.193523	-1.950186	3.465809
H	-4.731084	-1.796727	0.809941
H	-4.822004	-1.273918	3.250593
C	-0.265427	3.846069	-1.157751
C	0.973671	3.239781	-1.238835
C	-1.409502	3.084413	-1.297006
C	-1.321457	1.718200	-1.516483
C	1.076280	1.877163	-1.469383
C	2.401152	1.221541	-1.565728
C	-2.540969	0.888225	-1.647454
H	-0.339292	4.927289	-1.009178
H	1.882596	3.847316	-1.155460
H	-2.392393	3.569551	-1.267542
H	-3.352852	1.477085	-2.121235
H	-2.333207	0.015500	-2.291275
C	-0.075667	1.125421	-1.618229
H	3.161091	1.960754	-1.890248
H	2.373504	0.414998	-2.319524
H	3.571133	-2.271703	-0.131949
H	-2.166379	-3.059659	1.472862
H	-3.828554	-0.231800	-0.554398
H	-2.747144	0.240116	3.211447
H	2.505488	-0.249550	3.165443
H	3.758508	0.202310	-0.460854
H	-0.001864	0.049152	-1.828346
C	2.068550	-3.657286	-0.073167
C	-2.827147	-3.112892	-0.459665
C	-0.057391	-2.411406	-2.938278
C	1.054794	-2.776716	-2.201630
C	-1.323795	-2.524000	-2.388320
C	0.905448	-3.276469	-0.915328
C	-1.488520	-3.020557	-1.105950
C	-0.367287	-3.410851	-0.393315
H	0.059294	-2.055069	-3.966659
H	2.051220	-2.714535	-2.656127
H	-2.203176	-2.256244	-2.986690
H	-0.469377	-3.844179	0.609651
H	2.781105	-4.289007	-0.636802
H	1.715880	-4.263618	0.778769
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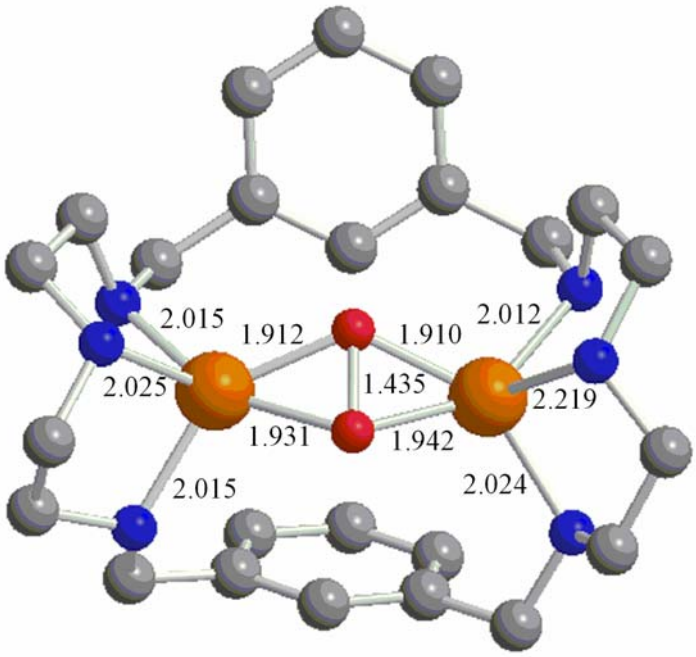

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Cu	-1.774296	-0.385564	0.810617
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N	-2.810320	1.066580	-0.104658
N	2.856120	1.113063	-0.127994
N	3.004262	-1.954967	-0.247575
N	-2.760705	-0.304339	2.559199
N	2.705466	-0.361091	2.511505
O	0.007361	-0.187439	0.189315
O	0.053096	-1.023919	1.346914
C	2.931761	2.263230	0.776245
C	3.571117	1.931357	2.078477
C	2.796360	1.019458	2.993797
H	3.504052	3.078126	0.283118
H	1.900940	2.642338	0.919567
H	3.728589	2.879963	2.622826
H	4.594646	1.538992	1.913268
H	1.763688	1.401021	3.102091
H	3.263446	1.029140	4.000967
C	4.184972	-2.369562	0.520428
C	3.961372	-2.431160	1.992743
C	3.952957	-1.105061	2.683645
H	5.004596	-1.655254	0.311920
H	4.537194	-3.353669	0.148459
H	3.036072	-2.995768	2.225117
H	4.777973	-3.030175	2.434473
H	4.777190	-0.482783	2.286812
H	4.153458	-1.225143	3.768291
C	-2.814958	1.090060	3.016566
C	-2.879865	2.252437	0.754405
C	-3.538480	1.995939	2.075149
H	-3.644934	2.973660	2.578959
H	-4.581206	1.656032	1.921659
H	-1.772184	1.437921	3.141565
H	-3.302156	1.132273	4.013479
H	-3.436376	3.054287	0.224171
H	-1.845338	2.622216	0.892619
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C	-4.114556	-2.344944	2.081937
C	-4.070534	-0.951941	2.643777
H	-4.407446	-3.447084	0.266073
H	-5.065774	-2.796356	2.415685
H	-4.403395	-0.955137	3.702624
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H	-3.327315	-2.974467	2.544886
H	-4.796682	-0.324868	2.094877
C	-0.020931	4.297887	-1.574177
C	1.186752	3.626024	-1.562665
C	-1.204711	3.584773	-1.564674
C	-1.189388	2.197907	-1.582288
C	1.217042	2.239992	-1.584286
C	2.502052	1.502103	-1.511186
C	-2.450032	1.419562	-1.499189
H	-0.040194	5.391412	-1.594569
H	2.124583	4.193394	-1.559987
H	-2.160846	4.120850	-1.566966
H	-3.281022	2.009643	-1.936288
H	-2.354054	0.478862	-2.070374
C	0.025491	1.540131	-1.648611
H	3.316956	2.131188	-1.923331
H	2.440502	0.577441	-2.115632
H	3.336035	-1.517488	-1.122683
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H	-2.119176	-0.816055	3.189010
H	1.974830	-0.840269	3.065260
H	3.811394	0.713620	-0.176814
H	0.043330	0.446837	-1.749991
C	2.204836	-3.107712	-0.670334
C	-2.648674	-2.356540	-1.361668
C	0.316704	-1.650545	-3.581593
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C	-0.983939	-1.712883	-3.111880
C	1.097749	-2.659802	-1.549214
C	-1.255669	-2.258378	-1.868533
C	-0.204954	-2.731620	-1.104386
H	0.516728	-1.242032	-4.576814
H	2.380625	-2.108343	-3.197281
H	-1.806312	-1.350900	-3.741160
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H	2.847154	-3.849777	-1.192582
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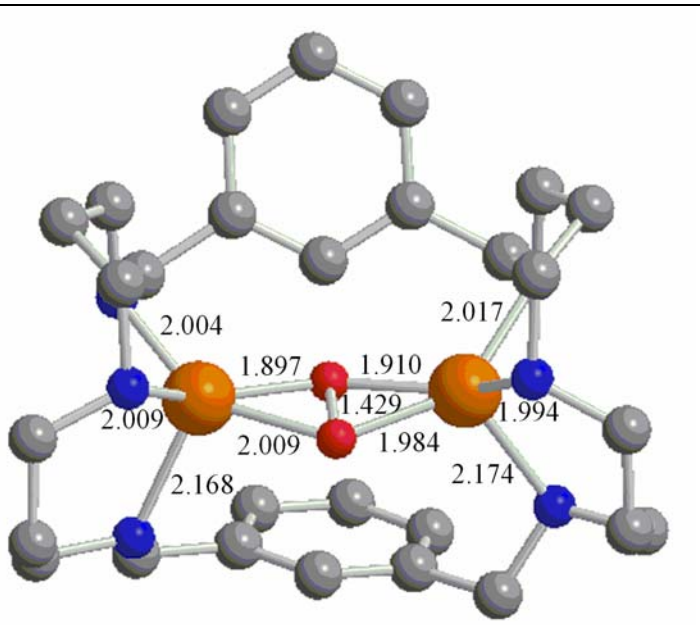

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Cu	-1.856976	-0.780082	0.525011
Cu	1.706554	-0.765446	0.158322
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N	2.925816	0.748875	-0.371140
N	2.775965	-2.665931	0.244442
N	-3.134606	-0.142381	2.314737
N	2.440711	-0.558790	2.197547
O	-0.085221	0.026309	0.361819
O	-0.036376	-1.303818	0.852037
C	3.103785	1.419657	0.929865
C	3.472988	0.454912	2.026180
H	3.882128	2.208802	0.837312
H	2.146531	1.919958	1.172526
H	3.643763	1.027683	2.963605
H	4.430135	-0.043870	1.791459
C	2.417085	-2.956044	1.639181
C	2.910526	-1.882264	2.586244
H	1.314142	-3.022930	1.697490
H	2.840405	-3.939183	1.944092
H	4.014325	-1.887829	2.630338
H	2.574800	-2.136028	3.610871
C	-4.132993	0.724427	1.704861
C	-3.561979	1.447403	0.537683
H	-4.524845	1.457484	2.442270
H	-4.999120	0.113926	1.394113
H	-4.308863	2.156949	0.118713
H	-2.685149	2.038741	0.858170
C	-3.913398	-2.387171	1.817859
C	-3.757678	-1.334933	2.866859
H	-4.305726	-3.322022	2.271254
H	-3.132118	-1.706778	3.695115
H	-4.643706	-2.077153	1.047814
H	-4.745382	-1.111012	3.321612
C	-0.302447	4.079465	-0.285677
C	0.951687	3.533601	-0.485385
C	-1.427752	3.370836	-0.662035
C	-1.311432	2.114166	-1.242157
C	1.086803	2.297971	-1.099750
C	2.419241	1.716586	-1.373213
C	-2.499362	1.309235	-1.614483
H	-0.403743	5.078306	0.148390
H	1.845440	4.100716	-0.198715
H	-2.417726	3.823123	-0.530828
H	-3.291210	1.969295	-2.032997
H	-2.228488	0.589060	-2.406183
C	-0.047865	1.617614	-1.503792
H	3.174485	2.527532	-1.457199
H	2.409362	1.191543	-2.345106
H	0.054131	0.656520	-2.019938
C	-4.279880	-0.136360	-1.095783
H	-4.735464	-0.846125	-0.390233
H	-3.986799	-0.682899	-2.004256
H	-5.047004	0.611387	-1.386742
C	-2.361529	0.583323	3.303002
H	-1.897748	1.470173	2.837238
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H	-1.546396	-0.053127	3.688115
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H	-2.108718	-4.118854	2.566061
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H	4.550395	-3.813918	0.317663
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H	4.876117	1.158245	-1.072127
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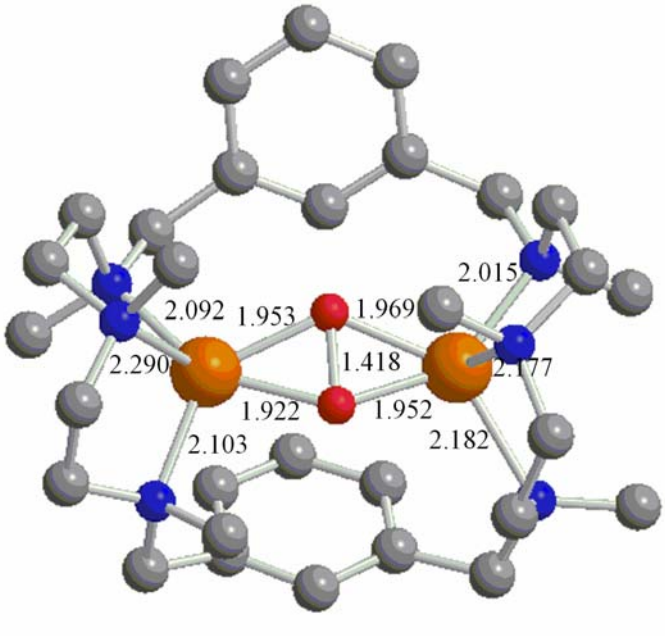

6

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C	2.911265	1.423594	2.916377
C	2.211678	0.157609	3.331743
H	2.893221	3.101556	1.587668
H	1.382723	2.141903	1.549541
H	2.689711	2.160294	3.712468
H	4.010511	1.313262	2.962374
H	1.123341	0.351641	3.358861
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C	3.722199	-1.569607	2.544385
H	4.793016	-1.190515	0.069505
H	4.685442	-2.850467	-0.532916
H	3.318273	-3.439229	1.546367
H	5.000554	-3.044683	1.751400
H	4.447948	-0.740180	2.477412
H	3.868473	-2.023936	3.551111
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C	0.889836	-2.868765	-1.584553
C	-1.485803	-2.917154	-1.153633
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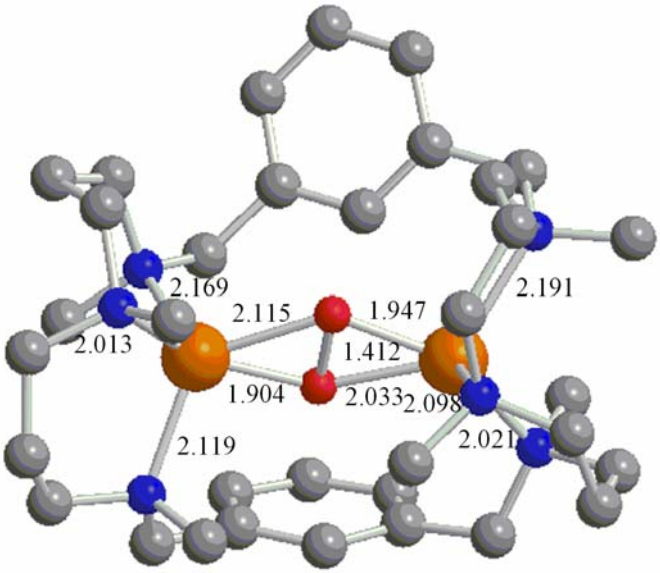
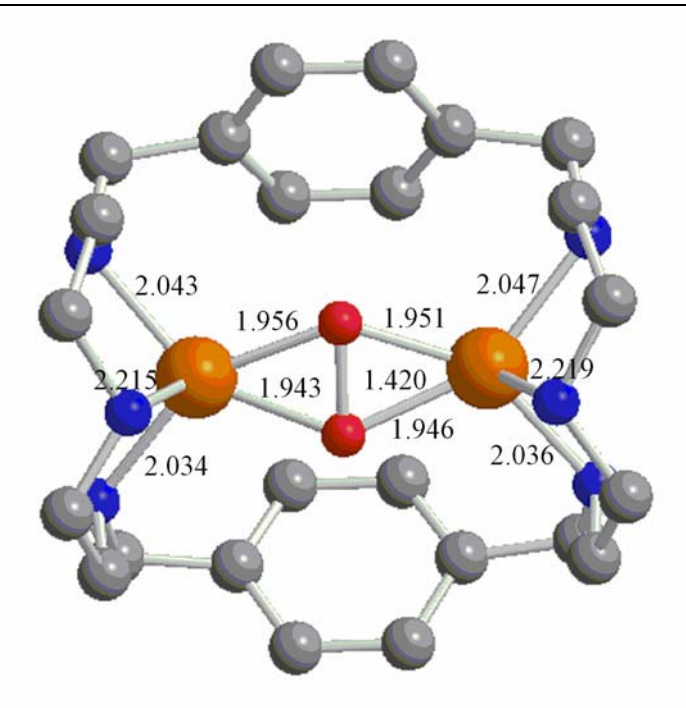


7		

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8

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C	-5.422548	-0.506574	-1.187776
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H	-2.970997	0.523461	-1.506783
H	-5.266345	0.347475	-1.868975
H	-6.153315	-1.180635	-1.687631
H	-5.026282	-3.128974	-0.609612
C	-4.094323	-2.555008	-0.668758
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C	-2.945091	-0.523125	-1.181402
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H	-0.383717	-4.194847	-0.685751
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C	-1.736014	-1.163215	-1.008833
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C	-1.695000	-2.494759	-0.626586

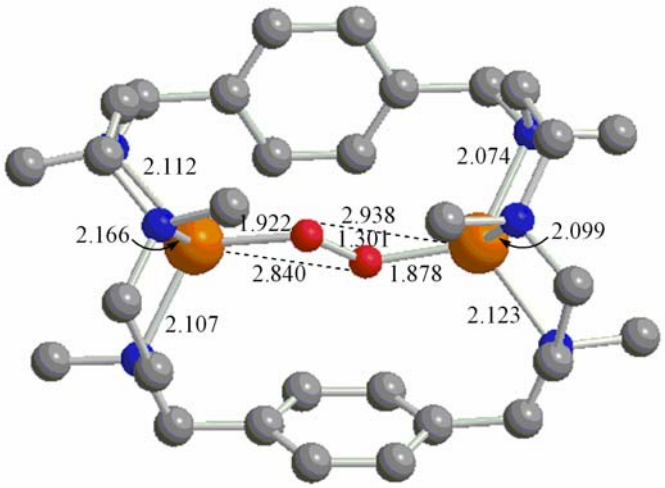

Table S2. Comparison between the X-ray data of complex **5e** and the corresponding geometry (distances in Å and angles in degrees).

Distances	dist(RX)	dist(LDA)		Angles	ang(RX)	ang(LDA)
O1-O2	2.329	2.409		N12-Cu12-N32	112.030	111.115
Cu1-Cu12	3.114	3.011		N12-Cu12-N22	75.200	72.703
Cu1-O2	1.950	1.935		N22-Cu12-N32	88.083	86.738
Cu1-O1	1.940	1.922		N3-Cu1-N1	112.153	111.115
Cu12-O2	1.949	1.935		N3-Cu1-N2	87.999	86.738
Cu12-O1	1.939	1.922		N2-Cu12-N1	75.246	72.703
Cu12-N32	2.030	2.055		O2-Cu1-N3	97.665	97.732
Cu12-N22	1.985	2.014		O2-Cu1-N2	174.323	174.656
Cu12-N12	2.851	3.018		O2-Cu1-N1	102.776	102.823
Cu1-N1	2.853	2.853		O1-Cu12-N12	89.787	88.263
Cu1-N3	2.030	2.055		O1-Cu12-N32	157.956	160.620
Cu1-N2	1.983	2.014		O1-Cu12-N22	101.083	99.388
				O1-Cu1-N3	157.92213	160.62058
				O1-Cu1-N2	100.98165	99.38807
				O1-Cu1-N1	89.72676	88.26334
				O2-Cu12-N12	102.89942	102.82294
				O2-Cu12-N32	97.47148	97.73175
				O2-Cu12-N22	174.43134	174.65577

*Standard deviations for the distances and for the angles, $s_{n-1} = \sqrt{\frac{\sum_{i=1}^{N} (CV - EV)^2}{N-1}}$,

where CV means calculated value, EV experimental value (X-ray data), and N is the number of distances or angles taken into account.

	BP86
Distances	0.0669
Angles	1.5370

The standard deviation for the distances is 0.067 Å, and for the angles 1.5º.