

## Supporting Information

### A Broken-Symmetry Density Functional Study of Structures, Energies, and Protonation States along the Catalytic O-O Bond Cleavage Pathway in $ba_3$ Cytochrome *c* Oxidase from *Thermus thermophilus*

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### Cartesian Coordinates of the Optimized Structures with His376<sup>+</sup> Given in Table 1:

PW91-Fe<sup>3+</sup>-(O-OH)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	H	-4.689169	4.854978	21.111165
C	1.112882	6.047243	23.575569	H	-5.260390	4.080554	22.611008
O	1.258232	5.021139	24.281579	H	-3.987062	1.714316	23.252380
H	1.545170	7.706669	24.815058	H	-2.092312	4.089402	20.280693
H	-0.148993	7.175394	24.867136	H	-1.624967	0.805554	22.870326
H	0.451023	8.118105	23.462987	C	-8.404976	-3.813731	17.749513
N	1.335379	6.062702	22.248212	C	-8.076809	-3.041892	18.989482
C	2.027795	4.993943	21.553463	O	-8.083027	-1.806179	19.031267
C	1.482159	4.694047	20.150517	O	-7.750571	-3.809341	20.027030
C	2.310128	3.581443	19.608739	H	-7.457757	-4.150224	17.302538
N	1.964514	2.242314	19.750243	H	-8.918507	-3.164588	17.034229
C	3.608589	3.650447	19.188614	C	-10.828653	-3.317140	22.671861
C	3.028424	1.522044	19.414917	C	-10.686145	-1.996875	23.328355
N	4.063696	2.348337	19.076044	N	-9.478377	-1.327168	23.347744
H	1.271758	6.964514	21.777458	C	-11.576600	-1.192400	23.983715
H	1.961852	4.091111	22.168632	C	-9.606897	-0.163783	23.983046
H	0.422984	4.406207	20.206314	N	-10.879629	-0.069978	24.372830
H	1.557223	5.584543	19.510366	H	-10.691906	-3.225458	21.584059
H	4.245143	4.499470	18.976886	H	-11.823400	-3.731600	22.866174
H	3.105302	0.443698	19.417258	H	-8.584904	-1.729909	22.925603
H	3.094845	5.256581	21.465471	H	-12.627921	-1.318868	24.203097
C	8.822075	3.453037	19.812969	H	-8.828846	0.583982	24.135516
C	7.771053	2.531732	19.266854	C	-0.023531	-7.192567	24.252404
C	8.109674	1.334875	18.606899	C	0.687327	-6.113456	23.493040
C	6.412290	2.830613	19.408716	N	1.664894	-6.341803	22.543050
C	7.142289	0.482848	18.110047	C	0.455990	-4.756551	23.421819
C	5.426818	1.992212	18.902670	C	1.993041	-5.177289	21.943350
C	5.747527	0.766452	18.223790	N	1.270613	-4.184386	22.452178
O	4.827362	-0.000431	17.755539	H	-0.631833	-7.784946	23.551157
H	8.593960	4.498924	19.562299	H	-0.712010	-6.716925	24.961306
H	9.808819	3.204456	19.402729	H	2.078301	-7.246549	22.316230
H	9.162794	1.076954	18.484710	H	-0.245379	-4.168606	23.999885
H	6.121862	3.736102	19.940332	H	2.741982	-5.092991	21.168433
H	7.427454	-0.434769	17.594539	C	-7.209370	-2.964134	29.396675
C	-3.887222	1.561759	16.393100	N	-6.022980	-2.335531	29.945273
C	-2.593745	1.569136	17.126442	C	-5.303869	-1.408183	29.304904
N	-1.372145	1.499255	16.486011	N	-5.636112	-1.019568	28.077626
C	-2.285013	1.591699	18.462648	N	-4.239794	-0.869918	29.920527
C	-0.385037	1.497129	17.405739	H	-6.957697	-3.732213	28.651843
N	-0.911672	1.550781	18.624795	H	-7.859720	-2.207554	28.941280
H	-4.230820	0.530181	16.226146	H	-5.625639	-2.724876	30.798489
H	-3.771216	2.042454	15.412877	H	-6.278171	-1.549534	27.462933
H	-1.232150	1.483363	15.475635	H	-5.123341	-0.232299	27.648106
H	-2.955786	1.636276	19.309741	H	-4.180577	-0.938966	30.934366
H	0.669217	1.481139	17.164036	H	-3.718217	-0.096621	29.465980
C	-4.818929	3.894099	21.622262	Fe	1.495381	-2.153224	21.953461
C	-3.511928	3.198850	21.732443	C	-1.428697	-1.564577	23.591197
N	-3.301609	2.121232	22.567481	C	-0.146324	-2.183561	18.972447
C	-2.331063	3.363920	21.048553	C	4.429541	-2.873938	20.307041
C	-2.050906	1.663172	22.369334	C	3.218437	-1.812420	24.850117
N	-1.429510	2.392474	21.443083	N	0.989114	-1.770352	23.830410

C	-0.266128	-1.535489	24.327946	H	-7.075928	-0.588623	19.944398
C	-0.206063	-1.228421	25.735458	O	-7.327305	-2.127129	26.074788
C	1.115627	-1.272391	26.089351	H	-6.989661	-1.827697	25.181544
C	1.845973	-1.627568	24.890420	H	-7.273263	-3.106142	26.030979
C	1.732606	-0.982397	27.409712	O	1.491884	2.492147	26.842736
O	-2.942050	-1.732618	17.811720	H	1.255990	2.373628	25.885487
C	-1.380973	-0.858736	26.573005	H	0.624190	2.473202	27.301534
C	-1.849544	0.591691	26.330068	O	-7.459938	2.187356	24.067685
C	-2.960243	0.923736	27.304653	H	-6.552764	1.785439	24.216782
O	-2.668774	1.010956	28.521325	H	-7.487160	2.358031	23.102437
O	-4.165471	1.023755	26.849594	O	-5.023802	0.985751	24.365170
N	2.018707	-2.566719	20.409897	H	-4.650591	0.970758	25.312181
C	1.197479	-2.485399	18.952544	H	-5.372980	0.074360	24.153092
C	1.937711	-2.731251	17.735042	O	-5.655124	2.868892	28.240540
C	3.235317	-2.951805	18.107400	H	-5.082994	2.195460	27.776218
C	3.274949	-2.821071	19.551327	H	-5.017011	3.552950	28.535121
C	1.333451	-2.738551	16.375673	O	0.928339	2.370263	24.062521
N	3.432502	-2.361752	22.482696	H	1.117002	3.357184	23.994079
C	4.500549	-2.644497	21.667726	H	-0.049795	2.335848	24.031279
C	5.735756	-2.631841	22.414034	H	-7.540308	-3.225774	20.863785
C	5.399199	-2.327189	23.713828	H	-2.186622	0.728626	25.294793
C	3.952174	-2.163645	23.731913	H	-1.007512	1.274960	26.508048
C	7.080322	-2.903775	21.839668	H	-1.124998	-0.963676	27.636284
C	6.245522	-2.192594	24.880875	H	-2.220335	-1.547649	26.378998
C	7.554148	-1.889551	24.887084	H	2.475870	-1.743858	27.684756
N	-0.416459	-1.982215	21.397641	H	2.236314	-0.003482	27.389182
C	-0.892835	-1.954139	20.114292	H	0.971590	-0.947925	28.198978
C	-2.304153	-1.645187	20.117228	H	-2.362013	-1.403300	24.124918
C	-2.677461	-1.503374	21.441877	H	3.761558	-1.658065	25.777783
C	-1.493601	-1.720137	22.216445	H	5.754090	-2.349074	25.847166
C	-3.201928	-1.491472	18.994521	H	8.099315	-1.824830	25.828128
C	-4.013842	-1.163794	21.987393	H	8.108516	-1.672885	23.973944
C	-5.006192	-2.330153	21.940753	H	7.722749	-3.401521	22.578627
C	-6.286773	-2.011611	22.673216	H	7.019090	-3.544442	20.951923
O	-7.378073	-2.498642	22.214777	H	7.579994	-1.966779	21.545224
O	-6.246599	-1.315977	23.728058	H	5.354795	-3.032041	19.761639
C	4.394190	-3.271879	17.203941	H	4.064643	-3.054133	16.171551
O	5.561028	-2.505550	17.508843	H	3.933922	-5.381183	16.989057
C	4.783601	-4.742668	17.268750	H	5.105989	-5.009611	18.286332
H	5.616040	-4.928829	16.574000	H	2.101335	-2.817235	15.597114
Cu	0.114650	1.684296	20.343689	H	0.646228	-3.590367	16.256826
H	8.891071	3.392424	20.913367	H	0.753905	-1.821520	16.193146
H	-4.673317	2.104938	16.938341	H	-0.680739	-2.122080	18.029600
H	-5.531461	3.294705	21.032081	H	-4.213364	-1.119993	19.274522
H	-9.006488	-4.710142	17.956796	H	-4.454982	-0.319686	21.435432
H	-10.071118	-4.017669	23.050776	H	-3.913195	-0.845075	23.028656
H	0.595658	-7.919074	24.825696	H	-4.569850	-3.213728	22.438886
H	-7.746921	-3.426171	30.227401	H	-5.227630	-2.619886	20.905958
O	1.881731	-0.437422	21.665290	H	5.279419	-1.530384	17.578887
O	0.746088	0.534990	21.984045	H	1.157254	1.132278	22.679442
O	-6.539629	0.176354	20.280609	H	-11.271983	0.719188	24.886685
H	-6.382397	0.708823	19.472708				

PW91-Fe<sup>3+</sup>-(HO-O)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	H	-2.102470	3.985900	20.240435
C	1.168465	6.054733	23.589494	H	-1.594023	0.817582	22.959141
O	1.438163	5.071871	24.316429	C	-8.444472	-3.786032	17.766494
H	1.501454	7.718111	24.861085	C	-8.158778	-3.033685	19.028729
H	-0.180426	7.148972	24.818067	O	-8.276691	-1.805726	19.122690
H	0.467808	8.118576	23.455280	O	-7.739887	-3.808828	20.026727
N	1.290638	6.019897	22.246368	H	-7.482615	-4.075989	17.318788
C	1.995816	4.949434	21.561227	H	-8.984680	-3.145853	17.063078
C	1.428620	4.602785	20.177985	C	-10.810069	-3.337614	22.603819
C	2.275367	3.508147	19.623091	C	-10.713343	-1.999275	23.231360
N	1.951957	2.163011	19.731207	N	-9.510813	-1.323551	23.300031
C	3.569472	3.603841	19.187856	C	-11.639284	-1.187348	23.825801
C	3.023621	1.466095	19.363571	C	-9.676293	-0.148164	23.905320
N	4.042154	2.313643	19.039215	N	-10.967284	-0.054401	24.229137
H	1.150200	6.894457	21.738172	H	-10.607268	-3.276156	21.524435
H	1.963649	4.061784	22.203396	H	-11.811307	-3.756506	22.748880
H	0.382573	4.280437	20.266476	H	-8.600905	-1.733347	22.923012
H	1.453812	5.483934	19.520307	H	-12.699665	-1.318132	23.995772
H	4.191352	4.465878	18.987179	H	-8.908393	0.603093	24.083879
H	3.116612	0.390103	19.311115	C	-0.011750	-7.165435	24.270532
H	3.054263	5.233873	21.443751	C	0.706667	-6.082644	23.520725
C	8.787514	3.477157	19.814675	N	1.703464	-6.305958	22.588524
C	7.749620	2.544588	19.248342	C	0.460287	-4.728668	23.438985
C	8.100902	1.379803	18.544656	C	2.035500	-5.148270	21.987343
C	6.385271	2.810361	19.395396	N	1.289600	-4.158531	22.479015
C	7.142621	0.530639	18.011745	H	-0.636663	-7.729651	23.561620
C	5.414441	1.975907	18.848905	H	-0.686165	-6.691042	24.993655
C	5.745121	0.783768	18.127386	H	2.128693	-7.208341	22.373533
O	4.830259	0.016498	17.627344	H	-0.257484	-4.143582	23.999025
H	8.529080	4.524235	19.599278	H	2.795686	-5.061753	21.223667
H	9.771873	3.271538	19.374249	C	-7.198087	-3.014421	29.378082
H	9.157122	1.138790	18.411431	N	-5.972441	-2.436223	29.893851
H	6.072123	3.688667	19.959664	C	-5.252675	-1.512005	29.252878
H	7.446620	-0.362699	17.464150	N	-5.602230	-1.102042	28.038392
C	-3.858092	1.553705	16.440441	N	-4.161058	-1.005700	29.854973
C	-2.570022	1.622383	17.187838	H	-6.999984	-3.809574	28.645977
N	-1.350695	1.757018	16.552598	H	-7.814754	-2.234168	28.916019
C	-2.255357	1.523332	18.519671	H	-5.573066	-2.831756	30.743228
C	-0.362372	1.750587	17.469801	H	-6.259479	-1.621748	27.429439
N	-0.883685	1.608707	18.684982	H	-5.095427	-0.307974	27.611616
H	-4.176854	0.507619	16.318680	H	-4.110086	-1.064810	30.870533
H	-3.732919	1.986437	15.439281	H	-3.674653	-0.199109	29.420046
H	-1.213361	1.863478	15.547170	Fe	1.456415	-2.231918	21.944368
H	-2.921064	1.402995	19.363673	C	-1.468247	-1.590496	23.548892
H	0.686093	1.866963	17.231065	C	-0.180415	-2.318313	18.951421
C	-4.806940	3.865490	21.633639	C	4.419401	-2.799919	20.293845
C	-3.508953	3.151387	21.736680	C	3.186519	-1.656378	24.807908
N	-3.292820	2.099374	22.606788	N	0.958168	-1.738177	23.786899
C	-2.336143	3.290474	21.037356	C	-0.307791	-1.537287	24.285634
C	-2.043041	1.636759	22.416662	C	-0.256594	-1.213890	25.685042
N	-1.432421	2.334292	21.463378	C	1.068389	-1.195361	26.036087
H	-4.659999	4.835974	21.145168	C	1.808256	-1.541927	24.845631
H	-5.245261	4.040178	22.625516	C	1.669929	-0.848960	27.348526
H	-3.984495	1.698256	23.287962	O	-2.949208	-1.833180	17.766826

C	-1.434519	-0.864549	26.521055	H	-7.276203	-3.176987	26.015324
C	-1.863524	0.605809	26.324610	O	1.287071	2.633636	27.198250
C	-2.975278	0.919885	27.299064	H	1.075716	2.464936	26.239902
O	-2.688743	1.014250	28.516285	H	0.412304	2.612761	27.645811
O	-4.181629	0.989160	26.842050	O	-7.490991	2.154529	24.058943
N	1.992270	-2.591000	20.047406	H	-6.592707	1.739084	24.210852
C	1.168890	-2.585743	18.944545	H	-7.511429	2.322141	23.094387
C	1.919554	-2.840448	17.736979	O	-5.054238	0.950640	24.369266
C	3.228258	-2.985121	18.112853	H	-4.680213	0.928054	25.313918
C	3.262374	-2.812466	19.546102	H	-5.393451	0.036046	24.147872
C	1.320357	-2.921433	16.378267	O	-5.744458	2.746894	28.255037
N	3.403884	-2.253292	22.453342	H	-5.145639	2.105987	27.778033
C	4.484722	-2.526536	21.644788	H	-5.156526	3.507314	28.448333
C	5.718245	-2.442464	22.380921	O	0.761196	2.424883	24.496928
C	5.376218	-2.100244	23.671359	H	1.061472	3.329001	24.206951
C	3.927703	-1.997648	23.696284	H	0.924665	1.810686	23.741543
C	7.066505	-2.694539	21.808972	H	-7.556297	-3.240558	20.881796
C	6.223066	-1.897708	24.827971	H	-2.184444	0.782242	25.290557
C	7.526765	-1.572671	24.810989	H	-1.004369	1.258042	26.528170
N	-0.444535	-2.030914	21.367570	H	-1.191723	-1.016121	27.582669
C	-0.923698	-2.044960	20.084028	H	-2.283110	-1.528983	26.289958
C	-2.333037	-1.733145	20.077604	H	2.472487	-1.547388	27.622391
C	-2.708736	-1.555424	21.397043	H	2.092423	0.168347	27.320009
C	-1.527320	-1.753709	22.177664	H	0.912763	-0.866783	28.142174
C	-3.225244	-1.596973	18.946295	H	-2.404248	-1.436327	24.080019
C	-4.046341	-1.198366	21.933136	H	3.723073	-1.452199	25.729636
C	-5.037900	-2.364299	21.909271	H	5.740049	-2.020314	25.800648
C	-6.300128	-2.054177	22.677546	H	8.074995	-1.456973	25.745435
O	-7.401123	-2.541428	22.242806	H	8.072829	-1.387729	23.887911
O	-6.232844	-1.373035	23.739330	H	7.726000	-3.150492	22.559623
C	4.401986	-3.272013	17.215818	H	7.018774	-3.366952	20.943930
O	5.548581	-2.478571	17.525426	H	7.539059	-1.755095	21.480036
C	4.825158	-4.734669	17.285796	H	5.346205	-2.935056	19.745268
H	5.661656	-4.902604	16.592561	H	4.073044	-3.063129	16.182057
Cu	0.131758	1.579252	20.426520	H	3.990929	-5.394605	17.008993
H	8.891071	3.392424	20.913369	H	5.152996	-4.988385	18.304889
H	-4.673316	2.104938	16.938340	H	2.094466	-3.006854	15.606305
H	-5.531460	3.294705	21.032081	H	0.661040	-3.798792	16.293721
H	-9.006486	-4.710143	17.956794	H	0.712937	-2.031590	16.157778
H	-10.071117	-4.017669	23.050774	H	-0.717744	-2.309927	18.007815
H	0.595658	-7.919074	24.825694	H	-4.244808	-1.243450	19.214541
H	-7.746921	-3.426169	30.227399	H	-4.486245	-0.362311	21.367222
O	1.773066	-0.284913	21.595990	H	-3.944723	-0.857822	22.967676
O	0.789197	0.714707	22.038341	H	-4.588351	-3.248338	22.394536
O	-6.748606	0.132908	20.458795	H	-5.284951	-2.652663	20.879743
H	-6.646462	0.735238	19.692183	H	5.260264	-1.493975	17.542712
H	-7.286420	-0.614796	20.086115	H	2.589938	-0.013035	22.086582
O	-7.344149	-2.199272	26.065240	H	-11.384670	0.745601	24.706226
H	-6.994706	-1.891417	25.178171				

OLYP-Fe<sup>3+</sup>-(O-OH)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	H	1.480059	7.766850	24.856239
C	1.245503	6.095125	23.582198	H	-0.156315	7.093180	24.826395
O	1.496340	5.098305	24.286629	H	0.413272	8.106943	23.468872

N	1.451599	6.134231	22.251258	N	-9.602787	-1.325766	23.361344
C	2.184706	5.115026	21.530577	C	-11.709189	-1.264833	23.968020
C	1.664616	4.873647	20.107178	C	-9.785039	-0.168352	23.988139
C	2.456641	3.742991	19.551483	N	-11.061147	-0.118727	24.359927
N	2.072361	2.415699	19.697198	H	-10.779704	-3.284332	21.599756
C	3.747427	3.776931	19.117460	H	-11.837451	-3.835070	22.919638
C	3.112629	1.672435	19.357341	H	-8.688934	-1.680092	22.957503
N	4.166884	2.463880	19.005096	H	-12.755812	-1.427446	24.173977
H	1.319074	7.028145	21.786449	H	-9.044023	0.595055	24.168891
H	2.118926	4.189141	22.101400	C	-0.065414	-7.253187	24.246979
H	0.598778	4.631173	20.132755	C	0.644134	-6.188292	23.480671
H	1.788411	5.773052	19.492920	N	1.641583	-6.434448	22.561642
H	4.400457	4.604713	18.893071	C	0.442760	-4.832258	23.410373
H	3.159038	0.598335	19.366876	C	2.008923	-5.275112	21.982829
H	3.244794	5.397814	21.477410	N	1.294425	-4.273121	22.474222
C	8.912980	3.451140	19.816606	H	-0.646708	-7.883946	23.562297
C	7.867293	2.558524	19.224335	H	-0.763534	-6.782842	24.945005
C	8.199009	1.375349	18.535803	H	2.044312	-7.342436	22.346279
C	6.513036	2.869966	19.370368	H	-0.256585	-4.238436	23.973720
C	7.226059	0.556166	18.010800	H	2.776346	-5.206476	21.232075
C	5.517457	2.072624	18.831568	C	-7.181302	-2.976578	29.417842
C	5.828447	0.859831	18.109298	N	-6.008057	-2.360394	30.006462
O	4.923243	0.125798	17.595329	C	-5.254136	-1.442476	29.402301
H	8.728126	4.498006	19.546783	N	-5.547148	-1.017329	28.181176
H	9.914401	3.172036	19.477464	N	-4.175998	-0.962294	30.045993
H	9.245796	1.102717	18.420624	H	-6.912124	-3.746026	28.686447
H	6.238129	3.755428	19.933597	H	-7.810381	-2.217822	28.948887
H	7.501835	-0.351268	17.480909	H	-5.622056	-2.789441	30.841522
C	-3.910258	1.655401	16.292702	H	-6.206571	-1.508928	27.576891
C	-2.593399	1.644370	16.979977	H	-5.031658	-0.230369	27.773419
N	-1.388118	1.591381	16.315104	H	-4.177074	-1.000626	31.060273
C	-2.254519	1.668904	18.304841	H	-3.669749	-0.172928	29.631732
C	-0.386227	1.602998	17.214751	Fe	1.535679	-2.208047	21.969279
N	-0.883189	1.649700	18.442229	C	-1.391191	-1.587127	23.589269
H	-4.228463	0.638843	16.030932	C	-0.116268	-2.352794	18.998601
H	-3.860146	2.244586	15.370608	C	4.472090	-2.912373	20.332688
H	-1.266138	1.573506	15.306213	C	3.245704	-1.843036	24.864041
H	-2.905481	1.705998	19.161166	N	1.020233	-1.802717	23.850747
H	0.657687	1.595145	16.946143	C	-0.234726	-1.550648	24.336605
C	-4.844871	3.990783	21.533982	C	-0.177707	-1.233972	25.745174
C	-3.506566	3.362348	21.662103	C	1.142142	-1.291715	26.101645
N	-3.265223	2.306277	22.511781	C	1.872978	-1.658324	24.906404
C	-2.337017	3.532725	20.966993	C	1.759536	-1.023464	27.430314
C	-2.013456	1.864961	22.303062	O	-2.967921	-2.042388	17.832209
N	-1.413831	2.583098	21.361265	C	-1.347793	-0.857498	26.591799
H	-4.776942	4.901200	20.932832	C	-1.751856	0.623435	26.432045
H	-5.266442	4.246009	22.511810	C	-2.862084	0.982658	27.411582
H	-3.933333	1.916293	23.197119	O	-2.557680	1.076451	28.625851
H	-2.119670	4.246633	20.186962	O	-4.053152	1.106929	26.951617
H	-1.582968	1.024167	22.812695	N	2.065112	-2.652046	20.057562
C	-8.416619	-3.824326	17.699028	C	1.237740	-2.606622	18.969244
C	-8.128326	-2.994012	18.913167	C	1.980833	-2.845656	17.751290
O	-8.171846	-1.765400	18.927934	C	3.282037	-3.040050	18.123021
O	-7.794634	-3.737033	19.973124	C	3.321746	-2.887459	19.565506
H	-7.461131	-4.172116	17.286606	C	1.372046	-2.860119	16.390774
H	-8.931104	-3.223446	16.947148	N	3.479362	-2.397837	22.504629
C	-10.876159	-3.371208	22.687895	C	4.545764	-2.673435	21.692975
C	-10.783078	-2.039043	23.329628	C	5.780299	-2.652997	22.443463

C	5.437624	-2.349228	23.740285	O	-5.118194	1.212145	24.428590
C	3.990141	-2.194588	23.753040	H	-4.683939	1.145611	25.323484
C	7.129826	-2.924535	21.878006	H	-5.422951	0.300514	24.217472
C	6.276003	-2.218391	24.919585	O	-5.799633	2.917565	28.331146
C	7.559345	-1.828319	24.961477	H	-5.152531	2.303893	27.905979
N	-0.396462	-2.067567	21.406866	H	-5.245166	3.679083	28.589780
C	-0.873130	-2.108287	20.130806	O	1.166427	2.281019	24.319708
C	-2.289891	-1.824502	20.125388	H	1.294664	3.245280	24.157489
C	-2.659583	-1.620843	21.443137	H	0.202669	2.212068	24.455072
C	-1.466758	-1.784486	22.219280	H	-7.595391	-3.145911	20.781856
C	-3.200941	-1.734303	19.002526	H	-2.071499	0.823795	25.607557
C	-4.000672	-1.254850	21.976612	H	-0.882892	1.251552	26.649600
C	-5.004983	-2.412872	22.024516	H	-1.107723	-1.038408	27.643897
C	-6.288905	-2.012933	22.734509	H	-2.206846	-1.499344	26.356362
O	-7.395903	-2.398937	22.227688	H	2.426147	-1.840280	27.731705
O	-6.205149	-1.348724	23.800380	H	2.354595	-0.101586	27.405339
C	4.428739	-3.367454	17.203990	H	0.997333	-0.907514	28.204159
O	5.603057	-2.585270	17.463244	H	-2.317903	-1.413677	24.116242
C	4.833441	-4.836396	17.265071	H	3.783377	-1.682141	25.787823
H	5.638640	-5.019546	16.543403	H	5.794545	-2.458407	25.867011
Cu	0.154502	1.884277	20.195636	H	8.082306	-1.783587	25.914547
H	8.891071	3.392424	20.913367	H	8.112848	-1.527334	24.078217
H	-4.673317	2.104938	16.938341	H	7.788034	-3.353210	22.638972
H	-5.531461	3.294705	21.032081	H	7.082594	-3.624585	21.039285
H	-9.006488	-4.710142	17.956796	H	7.596441	-1.997787	21.516328
H	-10.071118	-4.017669	23.050776	H	5.397363	-3.073739	19.803331
H	0.595658	-7.919074	24.825696	H	4.088106	-3.161078	16.180811
H	-7.746921	-3.426171	30.227401	H	3.978699	-5.472858	17.011549
O	1.911440	-0.484661	21.642428	H	5.186414	-5.105900	18.266289
O	0.802375	0.468318	21.921273	H	2.131439	-2.945164	15.610681
O	-6.718350	0.577150	20.237624	H	0.679648	-3.704370	16.279967
H	-6.511204	0.981489	19.371298	H	0.803914	-1.940641	16.208241
H	-7.161337	-0.256789	19.974991	H	-0.647812	-2.333311	18.059918
O	-7.454361	-2.152140	26.133583	H	-4.199143	-1.345120	19.268593
H	-7.079360	-1.872344	25.261020	H	-4.430152	-0.440455	21.382372
H	-7.356115	-3.123459	26.118154	H	-3.893698	-0.868967	22.987869
O	1.709132	2.992595	27.355089	H	-4.571996	-3.248940	22.592877
H	1.523304	2.739079	26.427435	H	-5.223513	-2.782841	21.020603
H	0.899143	2.715933	27.826385	H	5.327904	-1.632253	17.478466
O	-7.683262	2.507822	24.405197	H	1.192794	0.986201	22.665857
H	-6.788914	2.090847	24.434341	H	-11.484939	0.654621	24.866939
H	-7.773204	2.782016	23.471579				

OLYP-Fe<sup>3+</sup>-(HO-O)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	N	2.113978	2.327084	19.674633
C	1.401540	6.158014	23.599972	C	3.752985	3.737079	19.114228
O	1.907740	5.287096	24.332621	C	3.164953	1.618661	19.291628
H	1.401065	7.847841	24.884406	N	4.197492	2.440171	18.950795
H	-0.145741	6.990642	24.789697	H	1.102444	6.893207	21.729921
H	0.348915	8.068714	23.457404	H	2.210280	4.175784	22.137689
N	1.435243	6.089504	22.253975	H	0.602631	4.488424	20.211661
C	2.207794	5.087064	21.542166	H	1.715916	5.663189	19.502285
C	1.652382	4.775848	20.139781	H	4.386536	4.585476	18.906233
C	2.468023	3.663697	19.572131	H	3.235646	0.546509	19.246692

H	3.247153	5.424455	21.444333	N	1.322282	-4.258729	22.491198
C	8.947182	3.433036	19.814674	H	-0.566164	-7.906865	23.486960
C	7.904334	2.562313	19.169904	H	-0.795039	-6.812481	24.859515
C	8.238663	1.450978	18.378400	H	2.164866	-7.297155	22.419623
C	6.546308	2.838116	19.340913	H	-0.309655	-4.252352	23.906582
C	7.265404	0.657117	17.794358	H	2.897483	-5.154995	21.328443
C	5.556296	2.068776	18.738446	C	-7.148301	-3.009895	29.422158
C	5.869180	0.916137	17.938281	N	-5.965103	-2.425911	30.023264
O	4.958090	0.184134	17.399425	C	-5.204489	-1.493040	29.450618
H	8.807143	4.482652	19.526854	N	-5.478740	-1.045475	28.232116
H	9.953788	3.129669	19.512955	N	-4.142801	-1.018361	30.122521
H	9.286604	1.203597	18.220731	H	-6.892444	-3.797996	28.705864
H	6.252028	3.673146	19.968341	H	-7.740004	-2.236685	28.929673
H	7.555116	-0.195971	17.186796	H	-5.590647	-2.873612	30.853964
C	-3.846069	1.745364	16.310902	H	-6.119838	-1.534616	27.608583
C	-2.544117	1.759677	17.035758	H	-4.981111	-0.233742	27.852398
N	-1.334702	1.924167	16.392410	H	-4.159176	-1.068012	31.135989
C	-2.209400	1.610271	18.355265	H	-3.618712	-0.235994	29.716536
C	-0.339598	1.889540	17.298073	Fe	1.482102	-2.330649	21.963158
N	-0.839753	1.701764	18.512257	C	-1.434931	-1.599778	23.555582
H	-4.091905	0.732867	15.967265	C	-0.172413	-2.615164	19.011065
H	-3.795672	2.395042	15.430645	C	4.458585	-2.813260	20.304526
H	-1.208443	2.057532	15.392183	C	3.205550	-1.775361	24.833686
H	-2.862662	1.458003	19.197183	N	0.980935	-1.796504	23.812456
H	0.700850	2.016473	17.046853	C	-0.278840	-1.553935	24.302850
C	-4.807652	4.005072	21.452335	C	-0.226809	-1.236990	25.707966
C	-3.484476	3.350843	21.615525	C	1.095123	-1.277674	26.065063
N	-3.259287	2.341574	22.527605	C	1.828582	-1.636832	24.874392
C	-2.307953	3.469673	20.921970	C	1.709314	-0.993771	27.389311
C	-2.005996	1.882987	22.359978	O	-2.992134	-2.303916	17.820363
N	-1.396072	2.540089	21.383752	C	-1.393529	-0.874118	26.563079
H	-4.722601	4.851922	20.766246	C	-1.746187	0.626151	26.479776
H	-5.198685	4.368075	22.409066	C	-2.845273	0.971505	27.475514
H	-3.933928	1.997944	23.227415	O	-2.539692	1.006480	28.692957
H	-2.079683	4.131964	20.100482	O	-4.031929	1.146220	27.021216
H	-1.571752	1.082081	22.928938	N	2.032291	-2.709256	20.062050
C	-8.467763	-3.797574	17.685879	C	1.193529	-2.785098	18.981262
C	-8.185682	-2.960258	18.896650	C	1.940259	-3.012518	17.765556
O	-8.236563	-1.733149	18.906131	C	3.260292	-3.070969	18.123270
O	-7.853508	-3.695858	19.961885	C	3.302318	-2.872475	19.553969
H	-7.509077	-4.095584	17.242579	C	1.322499	-3.136088	16.415475
H	-9.032303	-3.220083	16.951455	N	3.440415	-2.314516	22.470286
C	-10.905050	-3.419497	22.671314	C	4.523263	-2.555345	21.659070
C	-10.856125	-2.056671	23.250976	C	5.753981	-2.480402	22.404674
N	-9.693338	-1.314260	23.275918	C	5.402389	-2.180486	23.700282
C	-11.816473	-1.274371	23.825455	C	3.952880	-2.092284	23.720060
C	-9.919361	-0.131252	23.837114	C	7.109097	-2.719853	21.839288
N	-11.205747	-0.094384	24.174470	C	6.240770	-2.008177	24.873726
H	-10.826707	-3.378057	21.579146	C	7.497759	-1.540387	24.901421
H	-11.844437	-3.909050	22.938155	N	-0.434847	-2.176456	21.399216
H	-8.762010	-1.656119	22.899848	C	-0.922328	-2.310206	20.130387
H	-12.863939	-1.453034	24.013826	C	-2.337677	-2.028278	20.114244
H	-9.198974	0.655123	24.001884	C	-2.700715	-1.730269	21.415275
C	-0.043379	-7.264006	24.206647	C	-1.506681	-1.843050	22.196662
C	0.676736	-6.178990	23.475846	C	-3.247819	-1.998691	18.985994
N	1.728354	-6.399407	22.610785	C	-4.036552	-1.311012	21.923385
C	0.434511	-4.830499	23.388210	C	-5.053239	-2.453155	22.051321
C	2.096074	-5.242038	22.040797	C	-6.337345	-1.981818	22.717714



O	-7.445003	-2.355815	22.201099	H	1.421073	3.396264	24.529868
O	-6.251319	-1.279345	23.755880	H	1.143702	1.910187	24.183177
C	4.421871	-3.322216	17.193474	H	-7.657970	-3.100579	20.769041
O	5.562547	-2.502389	17.459753	H	-2.057200	0.884763	25.465732
C	4.886797	-4.776821	17.235098	H	-0.854473	1.212511	26.719628
H	5.686297	-4.919663	16.499155	H	-1.164692	-1.122878	27.604477
Cu	0.207308	1.652363	20.309757	H	-2.269097	-1.475473	26.288669
H	8.891071	3.392424	20.913369	H	2.392691	-1.796283	27.690246
H	-4.673316	2.104938	16.938340	H	2.284482	-0.060146	27.358682
H	-5.531460	3.294705	21.032081	H	0.947464	-0.889638	28.165397
H	-9.006486	-4.710143	17.956794	H	-2.362057	-1.414374	24.076291
H	-10.071117	-4.017669	23.050774	H	3.738423	-1.594253	25.755050
H	0.595658	-7.919074	24.825694	H	5.784280	-2.282537	25.824991
H	-7.746921	-3.426169	30.227399	H	8.031878	-1.468230	25.844890
O	1.769881	-0.322030	21.517011	H	8.017058	-1.200547	24.010123
O	0.824257	0.694846	21.926004	H	7.787782	-3.087819	22.614187
O	-6.958372	0.765183	20.152571	H	7.082974	-3.459531	21.034751
H	-6.749854	1.154820	19.281733	H	7.535815	-1.793212	21.432085
H	-7.345947	-0.100111	19.908274	H	5.386385	-2.930110	19.767120
O	-7.384338	-2.139472	26.136270	H	4.066619	-3.117318	16.176302
H	-7.051362	-1.852591	25.250082	H	4.055098	-5.446231	16.992160
H	-7.355227	-3.114469	26.083580	H	5.267262	-5.035971	18.228290
O	1.805123	3.103492	27.856685	H	2.079077	-3.211473	15.632311
H	1.574144	2.848325	26.939932	H	0.687490	-4.028642	16.357478
H	0.936378	3.134713	28.302567	H	0.693137	-2.266401	16.194192
O	-7.790995	2.552825	24.461067	H	-0.711328	-2.687909	18.080058
H	-6.895413	2.143264	24.499466	H	-4.267136	-1.659086	19.241772
H	-7.832296	2.917347	23.555574	H	-4.452744	-0.533913	21.272492
O	-5.154508	1.293160	24.489541	H	-3.925885	-0.850237	22.902403
H	-4.709433	1.204488	25.374311	H	-4.634736	-3.245399	22.688206
H	-5.451798	0.386788	24.255918	H	-5.267300	-2.901398	21.079141
O	-5.846651	2.930776	28.280755	H	5.284792	-1.545194	17.414586
H	-5.163656	2.327250	27.897738	H	2.578760	-0.060717	22.013808
H	-5.323410	3.696299	28.587057	H	-11.660536	0.692286	24.631536
O	1.150718	2.541597	24.928511				

### Cartesian Coordinates of the Optimized Structures with His376<sup>+</sup> Given in Table 2:

PW91-Fe<sup>4+</sup>=O<sup>2-</sup>...OH<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>\*</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	N	4.087524	2.372471	19.051164
C	1.256790	6.120582	23.547488	H	1.135968	6.971756	21.704049
O	1.630513	5.147877	24.246450	H	1.870089	4.103008	22.049996
H	1.471516	7.748692	24.880764	H	0.514389	4.619111	20.009651
H	-0.162338	7.062241	24.809735	H	1.767993	5.752782	19.456144
H	0.410710	8.128717	23.487605	H	4.389380	4.513836	18.973425
N	1.344758	6.108154	22.206281	H	2.991797	0.523370	19.352028
C	2.042275	5.041782	21.505130	H	3.125337	5.249427	21.511455
C	1.590201	4.845399	20.051401	C	8.858668	3.326635	19.810323
C	2.385824	3.701380	19.522079	C	7.789811	2.394777	19.338394
N	1.953253	2.384133	19.613104	C	8.100780	1.113987	18.827412
C	3.702106	3.700354	19.158989	C	6.440605	2.774709	19.400019
C	2.982110	1.604509	19.332558	C	7.114590	0.263989	18.388148

C	5.428626	1.941564	18.957406	C	-7.222993	-2.932811	29.407059
C	5.726791	0.634510	18.404746	N	-6.083323	-2.243934	29.982022
O	4.807989	-0.121997	17.949814	C	-5.339445	-1.346604	29.328642
H	8.670217	4.344602	19.441043	N	-5.604449	-1.037899	28.062804
H	9.846110	2.998223	19.464692	N	-4.327188	-0.751680	29.968260
H	9.144274	0.801994	18.779575	H	-6.915699	-3.685435	28.667099
H	6.192872	3.742884	19.832249	H	-7.904535	-2.211565	28.938546
H	7.362821	-0.717705	17.985551	H	-5.715762	-2.589853	30.868630
C	-3.934539	1.309171	16.728460	H	-6.246463	-1.579223	27.456890
C	-2.630745	1.489263	17.432302	H	-5.095984	-0.251279	27.626763
N	-1.436212	1.631211	16.754084	H	-4.276676	-0.809218	30.983846
C	-2.273120	1.501156	18.759237	H	-3.714983	-0.068268	29.478430
C	-0.424075	1.731783	17.639352	Fe	1.603568	-2.168634	21.813823
N	-0.901806	1.657422	18.878931	C	-1.335044	-1.526543	23.428365
H	-4.388838	0.347247	17.005031	C	-0.056427	-2.397326	18.847851
H	-3.770202	1.291045	15.643681	C	4.510901	-3.018504	20.241712
H	-1.331631	1.670593	15.739905	C	3.297011	-1.765400	24.736619
H	-2.909666	1.409436	19.627983	N	1.082512	-1.752681	23.697951
H	0.610892	1.872390	17.360627	C	-0.181935	-1.521404	24.178851
C	-4.915391	3.886823	21.725488	C	-0.139483	-1.217685	25.589411
C	-3.575238	3.264709	21.852384	C	1.179113	-1.228440	25.952848
N	-3.316654	2.197808	22.687999	C	1.925423	-1.587302	24.763744
C	-2.415113	3.471340	21.148609	C	1.770515	-0.898471	27.275890
C	-2.051195	1.783901	22.472188	O	-2.824632	-1.903032	17.647413
N	-1.480299	2.534882	21.539545	C	-1.323352	-0.902819	26.434651
H	-4.827057	4.898118	21.311888	C	-1.797395	0.557457	26.282196
H	-5.428567	3.948286	22.693364	C	-2.872587	0.852899	27.305142
H	-3.986806	1.753006	23.366251	O	-2.552374	0.833280	28.517578
H	-2.213388	4.195477	20.368491	O	-4.079701	1.055925	26.890568
H	-1.566589	0.965737	22.988327	N	2.098386	-2.767875	19.952730
C	-8.521465	-3.725956	17.854377	C	1.280836	-2.728250	18.852012
C	-8.311124	-3.080169	19.190914	C	2.032807	-3.021713	17.649881
O	-8.883830	-2.044848	19.547570	C	3.330572	-3.202758	18.039788
O	-7.433355	-3.726684	19.958424	C	3.358943	-3.017091	19.478194
H	-7.548286	-3.895751	17.374676	C	1.437856	-3.092934	16.288156
H	-9.140172	-3.081720	17.222861	N	3.511436	-2.427541	22.399204
C	-10.700966	-3.292626	22.518074	C	4.579557	-2.730085	21.591401
C	-10.554604	-1.947517	23.118370	C	5.816522	-2.661630	22.333076
N	-9.326571	-1.322544	23.207257	C	5.477320	-2.299587	23.617575
C	-11.461732	-1.081995	23.662662	C	4.030824	-2.159543	23.634013
C	-9.459492	-0.125404	23.776328	C	7.162697	-2.944947	21.771281
N	-10.754305	0.031351	24.057936	C	6.324190	-2.094334	24.776205
H	-10.389469	-3.277370	21.463964	C	7.616872	-1.730830	24.758142
H	-11.743821	-3.621693	22.574252	N	-0.334821	-2.035392	21.250745
H	-8.421312	-1.779631	22.890622	C	-0.802206	-2.066876	19.967596
H	-12.531196	-1.163005	23.802055	C	-2.204424	-1.721374	19.952150
H	-8.673274	0.606923	23.953861	C	-2.574485	-1.490647	21.266873
C	-0.049509	-7.196989	24.285053	C	-1.397168	-1.698299	22.053055
C	0.653251	-6.159582	23.469961	C	-3.091664	-1.616155	18.817961
N	1.569303	-6.447054	22.477686	C	-3.915518	-1.136670	21.805249
C	0.486779	-4.793594	23.394082	C	-4.844313	-2.354172	21.885262
C	1.919831	-5.303372	21.848040	C	-6.093719	-2.103064	22.700110
N	1.275813	-4.271168	22.379486	O	-7.181897	-2.648876	22.305057
H	-0.712938	-7.788371	23.635069	O	-6.015578	-1.421357	23.761192
H	-0.679683	-6.692639	25.027166	C	4.507288	-3.509996	17.162173
H	1.929397	-7.372716	22.246374	O	5.628880	-2.649050	17.433365
H	-0.152359	-4.166273	24.002483	C	4.992744	-4.944923	17.310430
H	2.632292	-5.265178	21.035794	H	5.847640	-5.111901	16.640066

Cu	0.180777	1.958553	20.582633	H	-2.165129	0.747584	25.266441
H	8.891071	3.392424	20.913366	H	-0.940080	1.218562	26.468526
H	-4.673317	2.104938	16.938341	H	-1.068650	-1.065416	27.491575
H	-5.531461	3.294704	21.032081	H	-2.154369	-1.588758	26.200477
H	-9.006487	-4.710143	17.956795	H	2.627438	-1.542092	27.513850
H	-10.071116	-4.017670	23.050776	H	2.111053	0.149198	27.290925
H	0.595658	-7.919075	24.825694	H	1.026296	-1.010657	28.074505
H	-7.746918	-3.426173	30.227400	H	-2.268078	-1.338385	23.953476
O	1.877228	-0.606561	21.372848	H	3.838548	-1.572432	25.657917
O	1.168958	1.919364	22.189882	H	5.847947	-2.246436	25.748379
O	-7.554251	0.174691	20.795631	H	8.167574	-1.614031	25.690996
H	-7.380152	0.666525	19.965524	H	8.149785	-1.514708	23.833841
H	-7.982639	-0.657962	20.471600	H	7.825343	-3.357057	22.544193
O	-7.291220	-2.152026	26.040599	H	7.111980	-3.663921	20.943241
H	-6.884198	-1.887870	25.163640	H	7.631984	-2.024253	21.388676
H	-7.301293	-3.132308	26.004677	H	5.442083	-3.182997	19.709194
O	0.990310	2.670390	27.276717	H	4.184050	-3.364434	16.117332
H	0.626716	2.776953	26.354883	H	4.189839	-5.648042	17.047608
H	0.228221	2.889932	27.854283	H	5.308369	-5.142316	18.345083
O	-7.386767	2.228339	24.048464	H	2.209102	-3.245039	15.524079
H	-6.504560	1.786867	24.219440	H	0.722385	-3.926020	16.217262
H	-7.378597	2.412534	23.083765	H	0.893114	-2.168906	16.044883
O	-4.996059	0.966248	24.436954	H	-0.582946	-2.381754	17.898731
H	-4.612277	0.964277	25.379666	H	-4.106703	-1.238211	19.073528
H	-5.279577	0.035747	24.205923	H	-4.394316	-0.356105	21.193869
O	-5.446589	2.727721	28.591230	H	-3.809046	-0.715055	22.810142
H	-4.926789	2.120728	27.994651	H	-4.316096	-3.184150	22.385944
H	-5.420929	3.588662	28.123798	H	-5.109825	-2.707281	20.880207
O	0.097826	3.010521	24.676302	H	5.281872	-1.718081	17.577655
H	0.639157	3.831526	24.473136	H	0.604771	2.197281	22.949483
H	-0.832732	3.317668	24.641310	H	-11.157723	0.855184	24.504615
H	-7.336047	-3.252136	20.880581				

PW91-Fe<sup>4+</sup>=O<sup>2-</sup>...HO<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>•</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	H	4.342081	4.387027	19.049312
C	1.250167	6.082188	23.614665	H	2.987239	0.385873	19.507079
O	1.737893	5.196249	24.352194	H	2.968947	4.959115	21.731940
H	1.502042	7.828999	24.784878	C	8.848157	3.232437	19.815684
H	-0.110018	7.092858	24.890417	C	7.768522	2.289455	19.395972
H	0.335158	8.052889	23.444319	C	8.079943	1.003553	18.878874
N	1.198059	5.940027	22.276660	C	6.416052	2.666109	19.481485
C	1.878930	4.830718	21.626214	C	7.095645	0.150042	18.456386
C	1.544356	4.702493	20.135106	C	5.402808	1.828724	19.056840
C	2.352399	3.562110	19.623372	C	5.703715	0.519123	18.493095
N	1.934664	2.239476	19.741849	O	4.787342	-0.228741	18.043952
C	3.664813	3.569666	19.253768	H	8.670190	4.222378	19.370597
C	2.967728	1.466192	19.462332	H	9.829668	2.866664	19.492846
N	4.062524	2.244391	19.160737	H	9.124777	0.700580	18.813339
H	0.905903	6.738060	21.712403	H	6.172706	3.634735	19.912433
H	1.606168	3.897023	22.135967	H	7.339246	-0.830747	18.047907
H	0.469504	4.518249	19.990121	C	-3.939205	1.313401	16.699752
H	1.805116	5.624554	19.596468	C	-2.640057	1.467614	17.417981

N	-1.431635	1.551452	16.753954	H	-4.220448	-0.832749	30.949273
C	-2.304311	1.511793	18.748785	H	-3.722511	-0.045507	29.444943
C	-0.430206	1.652757	17.651586	Fe	1.545939	-2.292030	21.798977
N	-0.930846	1.633910	18.883266	C	-1.352101	-1.540891	23.451740
H	-4.396470	0.341657	16.934805	C	-0.179409	-2.480864	18.860005
H	-3.769910	1.340947	15.615823	C	4.404981	-3.174824	20.177409
H	-1.309705	1.548694	15.741371	C	3.266565	-2.034594	24.723591
H	-2.956713	1.466328	19.610253	N	1.054606	-1.866935	23.694420
H	0.613301	1.752491	17.385637	C	-0.190377	-1.568796	24.187475
C	-4.930563	3.926474	21.696842	C	-0.123191	-1.276185	25.600713
C	-3.587735	3.319947	21.830593	C	1.193480	-1.384085	25.956742
N	-3.312880	2.281152	22.696947	C	1.909734	-1.771313	24.758610
C	-2.436367	3.513075	21.109037	C	1.826590	-1.149655	27.280450
C	-2.044414	1.878958	22.493308	O	-2.972665	-1.960572	17.714661
N	-1.487315	2.606978	21.531441	C	-1.289480	-0.927207	26.459683
H	-4.858039	4.921350	21.242530	C	-1.890351	0.463015	26.173195
H	-5.443347	4.008985	22.662777	C	-2.903011	0.827370	27.241552
H	-3.981267	1.832686	23.370619	O	-2.530105	0.827404	28.438723
H	-2.249684	4.213128	20.303517	O	-4.116396	1.083166	26.875427
H	-1.534074	1.090658	23.028826	N	1.996075	-2.862710	19.921483
C	-8.210373	-3.977049	17.765098	C	1.157163	-2.817410	18.837462
C	-7.898405	-3.124164	18.957590	C	1.885631	-3.111360	17.621134
O	-7.701047	-1.907083	18.877070	C	3.191676	-3.292914	17.986562
O	-7.818311	-3.807260	20.097193	C	3.246492	-3.122217	19.425352
H	-7.301119	-4.541150	17.510296	C	1.261768	-3.200889	16.273571
H	-8.479908	-3.341162	16.916737	N	3.444232	-2.635373	22.364327
C	-10.820488	-3.325634	22.646256	C	4.493874	-2.945250	21.537971
C	-10.701665	-2.005245	23.304756	C	5.734003	-2.959567	22.274214
N	-9.502048	-1.321299	23.348666	C	5.415118	-2.639792	23.576836
C	-11.614196	-1.213507	23.944000	C	3.976598	-2.436258	23.606095
C	-9.660214	-0.159916	23.981377	C	7.065123	-3.274148	21.692973
N	-10.940276	-0.082558	24.348798	C	6.272268	-2.526508	24.739208
H	-10.650691	-3.235964	21.563328	C	7.588016	-2.256091	24.734132
H	-11.817415	-3.746575	22.813088	N	-0.396766	-2.082112	21.261170
H	-8.590307	-1.700880	22.943502	C	-0.896029	-2.129642	19.990718
H	-12.668030	-1.356364	24.140901	C	-2.296479	-1.773085	20.002394
H	-8.894990	0.599203	24.129840	C	-2.637014	-1.526761	21.321971
C	-0.100704	-7.243146	24.296570	C	-1.439827	-1.728048	22.083051
C	0.556503	-6.220619	23.434383	C	-3.208963	-1.659452	18.889094
N	1.405510	-6.528130	22.390839	C	-3.962059	-1.146441	21.879608
C	0.426171	-4.851370	23.381428	C	-4.966144	-2.308407	21.888234
C	1.753995	-5.391175	21.749956	C	-6.218185	-1.991274	22.679481
N	1.172319	-4.346826	22.328274	O	-7.337551	-2.417152	22.226942
H	-0.768245	-7.874199	23.690482	O	-6.114809	-1.363086	23.771170
H	-0.713703	-6.733451	25.048839	C	4.346880	-3.611223	17.085393
H	1.717180	-7.463048	22.128892	O	5.502426	-2.795076	17.362867
H	-0.156456	-4.211724	24.031792	C	4.786672	-5.064546	17.188825
H	2.417334	-5.366166	20.896606	H	5.627552	-5.242661	16.503827
C	-7.258219	-2.875921	29.419664	Cu	0.114630	1.854768	20.605464
N	-6.097872	-2.209725	29.982800	H	8.891071	3.392426	20.913366
C	-5.381985	-1.284659	29.331058	H	-4.673317	2.104936	16.938341
N	-5.711073	-0.918171	28.095296	H	-5.531461	3.294704	21.032081
N	-4.343739	-0.708703	29.947677	H	-9.006486	-4.710145	17.956797
H	-6.977487	-3.580947	28.624377	H	-10.071115	-4.017670	23.050778
H	-7.963414	-2.134927	29.023067	H	0.595660	-7.919073	24.825699
H	-5.687434	-2.599127	30.829716	H	-7.746918	-3.426168	30.227401
H	-6.344864	-1.461577	27.484330	O	1.909774	-0.714211	21.415188
H	-5.189398	-0.140878	27.657510	O	0.871037	1.536690	22.332216

O	-6.497481	0.227242	20.258657	H	2.455336	-0.247628	27.251660
H	-6.348033	0.784620	19.466180	H	1.068046	-0.999682	28.057051
H	-6.921255	-0.588067	19.878982	H	-2.272975	-1.327941	23.986008
O	-7.393314	-2.025484	26.071213	H	3.819350	-1.898348	25.648608
H	-6.983028	-1.781305	25.190472	H	5.784999	-2.673784	25.706669
H	-7.411114	-3.006380	26.053299	H	8.141038	-2.207448	25.671563
O	1.064333	2.306858	27.233104	H	8.139869	-2.052066	23.818687
H	0.872880	2.375067	26.247296	H	7.700144	-3.781250	22.431756
H	0.183229	2.402421	27.651405	H	6.979182	-3.923743	20.813414
O	-7.426152	2.052115	23.690309	H	7.588112	-2.355009	21.383641
H	-6.549391	1.711392	24.031463	H	5.325619	-3.353248	19.631438
H	-7.373572	1.891529	22.723853	H	4.016555	-3.424328	16.049562
O	-5.012301	1.000440	24.422775	H	3.957289	-5.732682	16.917156
H	-4.646618	1.000313	25.374887	H	5.105943	-5.300055	18.214441
H	-5.299405	0.069833	24.201641	H	2.017308	-3.337699	15.491262
O	-5.187769	3.203755	28.230160	H	0.567499	-4.053557	16.223963
H	-4.784182	2.413561	27.772252	H	0.686665	-2.293704	16.038564
H	-4.720483	3.963922	27.824725	H	-0.727316	-2.474648	17.922578
O	0.552008	2.702255	24.622063	H	-4.207995	-1.256972	19.167082
H	1.002389	3.569638	24.453809	H	-4.405745	-0.316369	21.307967
H	0.655836	2.185556	23.745444	H	-3.840484	-0.791359	22.908001
H	-7.566835	-3.184658	20.891585	H	-4.509653	-3.190683	22.369730
H	-2.360618	0.499767	25.184242	H	-5.233740	-2.601844	20.865036
H	-1.083772	1.210537	26.180046	H	5.192457	-1.864680	17.549979
H	-0.979263	-0.948061	27.512596	H	1.341645	0.669782	22.194942
H	-2.079020	-1.691043	26.347554	H	-11.352622	0.706743	24.845964
H	2.461318	-1.997034	27.576953				

OLYP-Fe<sup>4+</sup>=O<sup>2-</sup>...OH<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>•</sup>-H376<sup>+</sup>:

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C	0.705000	7.351000	24.202000	C	8.182253	1.286423	18.641374
C	1.475724	6.282899	23.478730	C	6.554715	2.963942	19.280203
O	2.028792	5.362395	24.114218	C	7.185761	0.503486	18.126984
H	1.356787	7.793659	24.960481	C	5.529163	2.203428	18.762982
H	-0.138011	6.879754	24.717923	C	5.801981	0.913753	18.132342
H	0.325555	8.135787	23.541512	O	4.893994	0.211000	17.616096
N	1.532341	6.354176	22.136627	H	8.835593	4.439691	19.497507
C	2.304099	5.399452	21.359299	H	9.957160	3.050133	19.529878
C	1.818229	5.229236	19.911838	H	9.212913	0.942651	18.606036
C	2.558856	4.058864	19.359277	H	6.332092	3.903719	19.771521
N	2.086175	2.756079	19.460765	H	7.412690	-0.456041	17.672878
C	3.863406	4.018217	18.968347	C	-3.870901	1.454761	16.552785
C	3.085011	1.953453	19.162807	C	-2.564155	1.671320	17.242539
N	4.207059	2.681192	18.856383	N	-1.375891	1.821515	16.559934
H	1.166590	7.183659	21.679098	C	-2.205190	1.738637	18.563321
H	2.227546	4.434377	21.863606	C	-0.371945	1.987930	17.440116
H	0.739437	5.047197	19.886261	N	-0.843736	1.947403	18.679580
H	2.018657	6.129681	19.319960	H	-4.197258	0.414058	16.659945
H	4.569512	4.806716	18.767002	H	-3.768093	1.661144	15.483094
H	3.069007	0.877828	19.182828	H	-1.267430	1.818958	15.549090
H	3.360555	5.699086	21.344710	H	-2.837838	1.658705	19.429219
C	8.961494	3.397709	19.815010	H	0.653506	2.145615	17.151069
C	7.892030	2.541714	19.227215	C	-4.948096	4.009584	21.624080

C	-3.575400	3.472906	21.773837	C	1.229888	-1.278097	26.006321
N	-3.278103	2.408578	22.596722	C	1.971821	-1.692696	24.832255
C	-2.426792	3.715216	21.068486	C	1.830779	-0.907794	27.318096
C	-2.006908	2.031160	22.369263	O	-2.819968	-2.383659	17.734421
N	-1.464683	2.802467	21.439585	C	-1.264179	-0.916158	26.495498
H	-4.927229	4.960921	21.087196	C	-1.644290	0.578616	26.456110
H	-5.441034	4.156991	22.589148	C	-2.734218	0.874214	27.479250
H	-3.915689	1.984617	23.291268	O	-2.416955	0.818040	28.693978
H	-2.253002	4.447704	20.294669	O	-3.920353	1.110020	27.052278
H	-1.509157	1.217226	22.867659	N	2.188199	-2.959741	20.022938
C	-8.569454	-3.733668	17.718052	C	1.358965	-2.991277	18.938357
C	-8.377930	-2.941889	18.976549	C	2.114146	-3.263619	17.733101
O	-8.918029	-1.863406	19.204387	C	3.421637	-3.383598	18.114714
O	-7.549355	-3.550523	19.832906	C	3.452933	-3.166498	19.551731
H	-7.595550	-3.916845	17.250610	C	1.513338	-3.354255	16.372257
H	-9.217718	-3.193164	17.026693	N	3.595027	-2.558564	22.480490
C	-10.824191	-3.365961	22.597498	C	4.667899	-2.816519	21.673973
C	-10.730706	-1.999394	23.163173	C	5.903410	-2.683160	22.413934
N	-9.542318	-1.297893	23.215749	C	5.550831	-2.316478	23.691690
C	-11.675695	-1.180622	23.711599	C	4.098536	-2.243090	23.707924
C	-9.740298	-0.107355	23.772071	C	7.263958	-2.917975	21.859467
N	-11.032394	-0.023658	24.075884	C	6.384658	-2.058816	24.854429
H	-10.658039	-3.350527	21.515355	C	7.626392	-1.551279	24.861207
H	-11.814385	-3.782716	22.794150	N	-0.290273	-2.287301	21.324819
H	-8.610863	-1.660529	22.864068	C	-0.760550	-2.408196	20.055383
H	-12.733088	-1.322226	23.874471	C	-2.170173	-2.088898	20.025823
H	-8.997236	0.652722	23.962640	C	-2.532649	-1.772394	21.324799
C	-0.116716	-7.347916	24.222849	C	-1.345563	-1.909418	22.113944
C	0.586643	-6.330339	23.406107	C	-3.070476	-2.048262	18.894129
N	1.555336	-6.640682	22.479369	C	-3.866997	-1.339391	21.830705
C	0.484533	-4.966247	23.357204	C	-4.870336	-2.486370	22.022214
C	1.998215	-5.502919	21.909057	C	-6.144952	-2.012732	22.710738
N	1.365034	-4.461111	22.423493	O	-7.261807	-2.336913	22.182688
H	-0.669493	-8.051352	23.589023	O	-6.034872	-1.353104	23.775860
H	-0.823431	-6.854748	24.895081	C	4.586192	-3.671998	17.208946
H	1.893175	-7.573195	22.258415	O	5.682591	-2.756421	17.405268
H	-0.161441	-4.331392	23.939001	C	5.138814	-5.083227	17.358883
H	2.758577	-5.481915	21.148152	H	5.955893	-5.229635	16.642381
C	-7.166609	-2.926930	29.456816	Cu	0.247606	2.299939	20.443334
N	-6.055180	-2.262365	30.112580	H	8.891071	3.392424	20.913366
C	-5.249600	-1.382033	29.514039	H	-4.673317	2.104938	16.938341
N	-5.449131	-1.027133	28.250858	H	-5.531461	3.294704	21.032081
N	-4.224188	-0.860706	30.199029	H	-9.006487	-4.710143	17.956795
H	-6.822702	-3.669876	28.728420	H	-10.071116	-4.017670	23.050776
H	-7.809144	-2.192408	28.966753	H	0.595658	-7.919075	24.825694
H	-5.715612	-2.666973	30.979669	H	-7.746918	-3.426173	30.227400
H	-6.104965	-1.514396	27.641934	O	1.901784	-0.791950	21.474618
H	-4.923452	-0.244470	27.848145	O	1.237412	2.220880	22.056352
H	-4.255314	-0.872070	31.211957	O	-8.170142	0.967256	20.206250
H	-3.622971	-0.158356	29.747302	H	-7.741809	1.244746	19.372385
Fe	1.665931	-2.369214	21.888628	H	-8.320486	0.011071	20.056659
C	-1.274098	-1.654361	23.476892	O	-7.354317	-2.062603	26.126632
C	0.000662	-2.752879	18.949763	H	-6.960161	-1.819657	25.252756
C	4.600622	-3.117589	20.324770	H	-7.380966	-3.038401	26.096738
C	3.347773	-1.845660	24.798095	O	1.552233	3.481619	27.782986
N	1.128782	-1.906897	23.783277	H	1.142310	3.381443	26.891781
C	-0.129872	-1.628750	24.242820	H	0.849815	3.177970	28.388454
C	-0.088035	-1.262495	25.643110	O	-7.654339	2.415046	24.691106

H	-6.743586	2.038253	24.651269	H	8.153702	-1.413979	25.802747
H	-7.682589	3.020831	23.925912	H	8.139584	-1.242482	23.956037
O	-5.033246	1.212198	24.539675	H	7.955625	-3.216620	22.651963
H	-4.578801	1.139556	25.423700	H	7.258890	-3.704639	21.099571
H	-5.306282	0.296976	24.303579	H	7.660833	-2.004539	21.396059
O	-5.592123	2.757638	28.812459	H	5.535013	-3.262767	19.807352
H	-4.996310	2.220110	28.240385	H	4.228063	-3.564563	16.177778
H	-5.465999	3.664718	28.466394	H	4.349564	-5.813026	17.148917
O	0.458582	3.282002	25.087349	H	5.518608	-5.259335	18.370442
H	0.958884	4.059681	24.744165	H	2.278199	-3.467742	15.601507
H	-0.464089	3.596340	25.125029	H	0.830401	-4.209689	16.299152
H	-7.452859	-3.012473	20.693746	H	0.937407	-2.450275	16.141733
H	-1.971153	0.861905	25.453857	H	-0.525666	-2.808881	18.009657
H	-0.760840	1.174634	26.702831	H	-4.080510	-1.671914	19.136820
H	-1.038708	-1.182693	27.533084	H	-4.296302	-0.596165	21.148936
H	-2.132150	-1.522243	26.206165	H	-3.747868	-0.832147	22.786810
H	2.639651	-1.589109	27.601100	H	-4.424228	-3.254702	22.668960
H	2.248955	0.107068	27.276509	H	-5.101132	-2.961991	21.066342
H	1.082337	-0.925576	28.114279	H	5.309310	-1.850118	17.399305
H	-2.200809	-1.429459	23.984083	H	0.691873	2.543060	22.794966
H	3.884960	-1.604280	25.703947	H	-11.470602	0.779232	24.521592
H	5.933571	-2.296602	25.817537				

OLYP-Fe<sup>4+</sup>=O<sup>2-</sup>...HO<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>\*</sup>-H376<sup>+</sup>:

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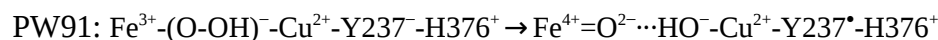
C	0.705000	7.351000	24.202000	C	5.785058	0.704085	18.287257
C	1.472310	6.229819	23.567718	O	4.878248	-0.001619	17.775298
O	2.119878	5.424316	24.265168	H	8.801219	4.300113	19.406099
H	1.380583	7.907175	24.858778	H	9.931115	2.926464	19.543024
H	-0.086416	6.917936	24.823295	H	9.203383	0.805642	18.679227
H	0.255287	8.035911	23.477563	H	6.289864	3.719680	19.887316
N	1.412858	6.128332	22.226819	H	7.409632	-0.647070	17.816353
C	2.167585	5.114245	21.513756	C	-3.882958	1.433877	16.568461
C	1.738444	4.952853	20.050648	C	-2.584042	1.618261	17.281291
C	2.496356	3.785082	19.521936	N	-1.375176	1.694458	16.622582
N	2.056094	2.474853	19.667005	C	-2.252500	1.710255	18.607515
C	3.795681	3.763591	19.116752	C	-0.383754	1.840674	17.519694
C	3.069541	1.686005	19.374183	N	-0.885201	1.859925	18.748329
N	4.167709	2.433424	19.034011	H	-4.237232	0.402008	16.670698
H	0.960293	6.869784	21.701317	H	-3.756845	1.635448	15.500068
H	2.030232	4.162720	22.031234	H	-1.243260	1.649829	15.615441
H	0.659631	4.786507	19.976464	H	-2.907033	1.683317	19.460169
H	1.973985	5.853818	19.473094	H	0.654127	1.942570	17.250205
H	4.479269	4.564813	18.889048	C	-4.962064	4.049032	21.583751
H	3.074927	0.611230	19.417411	C	-3.593779	3.515632	21.763271
H	3.237820	5.356970	21.544040	N	-3.310175	2.486494	22.633902
C	8.938539	3.291790	19.816924	C	-2.439443	3.719172	21.056337
C	7.866431	2.386495	19.311789	C	-2.039498	2.096478	22.439225
C	8.166633	1.126803	18.739086	N	-1.484092	2.823234	21.482051
C	6.519488	2.776709	19.405434	H	-4.941452	4.969694	20.995570
C	7.174525	0.314515	18.262244	H	-5.459867	4.243785	22.537994
C	5.500083	1.987391	18.922966	H	-3.966417	2.056948	23.304207

H	-2.256089	4.416241	20.252842	O	-3.975956	1.152650	26.966594
H	-1.541268	1.311419	22.978184	N	2.055779	-2.982547	19.952802
C	-8.236753	-3.968984	17.720569	C	1.214190	-2.959012	18.877007
C	-7.966251	-3.079644	18.896867	C	1.945588	-3.231696	17.658336
O	-7.871314	-1.856818	18.822718	C	3.252751	-3.404435	18.021586
O	-7.817136	-3.767765	20.033658	C	3.307287	-3.225631	19.461985
H	-7.316821	-4.516084	17.480467	C	1.320277	-3.293244	16.306931
H	-8.535904	-3.371430	16.857954	N	3.494029	-2.733409	22.409862
C	-10.883496	-3.398119	22.663463	C	4.548064	-3.017863	21.586645
C	-10.827644	-2.058550	23.290528	C	5.789513	-2.990876	22.326071
N	-9.663009	-1.319291	23.334016	C	5.461509	-2.663055	23.622211
C	-11.779960	-1.299729	23.907225	C	4.016040	-2.502147	23.647906
C	-9.881519	-0.160496	23.947387	C	7.132777	-3.278621	21.754651
N	-11.163611	-0.136259	24.298674	C	6.309597	-2.513697	24.792216
H	-10.767475	-3.322685	21.576825	C	7.597814	-2.137128	24.820033
H	-11.838140	-3.880125	22.884507	N	-0.384686	-2.266914	21.300416
H	-8.734761	-1.647036	22.951618	C	-0.874186	-2.350667	20.034666
H	-12.825415	-1.486923	24.098273	C	-2.281609	-2.022856	20.034522
H	-9.159926	0.622988	24.119417	C	-2.628142	-1.747433	21.347093
C	-0.159394	-7.363225	24.261605	C	-1.427416	-1.906189	22.114520
C	0.486598	-6.364514	23.377959	C	-3.194171	-1.935413	18.913905
N	1.387170	-6.691310	22.389752	C	-3.956907	-1.335620	21.885055
C	0.389549	-5.000847	23.324185	C	-4.986159	-2.473175	21.979897
C	1.797008	-5.562585	21.779576	C	-6.240901	-2.042585	22.732096
N	1.207280	-4.511474	22.326845	O	-7.374729	-2.340778	22.225196
H	-0.755963	-8.079335	23.684544	O	-6.095637	-1.443132	23.828491
H	-0.815648	-6.853526	24.971653	C	4.394739	-3.721607	17.095906
H	1.697367	-7.629157	22.151424	O	5.547992	-2.889040	17.322518
H	-0.208382	-4.357698	23.946078	C	4.855113	-5.170824	17.182373
H	2.501725	-5.553157	20.967001	H	5.661900	-5.337451	16.458585
C	-7.226036	-2.881839	29.444929	Cu	0.178504	2.083637	20.540418
N	-6.084372	-2.226264	30.055587	H	8.891071	3.392426	20.913366
C	-5.340043	-1.295437	29.452630	H	-4.673317	2.104936	16.938341
N	-5.639271	-0.880715	28.225466	H	-5.531461	3.294704	21.032081
N	-4.301859	-0.763599	30.102757	H	-9.006486	-4.710145	17.956797
H	-6.918699	-3.587185	28.665595	H	-10.071115	-4.017670	23.050778
H	-7.910574	-2.139595	29.028052	H	0.595660	-7.919073	24.825699
H	-5.695417	-2.646809	30.893376	H	-7.746918	-3.426168	30.227401
H	-6.254646	-1.413525	27.612215	O	1.886432	-0.845547	21.496071
H	-5.099720	-0.118174	27.803613	O	0.934722	1.735611	22.274351
H	-4.210454	-0.894198	31.103003	O	-6.716422	0.624986	20.182333
H	-3.680276	-0.092288	29.634748	H	-6.545921	1.070393	19.330311
Fe	1.576144	-2.432701	21.842671	H	-7.088448	-0.233798	19.898177
C	-1.330620	-1.679149	23.479819	O	-7.496309	-2.097705	26.129804
C	-0.135877	-2.681119	18.910505	H	-7.076432	-1.867273	25.263801
C	4.460210	-3.257001	20.226339	H	-7.468786	-3.073466	26.136226
C	3.289977	-2.106321	24.755806	O	1.213969	2.884542	27.643692
N	1.067761	-2.007292	23.749761	H	1.063668	2.770884	26.677935
C	-0.175189	-1.690504	24.228235	H	0.332062	2.714578	28.026050
C	-0.107022	-1.365616	25.637921	O	-7.709913	2.387163	23.979417
C	1.210535	-1.462519	25.991588	H	-6.828133	2.010632	24.210769
C	1.925738	-1.874672	24.800250	H	-7.703002	2.387065	23.002285
C	1.848992	-1.194230	27.309950	O	-5.115567	1.180374	24.475412
O	-2.961525	-2.237666	17.742003	H	-4.676986	1.133651	25.369706
C	-1.268635	-0.995603	26.502937	H	-5.372173	0.257361	24.258697
C	-1.770754	0.446522	26.297995	O	-5.211291	3.336090	28.369787
C	-2.793160	0.846813	27.357050	H	-4.759538	2.577244	27.928535
O	-2.429936	0.833114	28.559396	H	-4.777630	4.112724	27.965846



O	0.785962	2.871273	24.767471	H	7.615762	-2.355586	21.406611
H	1.241231	3.712892	24.562651	H	5.382187	-3.430600	19.695770
H	0.793185	2.392433	23.894251	H	4.038784	-3.545404	16.073454
H	-7.605992	-3.141537	20.813544	H	4.021404	-5.839612	16.943127
H	-2.204173	0.566924	25.305115	H	5.222025	-5.412324	18.185406
H	-0.919223	1.129313	26.367555	H	2.066055	-3.424979	15.520749
H	-0.980861	-1.109111	27.551258	H	0.613738	-4.130242	16.242456
H	-2.096113	-1.698628	26.332971	H	0.764855	-2.373022	16.092000
H	2.457797	-2.044727	27.638103	H	-0.676410	-2.699295	17.976948
H	2.505543	-0.317304	27.247896	H	-4.193095	-1.549608	19.182644
H	1.101481	-0.994416	28.080094	H	-4.375154	-0.529893	21.271337
H	-2.246385	-1.456648	24.006163	H	-3.829911	-0.919056	22.882001
H	3.838982	-1.935928	25.670767	H	-4.551273	-3.311835	22.542285
H	5.830105	-2.724063	25.747813	H	-5.243852	-2.848983	20.988019
H	8.123261	-2.071713	25.770089	H	5.233495	-1.962276	17.387447
H	8.152957	-1.864170	23.928421	H	1.320554	0.840219	22.170211
H	7.783231	-3.730172	22.509321	H	-11.612587	0.635489	24.785784
H	7.072578	-3.965604	20.906574				

### Cartesian Coordinates of the Highest-Energy Structures with His376<sup>+</sup> Given in Table 3:

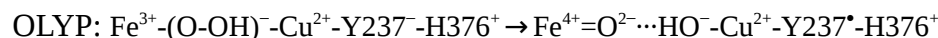


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C	0.705000	7.351000	24.202000	H	9.800813	3.137259	19.407047
C	1.057578	6.029864	23.577391	H	9.138479	0.999400	18.538935
O	1.197477	5.012761	24.293263	H	6.115288	3.714817	19.926802
H	1.563701	7.676256	24.804275	H	7.395015	-0.508120	17.662271
H	-0.149328	7.209274	24.873488	C	-3.929692	1.461205	16.444693
H	0.472202	8.125274	23.461224	C	-2.626204	1.496465	17.156450
N	1.240115	6.011451	22.241283	N	-1.411269	1.369779	16.514168
C	1.900518	4.904000	21.572470	C	-2.309047	1.595477	18.486324
C	1.466754	4.699324	20.115678	C	-0.417142	1.407316	17.425402
C	2.300764	3.589122	19.577964	N	-0.936196	1.542640	18.642141
N	1.939054	2.254868	19.706855	H	-4.323311	0.434324	16.411178
C	3.605567	3.645727	19.174919	H	-3.813051	1.813251	15.411721
C	2.999006	1.522998	19.383908	H	-1.280614	1.294046	15.505308
N	4.048014	2.339132	19.062853	H	-2.974026	1.698115	19.333264
H	1.216039	6.907530	21.752520	H	0.635077	1.359674	17.178818
H	1.695292	3.995346	22.149422	C	-4.847602	3.909426	21.636017
H	0.397428	4.451089	20.063779	C	-3.524427	3.249235	21.745942
H	1.628574	5.617950	19.533997	N	-3.279743	2.192923	22.600170
H	4.253876	4.487561	18.971117	C	-2.358446	3.428300	21.043203
H	3.066056	0.443824	19.386815	C	-2.020197	1.764475	22.398297
H	2.990483	5.066695	21.593093	N	-1.428316	2.488683	21.449153
C	8.817139	3.409845	19.809505	H	-4.743104	4.880222	21.138187
C	7.757035	2.482634	19.287252	H	-5.302972	4.066737	22.622868
C	8.087637	1.270754	18.649721	H	-3.957773	1.765030	23.277939
C	6.400155	2.797972	19.412254	H	-2.145573	4.142781	20.257371
C	7.115126	0.421105	18.159714	H	-1.562518	0.940741	22.925547
C	5.408364	1.963732	18.909351	C	-8.403219	-3.817082	17.746330
C	5.722243	0.723353	18.252991	C	-8.070605	-3.050354	18.988460
O	4.799708	-0.040436	17.783818	O	-8.081640	-1.815833	19.036171
H	8.599613	4.448298	19.521351	O	-7.737164	-3.823398	20.019528

H	-7.458630	-4.155759	17.295460	C	1.294102	-2.718956	16.354454
H	-8.918333	-3.165491	17.034287	N	3.393839	-2.361961	22.476348
C	-10.826141	-3.317854	22.667421	C	4.453174	-2.655889	21.655922
C	-10.673209	-1.988203	23.302791	C	5.689632	-2.664255	22.401250
N	-9.463280	-1.322246	23.300057	C	5.358681	-2.358324	23.702717
C	-11.555463	-1.168401	23.950562	C	3.915800	-2.171051	23.722852
C	-9.583308	-0.145969	23.913281	C	7.026158	-2.964727	21.825099
N	-10.852454	-0.040319	24.311336	C	6.206245	-2.258411	24.872973
H	-10.693685	-3.242643	21.577902	C	7.522402	-1.989446	24.880639
H	-11.821711	-3.725284	22.871256	N	-0.443580	-1.890889	21.374851
H	-8.571268	-1.744652	22.894310	C	-0.918230	-1.876736	20.089829
H	-12.605301	-1.288897	24.180806	C	-2.328345	-1.575722	20.094188
H	-8.802669	0.602718	24.042097	C	-2.701763	-1.425872	21.417277
C	-0.027088	-7.170892	24.281275	C	-1.519091	-1.628841	22.194397
C	0.668952	-6.085233	23.513200	C	-3.229150	-1.455711	18.966946
N	1.621854	-6.311130	22.537942	C	-4.044064	-1.115170	21.961646
C	0.432921	-4.727319	23.446176	C	-4.998178	-2.312430	21.923072
C	1.929966	-5.146660	21.928356	C	-6.275473	-2.033214	22.676599
N	1.218936	-4.152981	22.452892	O	-7.361767	-2.539060	22.225265
H	-0.662777	-7.743860	23.588092	O	-6.234069	-1.347737	23.737726
H	-0.690218	-6.699838	25.016947	C	4.341706	-3.308175	17.197223
H	2.036806	-7.213478	22.305704	O	5.521123	-2.552880	17.499726
H	-0.254048	-4.138922	24.041411	C	4.708385	-4.784150	17.280599
H	2.660638	-5.064798	21.135633	H	5.539508	-4.991605	16.591765
C	-7.227091	-2.942039	29.398842	Cu	0.073787	1.713258	20.344761
N	-6.045702	-2.302429	29.944929	H	8.891071	3.392425	20.913367
C	-5.332104	-1.378834	29.292981	H	-4.673316	2.104937	16.938340
N	-5.669523	-1.006422	28.063277	H	-5.531460	3.294702	21.032081
N	-4.267080	-0.831010	29.899732	H	-9.006487	-4.710145	17.956794
H	-6.970742	-3.694871	28.640157	H	-10.071117	-4.017673	23.050774
H	-7.895030	-2.189991	28.961553	H	0.595662	-7.919075	24.825693
H	-5.644599	-2.683547	30.799979	H	-7.746923	-3.426175	30.227399
H	-6.316873	-1.542028	27.459357	O	1.884312	-0.471587	21.613512
H	-5.161106	-0.220799	27.623518	O	0.837169	0.847255	22.014172
H	-4.207715	-0.885872	30.914490	O	-6.629739	0.177298	20.356379
H	-3.752757	-0.055742	29.440488	H	-6.493206	0.738975	19.565391
Fe	1.457130	-2.074936	21.936988	H	-7.134149	-0.598107	19.996267
C	-1.454468	-1.482251	23.569350	O	-7.380240	-2.119215	26.073841
C	-0.179165	-2.124376	18.948472	H	-7.022657	-1.838440	25.181811
C	4.377906	-2.885904	20.295042	H	-7.356407	-3.099419	26.037258
C	3.185096	-1.810619	24.839404	O	1.365551	2.428232	27.261786
N	0.961081	-1.712846	23.811890	H	1.166942	2.315110	26.292438
C	-0.294189	-1.472271	24.309365	H	0.482136	2.486805	27.680411
C	-0.231933	-1.188915	25.721648	O	-7.432470	2.187325	23.897954
C	1.088226	-1.255996	26.076748	H	-6.542177	1.778762	24.106686
C	1.818023	-1.601362	24.874675	H	-7.428760	2.265217	22.920192
C	1.705882	-1.003737	27.404116	O	-5.030589	0.981556	24.359334
O	-2.964016	-1.725730	17.792698	H	-4.677242	0.970985	25.313263
C	-1.404271	-0.825124	26.563279	H	-5.370687	0.065961	24.146085
C	-1.890909	0.618424	26.310795	O	-5.665840	2.872875	28.273032
C	-2.992835	0.951936	27.293695	H	-5.105774	2.197727	27.795629
O	-2.692235	1.054764	28.506196	H	-5.014645	3.548948	28.559061
O	-4.203954	1.041007	26.849750	O	1.066033	2.346099	24.550705
N	1.972301	-2.549349	20.027930	H	1.026949	3.295499	24.254262
C	1.158502	-2.451602	18.929490	H	0.616452	1.788131	23.876933
C	1.897098	-2.715962	17.714676	H	-7.525852	-3.248716	20.861706
C	3.188375	-2.958057	18.092780	H	-2.244160	0.739352	25.279333
C	3.226264	-2.822076	19.536697	H	-1.051952	1.311137	26.464461

H	-1.136663	-0.917404	27.625039	H	3.848763	-5.410565	17.003661
H	-2.236290	-1.527145	26.383869	H	5.020442	-5.045189	18.302457
H	2.455555	-1.767603	27.652390	H	2.060664	-2.832115	15.579014
H	2.197717	-0.018554	27.416282	H	0.579462	-3.548785	16.244410
H	0.945864	-1.000317	28.194669	H	0.746564	-1.785116	16.160278
H	-2.387717	-1.318307	24.101840	H	-0.717479	-2.064445	18.007611
H	3.727660	-1.669763	25.769971	H	-4.243543	-1.088489	19.237549
H	5.711449	-2.418341	25.834716	H	-4.511609	-0.286649	21.407721
H	8.069381	-1.954962	25.822083	H	-3.947578	-0.790196	23.000928
H	8.080477	-1.772412	23.971399	H	-4.525511	-3.183141	22.410702
H	7.661506	-3.471342	22.563792	H	-5.224966	-2.605719	20.890174
H	6.949690	-3.608798	20.940618	H	5.246744	-1.577334	17.579238
H	7.543218	-2.039435	21.523943	H	1.641236	1.400207	22.169683
H	5.301243	-3.056112	19.750469	H	-11.233893	0.759138	24.817711
H	4.022556	-3.095205	16.161396				



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C	0.705000	7.351000	24.202000	C	-2.579763	1.638761	17.045517
C	1.311140	6.129492	23.570757	N	-1.371122	1.596332	16.384572
O	1.692273	5.179210	24.281214	C	-2.241936	1.676322	18.371375
H	1.456099	7.801916	24.859228	C	-0.371023	1.629171	17.285823
H	-0.140615	7.038125	24.822351	N	-0.868536	1.679348	18.513386
H	0.367776	8.095391	23.475588	H	-4.206599	0.592162	16.126096
N	1.422912	6.129517	22.227664	H	-3.819443	2.156900	15.388775
C	2.174612	5.117000	21.508644	H	-1.244829	1.570076	15.376378
C	1.714174	4.921332	20.058104	H	-2.896571	1.705271	19.224015
C	2.503600	3.785608	19.503512	H	0.672765	1.631410	17.017286
N	2.105029	2.464131	19.642241	C	-4.851530	4.021304	21.497481
C	3.796936	3.805664	19.068531	C	-3.501561	3.421826	21.644603
C	3.135699	1.710076	19.303228	N	-3.243439	2.386140	22.515734
N	4.200146	2.488130	18.951152	C	-2.329830	3.607489	20.956925
H	1.208211	6.993925	21.738906	C	-1.977159	1.975124	22.330037
H	2.069571	4.177104	22.050373	N	-1.388630	2.689496	21.380166
H	0.642937	4.703804	20.026665	H	-4.801460	4.905693	20.857042
H	1.887728	5.831502	19.472707	H	-5.270997	4.313578	22.466021
H	4.460954	4.625567	18.847023	H	-3.905972	1.995453	23.204355
H	3.172269	0.635419	19.310532	H	-2.124840	4.307737	20.161083
H	3.241001	5.380815	21.508944	H	-1.517860	1.160960	22.858319
C	8.958003	3.389030	19.814926	C	-8.450331	-3.805755	17.690401
C	7.901770	2.512353	19.213307	C	-8.157167	-2.968107	18.897937
C	8.218192	1.334215	18.509911	O	-8.202914	-1.740465	18.905664
C	6.550622	2.843687	19.347984	O	-7.815770	-3.703541	19.962259
C	7.235031	0.534098	17.970809	H	-7.494213	-4.120830	17.253562
C	5.546703	2.070341	18.788719	H	-8.999938	-3.219036	16.952255
C	5.841148	0.852523	18.067911	C	-10.866779	-3.366047	22.675468
O	4.926951	0.123979	17.558282	C	-10.773264	-2.026175	23.302468
H	8.831853	4.427393	19.483748	N	-9.596365	-1.306624	23.319128
H	9.959601	3.054756	19.531219	C	-11.701399	-1.246923	23.932016
H	9.261269	1.048160	18.392846	C	-9.783058	-0.141012	23.928649
H	6.283549	3.729113	19.914980	N	-11.058356	-0.091295	24.303535
H	7.501495	-0.371463	17.432826	H	-10.759785	-3.291057	21.587494
C	-3.890466	1.620202	16.341203	H	-11.834022	-3.820328	22.901771

H	-8.676962	-1.658699	22.917721	C	-0.884888	-2.092116	20.106677
H	-12.746893	-1.411079	24.142493	C	-2.297554	-1.799607	20.094573
H	-9.043236	0.626362	24.097853	C	-2.667134	-1.550765	21.404588
C	-0.068908	-7.257547	24.244596	C	-1.479512	-1.701487	22.189150
C	0.631825	-6.186894	23.478368	C	-3.206728	-1.751231	18.966281
N	1.616238	-6.430612	22.545682	C	-4.009897	-1.175422	21.924443
C	0.431391	-4.829422	23.414996	C	-4.988458	-2.351870	22.036828
C	1.975034	-5.269848	21.963902	C	-6.281633	-1.941833	22.722642
N	1.269112	-4.268697	22.467836	O	-7.380306	-2.346996	22.211277
H	-0.641465	-7.893407	23.557336	O	-6.213238	-1.252458	23.772375
H	-0.774427	-6.794283	24.939684	C	4.420606	-3.408238	17.213371
H	2.015215	-7.338314	22.321617	O	5.584271	-2.608105	17.464981
H	-0.258720	-4.233305	23.988171	C	4.842241	-4.871175	17.300522
H	2.733146	-5.202359	21.204084	H	5.649738	-5.057467	16.582204
C	-7.187428	-2.940842	29.433125	Cu	0.204273	1.888036	20.288819
N	-6.033766	-2.310853	30.046414	H	8.891071	3.392425	20.913366
C	-5.261349	-1.404959	29.446070	H	-4.673318	2.104937	16.938341
N	-5.523220	-0.994903	28.213528	H	-5.531462	3.294703	21.032081
N	-4.193646	-0.922880	30.107625	H	-9.006487	-4.710144	17.956797
H	-6.893973	-3.685987	28.685833	H	-10.071117	-4.017671	23.050776
H	-7.830822	-2.186044	28.976659	H	0.595661	-7.919074	24.825694
H	-5.661368	-2.736453	30.889237	H	-7.746920	-3.426171	30.227401
H	-6.190553	-1.472225	27.606523	O	1.909509	-0.546118	21.608865
H	-5.000459	-0.209311	27.809160	O	0.889382	0.818831	21.948289
H	-4.228866	-0.930270	31.122163	O	-6.763865	0.630080	20.199074
H	-3.677058	-0.142366	29.688952	H	-6.611445	1.061439	19.336862
Fe	1.504517	-2.144280	21.958081	H	-7.204446	-0.204424	19.939983
C	-1.407797	-1.500878	23.558895	O	-7.443482	-2.006104	26.148525
C	-0.135579	-2.378482	18.979427	H	-7.072318	-1.750909	25.267961
C	4.445545	-2.918901	20.333009	H	-7.453371	-2.981802	26.109998
C	3.219912	-1.845804	24.859856	O	1.875543	3.064415	27.533154
N	0.995023	-1.768604	23.834357	H	1.700825	2.821170	26.598615
C	-0.256628	-1.495923	24.314395	H	1.021920	2.885035	27.973248
C	-0.196340	-1.194746	25.726166	O	-7.653578	2.556757	24.500064
C	1.121442	-1.270009	26.084454	H	-6.755616	2.147663	24.501671
C	1.850788	-1.641096	24.891079	H	-7.731165	2.928288	23.600661
C	1.743915	-1.017127	27.413110	O	-5.081397	1.266122	24.446040
O	-2.963638	-2.089980	17.807569	H	-4.652298	1.181521	25.339997
C	-1.361668	-0.823466	26.578779	H	-5.399504	0.362446	24.220234
C	-1.725882	0.672568	26.477484	O	-5.798927	2.899437	28.385631
C	-2.843464	1.006280	27.457192	H	-5.146661	2.297581	27.951790
O	-2.547323	1.077440	28.674575	H	-5.287729	3.720770	28.519277
O	-4.032322	1.129328	26.990353	O	1.442951	2.393596	24.542926
N	2.038729	-2.660474	20.041811	H	1.468780	3.358889	24.342391
C	1.216474	-2.638744	18.952229	H	0.490851	2.195989	24.582146
C	1.963552	-2.903157	17.740997	H	-7.606261	-3.107523	20.761376
C	3.265091	-3.077027	18.121291	H	-2.025863	0.922725	25.457604
C	3.297977	-2.897600	19.561926	H	-0.845736	1.270152	26.734669
C	1.358776	-2.957945	16.379634	H	-1.131994	-1.056793	27.623043
N	3.457452	-2.409326	22.509040	H	-2.234778	-1.432497	26.311640
C	4.519411	-2.682763	21.693504	H	2.377597	-1.857215	27.720725
C	5.754484	-2.669421	22.444398	H	2.373349	-0.119234	27.382290
C	5.413551	-2.366935	23.741662	H	0.985702	-0.866667	28.184418
C	3.967237	-2.207067	23.754885	H	-2.334627	-1.306807	24.078613
C	7.100748	-2.948944	21.875423	H	3.752959	-1.687511	25.786642
C	6.254424	-2.239256	24.919655	H	5.785304	-2.508996	25.865486
C	7.526846	-1.816338	24.956286	H	8.060026	-1.774572	25.903304
N	-0.412787	-2.016650	21.384240	H	8.060221	-1.484185	24.071228

H	7.770149	-3.345507	22.643501
H	7.049866	-3.677654	21.061521
H	7.554820	-2.031494	21.476360
H	5.372141	-3.082932	19.806572
H	4.082272	-3.223293	16.185418
H	3.995548	-5.522325	17.057816
H	5.198487	-5.120284	18.305806
H	2.120082	-3.063311	15.604026
H	0.670132	-3.807751	16.291110
H	0.788594	-2.045909	16.168640

H	-0.672181	-2.383553	18.043289
H	-4.212064	-1.370952	19.218177
H	-4.457070	-0.402428	21.289864
H	-3.903698	-0.731820	22.911559
H	-4.537812	-3.145532	22.649945
H	-5.194976	-2.780840	21.053916
H	5.304242	-1.656613	17.463892
H	1.495757	1.260414	22.581844
H	-11.485002	0.689338	24.797071

### Cartesian Coordinates of the Optimized Structures Given in Table 4:

PW91-Fe<sup>3+</sup>-(O-OH)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-Prop-A-H.1:

205

C	0.705000	7.351000	24.202000
C	1.116244	6.052175	23.565665
O	1.242684	5.015605	24.258215
H	1.543970	7.703470	24.818275
H	-0.151146	7.171450	24.862967
H	0.454022	8.123200	23.466828
N	1.366365	6.087051	22.243738
C	2.065783	5.026370	21.543391
C	1.515307	4.723318	20.142513
C	2.338812	3.609079	19.597907
N	1.986522	2.270758	19.734553
C	3.636454	3.673289	19.175258
C	3.045817	1.546867	19.393204
N	4.084712	2.369231	19.055567
H	1.314642	6.997278	21.784539
H	2.012050	4.122497	22.158920
H	0.456473	4.435888	20.203012
H	1.588613	5.612849	19.500689
H	4.276360	4.519482	18.962313
H	3.117713	0.468130	19.391137
H	3.129266	5.300683	21.450052
C	8.843582	3.448495	19.810756
C	7.791738	2.536115	19.251087
C	8.127510	1.340385	18.586073
C	6.434118	2.841912	19.387972
C	7.157621	0.493904	18.085638
C	5.445642	2.008411	18.880098
C	5.763055	0.780901	18.202050
O	4.840488	0.014386	17.738063
H	8.630754	4.495166	19.551909
H	9.834848	3.187658	19.419875
H	9.179653	1.078672	18.465275
H	6.146785	3.747438	19.920982
H	7.439358	-0.422493	17.566773
C	-3.882082	1.589455	16.373211
C	-2.584799	1.594126	17.099560
N	-1.365626	1.533017	16.453165

C	-2.268710	1.606193	18.433653
C	-0.374509	1.525621	17.368701
N	-0.895118	1.567434	18.591094
H	-4.212610	0.558511	16.178224
H	-3.778738	2.099030	15.406224
H	-1.230005	1.525761	15.442106
H	-2.935940	1.643934	19.283741
H	0.678893	1.515013	17.120874
C	-4.810352	3.892306	21.615348
C	-3.498275	3.203493	21.715656
N	-3.272278	2.135840	22.561095
C	-2.326109	3.367095	21.018108
C	-2.020631	1.682290	22.352495
N	-1.413985	2.405407	21.412760
H	-4.688595	4.853789	21.103021
H	-5.240768	4.081449	22.608112
H	-3.944865	1.737364	23.260330
H	-2.098956	4.085540	20.239773
H	-1.585464	0.829579	22.855445
C	-8.471578	-3.789581	17.694462
C	-8.046539	-3.034255	18.906438
O	-8.149277	-1.720908	18.769158
O	-7.606388	-3.595247	19.925931
H	-7.557933	-4.075596	17.152015
H	-9.084353	-3.164622	17.038186
C	-10.816553	-3.325131	22.633317
C	-10.819982	-2.017144	23.340233
N	-9.683053	-1.253239	23.492684
C	-11.815414	-1.271502	23.928890
C	-10.013098	-0.108951	24.148827
N	-11.309214	-0.082532	24.429409
H	-10.588848	-3.197157	21.563708
H	-11.803978	-3.794357	22.715170
H	-8.754603	-1.550508	23.185751
H	-12.866777	-1.525629	24.018537
H	-9.280636	0.659836	24.377148
C	-0.025784	-7.190899	24.258804

C	0.688762	-6.117770	23.495784	C	-3.159824	-1.504571	18.972607
N	1.659431	-6.354585	22.541696	C	-4.000761	-1.189569	21.965995
C	0.470389	-4.758270	23.428605	C	-5.006881	-2.339599	21.869654
C	1.997009	-5.192505	21.942988	C	-6.245565	-2.057029	22.663108
N	1.286108	-4.192824	22.456565	O	-7.388995	-2.581503	22.253759
H	-0.642244	-7.779728	23.561870	O	-6.237905	-1.386772	23.703498
H	-0.705726	-6.711744	24.973406	C	4.429513	-3.284387	17.216078
H	2.063504	-7.262747	22.312572	O	5.588260	-2.500199	17.524030
H	-0.221198	-4.164816	24.012281	C	4.841727	-4.749081	17.279229
H	2.743821	-5.114645	21.165066	H	5.676691	-4.921220	16.585191
C	-7.201562	-2.946833	29.412321	Cu	0.137386	1.716334	20.313718
N	-6.030862	-2.308723	29.984495	H	8.891071	3.392425	20.913367
C	-5.303611	-1.381767	29.351933	H	-4.673317	2.104938	16.938341
N	-5.626666	-0.990941	28.121296	H	-5.531461	3.294705	21.032081
N	-4.246849	-0.842226	29.975085	H	-9.006487	-4.710143	17.956796
H	-6.928445	-3.703574	28.663340	H	-10.071117	-4.017670	23.050776
H	-7.854851	-2.193590	28.955917	H	0.595659	-7.919073	24.825698
H	-5.634862	-2.707909	30.833922	H	-7.746919	-3.426172	30.227401
H	-6.263162	-1.527855	27.509726	O	1.904574	-0.448329	21.665170
H	-5.110520	-0.207228	27.690715	O	0.764235	0.524315	21.957954
H	-4.175629	-0.928745	30.986366	O	-7.043433	-0.127618	20.569889
H	-3.704657	-0.088046	29.513244	H	-6.938714	0.688898	20.029474
Fe	1.517555	-2.167183	21.956512	H	-7.747698	-1.195032	19.553734
C	-1.414484	-1.568933	23.583676	O	-7.322756	-2.180337	26.144218
C	-0.117973	-2.219640	18.972517	H	-6.982194	-1.903935	25.255761
C	4.455487	-2.894945	20.320459	H	-7.233776	-3.157806	26.131802
C	3.229598	-1.827613	24.856341	O	1.505372	2.527317	26.859115
N	1.004468	-1.778458	23.829453	H	1.277588	2.395118	25.902053
C	-0.253732	-1.542607	24.323837	H	0.641975	2.479114	27.318410
C	-0.195835	-1.242142	25.733988	O	-7.468568	2.217208	24.140354
C	1.124630	-1.287928	26.090246	H	-6.559305	1.822962	24.243259
C	1.857251	-1.640533	24.891260	H	-7.494641	2.542563	23.217499
C	1.740188	-1.003009	27.412897	O	-4.999082	1.002303	24.394633
O	-2.881100	-1.690907	17.785430	H	-4.610256	0.994598	25.340067
C	-1.369120	-0.874775	26.571818	H	-5.322382	0.088519	24.197900
C	-1.817993	0.585426	26.348474	O	-5.635775	2.872219	28.258422
C	-2.931379	0.919373	27.318604	H	-5.054567	2.208098	27.793603
O	-2.649324	0.970572	28.538547	H	-4.997527	3.512208	28.638959
O	-4.128462	1.062310	26.854414	O	0.947657	2.354363	24.059301
N	2.045415	-2.592302	20.056579	H	1.120302	3.346316	23.984708
C	1.225271	-2.521446	18.957202	H	-0.031725	2.312264	24.070203
C	1.969429	-2.770586	17.741915	H	-7.374764	-2.978792	21.285971
C	3.267559	-2.977489	18.117494	H	-2.142608	0.744221	25.312082
C	3.302960	-2.842705	19.561066	H	-0.967021	1.251323	26.546414
C	1.366455	-2.790377	16.381786	H	-1.117848	-0.997103	27.634670
N	3.451983	-2.377812	22.491877	H	-2.215054	-1.552251	26.367779
C	4.522519	-2.664949	21.681407	H	2.479769	-1.768285	27.687032
C	5.755963	-2.654570	22.432066	H	2.249513	-0.026546	27.395667
C	5.415632	-2.346462	23.729819	H	0.978046	-0.967116	28.200750
C	3.967287	-2.180026	23.742295	H	-2.347328	-1.405192	24.116894
C	7.100448	-2.931967	21.862296	H	3.768776	-1.674777	25.787541
C	6.258236	-2.211216	24.900163	H	5.763594	-2.359676	25.863796
C	7.569085	-1.916577	24.908276	H	8.110663	-1.851328	25.851270
N	-0.397055	-1.995356	21.394897	H	8.127864	-1.707678	23.998111
C	-0.866348	-1.975506	20.110152	H	7.740353	-3.429362	22.603442
C	-2.276227	-1.669690	20.103254	H	7.039389	-3.575190	20.976099
C	-2.656607	-1.526925	21.427578	H	7.604039	-1.997745	21.565410
C	-1.477226	-1.731599	22.208303	H	5.382424	-3.052509	19.778394

H	4.102463	-3.067858	16.183721	H	-4.413241	-0.312092	21.444446
H	4.001255	-5.398319	16.996562	H	-3.907167	-0.905845	23.018250
H	5.165607	-5.013448	18.296537	H	-4.575430	-3.257750	22.307507
H	2.135558	-2.876959	15.605346	H	-5.259266	-2.579205	20.828480
H	0.679353	-3.643140	16.270825	H	5.296340	-1.528970	17.578410
H	0.787883	-1.874836	16.190200	H	1.162001	1.116744	22.664653
H	-0.650628	-2.168290	18.027816	H	-7.735518	0.126304	21.220651
H	-4.186269	-1.173454	19.248778				

PW91-Fe<sup>3+</sup>-(O-OH)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-Prop-A-H.2:

205

C	0.705000	7.351000	24.202000	H	-2.941933	1.659187	19.299461
C	1.156922	6.066559	23.565884	H	0.680107	1.527927	17.148408
O	1.357163	5.047344	24.267211	C	-4.817257	3.903534	21.612353
H	1.533132	7.733202	24.815131	C	-3.500720	3.225117	21.723181
H	-0.139950	7.139126	24.867953	N	-3.270932	2.166745	22.578098
H	0.419813	8.113675	23.468638	C	-2.327134	3.387712	21.027395
N	1.356985	6.089587	22.235043	C	-2.018058	1.714683	22.375790
C	2.060786	5.035381	21.529028	N	-1.412695	2.432291	21.431005
C	1.504578	4.730784	20.131074	H	-4.700658	4.863042	21.095280
C	2.328072	3.615790	19.587162	H	-5.253722	4.093292	22.602424
N	1.979382	2.278154	19.735152	H	-3.944408	1.767517	23.272187
C	3.623529	3.679502	19.158712	H	-2.101152	4.100281	20.243291
C	3.038404	1.553534	19.395287	H	-1.581376	0.867217	22.886129
N	4.074010	2.375510	19.047219	C	-8.433564	-3.792874	17.766471
H	1.255385	6.987964	21.761685	C	-8.108004	-3.056607	19.024293
H	2.015351	4.130380	22.143596	O	-8.093070	-1.826946	19.108401
H	0.446846	4.441229	20.195999	O	-7.802831	-3.862088	20.048818
H	1.573905	5.619073	19.486985	H	-7.482831	-4.085612	17.296319
H	4.261436	4.525477	18.938535	H	-8.974347	-3.134412	17.080246
H	3.112112	0.474924	19.401958	C	-10.804829	-3.302545	22.648240
H	3.122061	5.315453	21.430193	C	-10.746638	-2.000600	23.360975
C	8.825933	3.470174	19.813656	N	-9.609603	-1.224438	23.385851
C	7.779478	2.550606	19.257031	C	-11.670632	-1.282576	24.086705
C	8.120661	1.346711	18.609472	C	-9.869461	-0.097662	24.106155
C	6.421220	2.855840	19.384271	N	-11.119610	-0.101692	24.552093
C	7.154141	0.493520	18.113279	H	-10.596163	-3.177440	21.574930
C	5.436687	2.015840	18.879759	H	-11.803872	-3.741412	22.752481
C	5.758674	0.782023	18.215990	H	-8.720471	-1.507036	22.955622
O	4.840407	0.011165	17.752635	H	-12.701012	-1.552269	24.295852
H	8.591536	4.517468	19.578061	H	-9.129513	0.685890	24.253666
H	9.814781	3.232445	19.402313	C	-0.010582	-7.183300	24.248043
H	9.173760	1.083682	18.499129	C	0.711030	-6.108567	23.489403
H	6.130799	3.766442	19.906688	N	1.681907	-6.343654	22.535060
H	7.439883	-0.430578	17.609933	C	0.489011	-4.749279	23.418349
C	-3.878408	1.578973	16.387266	C	2.015540	-5.181323	21.932534
C	-2.582799	1.601508	17.116553	N	1.301949	-4.181797	22.444297
N	-1.361949	1.538516	16.474163	H	-0.622598	-7.768295	23.543840
C	-2.271274	1.622645	18.451878	H	-0.697386	-6.700951	24.953998
C	-0.373776	1.538173	17.392757	H	2.089505	-7.250521	22.306517
N	-0.897948	1.586673	18.613103	H	-0.204610	-4.156385	24.000758
H	-4.205550	0.542364	16.217605	H	2.760082	-5.103691	21.153989
H	-3.773343	2.065319	15.408697	C	-7.247621	-2.930206	29.394260
H	-1.221827	1.522717	15.463738	N	-6.058444	-2.301644	29.934502

C	-5.326118	-1.399797	29.279451	H	-4.673317	2.104938	16.938341
N	-5.662985	-1.024192	28.046244	H	-5.531461	3.294705	21.032081
N	-4.240302	-0.884290	29.868437	H	-9.006487	-4.710143	17.956796
H	-7.003034	-3.671109	28.619862	H	-10.071117	-4.017670	23.050776
H	-7.929138	-2.172533	28.987186	H	0.595659	-7.919073	24.825698
H	-5.675063	-2.669036	30.803500	H	-7.746919	-3.426172	30.227401
H	-6.412346	-1.481255	27.528509	O	1.908991	-0.426983	21.640353
H	-5.157628	-0.242681	27.595797	O	0.766545	0.549947	21.970760
H	-4.137763	-0.994358	30.875205	O	-6.625749	0.062489	20.555100
H	-3.711981	-0.110774	29.420193	H	-6.583333	0.773766	19.879949
Fe	1.530746	-2.139138	21.934577	H	-7.146384	-0.648075	20.099113
C	-1.406998	-1.558003	23.545621	O	-7.597273	-1.986701	25.797777
C	-0.086423	-2.188625	18.938556	H	-8.477884	-1.551778	25.711600
C	4.476734	-2.869399	20.312988	H	-7.803272	-2.947409	25.863215
C	3.235094	-1.758243	24.834368	O	1.337253	2.653349	26.962238
N	1.011679	-1.753168	23.803414	H	1.147215	2.498835	26.001362
C	-0.250625	-1.528743	24.292867	H	0.464944	2.568147	27.398026
C	-0.201156	-1.219426	25.699935	O	-7.436609	2.277352	24.158620
C	1.119229	-1.241414	26.059789	H	-6.546524	1.844497	24.272818
C	1.860110	-1.593605	24.865722	H	-7.517285	2.400996	23.189803
C	1.725642	-0.932311	27.380880	O	-4.990457	1.012203	24.422007
O	-2.845894	-1.642564	17.743400	H	-4.604945	1.017266	25.373797
C	-1.381105	-0.865746	26.534803	H	-5.244723	0.081207	24.237404
C	-1.841023	0.592876	26.321352	O	-5.669738	2.783046	28.353796
C	-2.939832	0.913757	27.310411	H	-5.080572	2.151010	27.858344
O	-2.639260	0.980155	28.524202	H	-5.084648	3.546781	28.541399
O	-4.151419	1.023318	26.870031	O	0.934524	2.400161	24.117571
N	2.067799	-2.570616	20.035715	H	1.152659	3.377910	24.028419
C	1.254291	-2.503479	18.931887	H	-0.044401	2.395011	24.065903
C	2.003080	-2.768479	17.722369	H	-7.574979	-3.308960	20.870014
C	3.298372	-2.980497	18.106874	H	-2.182097	0.752649	25.290497
C	3.326454	-2.831101	19.549090	H	-0.991156	1.262814	26.507712
C	1.408057	-2.797269	16.359081	H	-1.132431	-0.993884	27.597677
N	3.464408	-2.341492	22.479071	H	-2.220773	-1.548479	26.322713
C	4.538947	-2.621443	21.670545	H	2.483010	-1.677387	27.661613
C	5.772581	-2.578193	22.419787	H	2.211842	0.055955	27.358815
C	5.427670	-2.254403	23.712565	H	0.961548	-0.908258	28.167540
C	3.978497	-2.113574	23.724358	H	-2.342935	-1.400179	24.074656
C	7.120936	-2.841147	21.852571	H	3.771424	-1.586779	25.763234
C	6.270495	-2.084256	24.878353	H	5.783390	-2.236641	25.845613
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N	-0.377845	-1.973007	21.360955	H	8.119187	-1.537567	23.960357
C	-0.838993	-1.940221	20.072543	H	7.774885	-3.302741	22.604411
C	-2.247330	-1.624023	20.060346	H	7.071413	-3.510592	20.985029
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C	-1.459836	-1.707833	22.168944	H	5.406304	-3.025389	19.774872
C	-3.129594	-1.446722	18.927501	H	4.141191	-3.104904	16.178223
C	-3.980266	-1.176594	21.921668	H	4.067379	-5.419794	17.035615
C	-4.930250	-2.382635	21.869054	H	5.218096	-4.994190	18.334920
C	-6.157263	-2.206672	22.701719	H	2.181687	-2.888300	15.587576
O	-7.286564	-2.572528	22.351588	H	0.721481	-3.650597	16.249927
O	-5.923168	-1.662039	23.890453	H	0.830213	-1.883443	16.157746
C	4.466265	-3.295647	17.216568	H	-0.613018	-2.131876	17.990881
O	5.615013	-2.491793	17.512767	H	-4.150958	-1.099055	19.200746
C	4.896750	-4.753394	17.311019	H	-4.451541	-0.347745	21.372088
H	5.738691	-4.927202	16.625813	H	-3.876324	-0.853278	22.961492
Cu	0.134101	1.725350	20.334994	H	-4.422967	-3.275589	22.276433
H	8.891071	3.392425	20.913367	H	-5.222848	-2.613873	20.838193



H 5.308341 -1.525393 17.576499  
H 1.177844 1.127448 22.680150

H -6.709173 -1.795439 24.564365

PW91-Fe<sup>4+</sup>=O<sup>2-</sup>...HO<sup>-</sup>-Cu<sup>2+</sup>-Y237\*-Prop-A-H.1:

205

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C	3.265653	-2.049900	24.715978	H	-7.885951	0.638778	20.396560
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C	-0.189243	-1.572635	24.168477	O	-7.378483	-2.118385	26.119657
C	-0.126504	-1.292536	25.585094	H	-6.961608	-1.900877	25.246199
C	1.188707	-1.405565	25.945591	H	-7.379041	-3.099635	26.140813
C	1.908409	-1.784863	24.746636	O	1.105059	2.289807	27.215536
C	1.816804	-1.178527	27.272034	H	0.915586	2.358327	26.229280
O	-2.922538	-1.914290	17.670579	H	0.230415	2.431917	27.631920
C	-1.292169	-0.943918	26.443624	O	-7.406309	2.157314	23.829108
C	-1.872754	0.458395	26.176221	H	-6.526801	1.758806	24.091709
C	-2.889277	0.816665	27.242495	H	-7.419706	2.102498	22.852100
O	-2.527294	0.794448	28.441489	O	-4.986221	0.986842	24.440018
O	-4.098833	1.091534	26.870686	H	-4.611591	1.001886	25.395235
N	2.012807	-2.862953	19.911104	H	-5.256389	0.057699	24.237275
C	1.180230	-2.806167	18.822092	O	-5.163649	3.224013	28.208648
C	1.910611	-3.104500	17.608524	H	-4.763226	2.432275	27.754620
C	3.213504	-3.299015	17.980083	H	-4.700686	3.980142	27.791347
C	3.262414	-3.131175	19.419301	O	0.572070	2.698049	24.613345
C	1.292870	-3.184765	16.258482	H	1.019779	3.566780	24.446221
N	3.451432	-2.643267	22.355201	H	0.674194	2.181547	23.735684
C	4.503355	-2.956385	21.534162	H	-7.287330	-3.074611	21.381767
C	5.741550	-2.973851	22.275224	H	-2.332869	0.518682	25.183856
C	5.417467	-2.654397	23.576902	H	-1.056539	1.194614	26.204277
C	3.979623	-2.446885	23.600127	H	-0.988083	-0.984578	27.497841
C	7.073504	-3.289858	21.698625	H	-2.090057	-1.696835	26.316686
C	6.268984	-2.548551	24.744349	H	2.458711	-2.019907	27.561843
C	7.585363	-2.284901	24.747995	H	2.434017	-0.270880	27.251746
N	-0.384255	-2.065662	21.238573	H	1.057542	-1.042036	28.048775
C	-0.873078	-2.102479	19.965206	H	-2.268178	-1.321231	23.963376
C	-2.269958	-1.739532	19.966207	H	3.814531	-1.919731	25.644005
C	-2.618575	-1.500287	21.285934	H	5.774260	-2.696655	25.708327
C	-1.431554	-1.709362	22.055262	H	8.133538	-2.242138	25.688831
C	-3.167187	-1.617547	18.842520	H	8.144098	-2.081674	23.835914
C	-3.953605	-1.131661	21.837459	H	7.706078	-3.797941	22.438996
C	-4.950979	-2.295676	21.790964	H	6.989496	-3.938828	20.818212
C	-6.136011	-2.107607	22.691938	H	7.598111	-2.370675	21.391368
O	-7.259073	-2.730098	22.369379	H	5.340325	-3.371428	19.631341
O	-6.090841	-1.460068	23.744433	H	4.049805	-3.423392	16.047304
C	4.371576	-3.619896	17.084036	H	3.968977	-5.737063	16.900908
O	5.529147	-2.811710	17.377417	H	5.114622	-5.320360	18.206271
C	4.801693	-5.076356	17.180691	H	2.050595	-3.326888	15.479467
H	5.644377	-5.255607	16.498247	H	0.590728	-4.030681	16.204101
Cu	0.119094	1.858219	20.596203	H	0.727655	-2.271437	16.023020
H	8.891071	3.392426	20.913366	H	-0.692819	-2.437863	17.895532
H	-4.673317	2.104936	16.938341	H	-4.169179	-1.211310	19.107028
H	-5.531461	3.294704	21.032081	H	-4.371262	-0.268100	21.295910
H	-9.006489	-4.710142	17.956797	H	-3.842193	-0.811194	22.878633
H	-10.071115	-4.017670	23.050778	H	-4.462535	-3.218324	22.155511
H	0.595660	-7.919073	24.825699	H	-5.277516	-2.513270	20.765261
H	-7.746918	-3.426168	30.227401	H	5.219174	-1.880109	17.558133
O	1.925536	-0.717242	21.405868	H	1.342897	0.661125	22.184251
O	0.870756	1.526007	22.321463	H	-8.713912	-0.037971	21.511661
O	-7.921761	-0.178821	20.943429				

C	0.705000	7.351000	24.202000	H	-2.234480	4.205857	20.270226
C	1.232111	6.065464	23.634751	H	-1.519920	1.126986	23.044252
O	1.693042	5.177688	24.387463	C	-8.213666	-3.975611	17.759962
H	1.517452	7.837877	24.756833	C	-7.908577	-3.153958	18.969246
H	-0.097645	7.115950	24.913426	O	-7.787578	-1.926896	18.953418
H	0.327556	8.038402	23.435461	O	-7.749411	-3.890634	20.075657
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C	1.869863	4.789277	21.662597	H	-8.493104	-3.323875	16.926213
C	1.557856	4.667280	20.166410	C	-10.823512	-3.317901	22.658474
C	2.367561	3.526901	19.656758	C	-10.761806	-2.009910	23.359490
N	1.947333	2.203620	19.759487	N	-9.624571	-1.234359	23.371381
C	3.680715	3.537013	19.292721	C	-11.681781	-1.288750	24.085606
C	2.980528	1.432332	19.475254	C	-9.881908	-0.101835	24.084113
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H	1.570373	3.861272	22.167936	H	-11.814234	-3.767464	22.791241
H	0.484364	4.491532	20.005327	H	-8.734529	-1.511464	22.938165
H	1.832689	5.590669	19.636488	H	-12.710227	-1.559052	24.303565
H	4.358375	4.356987	19.098522	H	-9.141090	0.683333	24.211282
H	2.998627	0.352017	19.508714	C	-0.093968	-7.238402	24.291386
H	2.959604	4.897975	21.788131	C	0.565180	-6.220840	23.423188
C	8.858507	3.219499	19.818701	N	1.409663	-6.533477	22.377094
C	7.783289	2.267076	19.408497	C	0.434622	-4.851207	23.362039
C	8.098834	0.980529	18.899688	C	1.756330	-5.400043	21.729219
C	6.430478	2.638053	19.499205	N	1.176909	-4.352316	22.303712
C	7.117056	0.123607	18.479514	H	-0.766254	-7.867014	23.687811
C	5.418276	1.797901	19.078174	H	-0.703987	-6.722045	25.041572
C	5.724438	0.491466	18.508792	H	1.722115	-7.469390	22.119759
O	4.814056	-0.255518	18.046082	H	-0.145831	-4.207867	24.010809
H	8.678949	4.202773	19.358953	H	2.418146	-5.379033	20.874605
H	9.843303	2.853323	19.506886	C	-7.290849	-2.849214	29.417189
H	9.144342	0.679115	18.837871	N	-6.141805	-2.153928	29.970688
H	6.187040	3.607367	19.928283	C	-5.433707	-1.230998	29.313789
H	7.362932	-0.857602	18.074132	N	-5.752242	-0.895301	28.062617
C	-3.934928	1.317836	16.696970	N	-4.419332	-0.613657	29.925449
C	-2.635791	1.467482	17.416653	H	-6.998724	-3.537113	28.610209
N	-1.424983	1.540644	16.755017	H	-8.030102	-2.128557	29.043953
C	-2.299987	1.506456	18.748418	H	-5.759998	-2.487569	30.853884
C	-0.423567	1.630505	17.653012	H	-6.436909	-1.417143	27.516711
N	-0.925148	1.614544	18.884599	H	-5.236533	-0.126450	27.603631
H	-4.390348	0.343600	16.925618	H	-4.221410	-0.819003	30.901997
H	-3.765297	1.349918	15.613373	H	-3.758001	-0.005511	29.403241
H	-1.302254	1.540491	15.742308	Fe	1.572939	-2.298881	21.774820
H	-2.952844	1.468123	19.609725	C	-1.323396	-1.536171	23.412448
H	0.620661	1.721976	17.388305	C	-0.127772	-2.449784	18.820618
C	-4.918789	3.943504	21.670551	C	4.438025	-3.201854	20.166857
C	-3.575285	3.338407	21.809757	C	3.284145	-2.054381	24.707209
N	-3.300274	2.314302	22.693322	N	1.079894	-1.870430	23.668714
C	-2.423284	3.518648	21.086173	C	-0.167061	-1.566922	24.154959
C	-2.030729	1.906475	22.496589	C	-0.105530	-1.275395	25.568580
N	-1.474435	2.617933	21.522839	C	1.208596	-1.391054	25.931855
H	-4.848249	4.923697	21.185536	C	1.929215	-1.781100	24.736691
H	-5.418747	4.060070	22.640048	C	1.834204	-1.167171	27.260942
H	-3.963139	1.886255	23.377810	O	-2.923020	-1.902643	17.659678

C	-1.273625	-0.929640	26.426335	H	-7.820211	-2.897045	25.818438
C	-1.899360	0.448439	26.133853	O	1.148401	2.293672	27.232063
C	-2.895721	0.810749	27.219064	H	0.936758	2.335016	26.250938
O	-2.509963	0.799988	28.410260	H	0.311819	1.998137	27.644825
O	-4.114795	1.076193	26.871852	O	-7.439328	2.148303	23.812164
N	2.034590	-2.867034	19.898571	H	-6.554668	1.776032	24.092048
C	1.203787	-2.804892	18.807855	H	-7.405479	2.142444	22.832933
C	1.935339	-3.103701	17.595780	O	-5.005138	1.030625	24.456336
C	3.236053	-3.303222	17.968486	H	-4.620409	1.045703	25.412248
C	3.284290	-3.138890	19.408455	H	-5.200283	0.089114	24.253829
C	1.318421	-3.180067	16.244341	O	-5.130496	3.273764	28.184431
N	3.467889	-2.655396	22.346916	H	-4.750497	2.462044	27.740341
C	4.520481	-2.970911	21.526921	H	-4.609643	4.012604	27.799240
C	5.757342	-2.990897	22.270040	O	0.579093	2.661222	24.635528
C	5.432415	-2.670030	23.570625	H	1.003087	3.542004	24.463103
C	3.995226	-2.459125	23.592529	H	0.675823	2.145334	23.759304
C	7.090605	-3.309382	21.696531	H	-7.523006	-3.285141	20.861334
C	6.281779	-2.565470	24.739314	H	-2.391550	0.466115	25.155412
C	7.598100	-2.300176	24.744836	H	-1.111798	1.217294	26.105870
N	-0.358747	-2.067047	21.222353	H	-0.961353	-0.940915	27.478640
C	-0.849557	-2.101667	19.949000	H	-2.053778	-1.705217	26.324253
C	-2.249368	-1.742261	19.953370	H	2.469574	-2.016359	27.552811
C	-2.593633	-1.508366	21.274262	H	2.459678	-0.261746	27.245129
C	-1.405154	-1.715696	22.041349	H	1.071170	-1.027267	28.035905
C	-3.160808	-1.622220	18.837600	H	-2.245983	-1.326092	23.944738
C	-3.925794	-1.155659	21.832536	H	3.833965	-1.924205	25.634866
C	-4.881949	-2.362227	21.834766	H	5.786824	-2.717205	25.702263
C	-6.104948	-2.162973	22.670764	H	8.144837	-2.260257	25.686557
O	-7.244969	-2.479845	22.309092	H	8.157109	-2.094231	23.834159
O	-5.852756	-1.657156	23.873050	H	7.718973	-3.820590	22.438202
C	4.393229	-3.627146	17.071872	H	7.008258	-3.956036	20.814538
O	5.550073	-2.815128	17.356654	H	7.618448	-2.391007	21.393458
C	4.823367	-5.082962	17.175360	H	5.360947	-3.385989	19.625824
H	5.666311	-5.266083	16.494444	H	4.069169	-3.437020	16.034799
Cu	0.119953	1.825301	20.605878	H	3.990277	-5.743975	16.897601
H	8.891071	3.392426	20.913366	H	5.134682	-5.323288	18.202187
H	-4.673317	2.104936	16.938341	H	2.077326	-3.317425	15.465503
H	-5.531461	3.294704	21.032081	H	0.618657	-4.027676	16.185941
H	-9.006486	-4.710145	17.956797	H	0.750937	-2.267558	16.011661
H	-10.071115	-4.017670	23.050778	H	-0.668626	-2.431517	17.879236
H	0.595660	-7.919073	24.825699	H	-4.164157	-1.232037	19.119981
H	-7.746918	-3.426168	30.227401	H	-4.401756	-0.343659	21.263043
O	1.953427	-0.724143	21.397983	H	-3.800672	-0.794858	22.858146
O	0.852840	1.488145	22.336939	H	-4.368662	-3.239774	22.266119
O	-6.489478	0.147001	20.334822	H	-5.184216	-2.626894	20.814833
H	-6.336657	0.745235	19.568686	H	5.239346	-1.884385	17.540701
H	-6.951408	-0.628404	19.926055	H	1.348723	0.637187	22.196176
O	-7.567248	-1.946055	25.758509	H	-6.649685	-1.771403	24.536505
H	-8.424804	-1.468921	25.683830				

OLYP-Fe<sup>3+</sup>-(O-OH)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-Prop-A-H.1:

205

C	0.705000	7.351000	24.202000	H	1.494256	7.764678	24.841693
C	1.223876	6.086319	23.584489	H	-0.149653	7.108379	24.842044
O	1.458426	5.085738	24.289714	H	0.410732	8.104596	23.468055

N	1.429465	6.119288	22.253116	N	-9.895563	-1.271769	23.563279
C	2.161856	5.094471	21.538843	C	-12.027229	-1.412841	23.942857
C	1.664150	4.872268	20.104958	C	-10.303802	-0.159284	24.221389
C	2.460647	3.745522	19.547769	N	-11.602802	-0.206771	24.469770
N	2.075726	2.417642	19.685873	H	-10.694211	-3.239551	21.586794
C	3.753106	3.781510	19.119024	H	-11.823401	-3.945440	22.757759
C	3.117074	1.675803	19.346579	H	-8.948786	-1.498286	23.280370
N	4.173047	2.468662	19.001622	H	-13.063183	-1.722115	24.001965
H	1.312999	7.015502	21.788930	H	-9.625765	0.640200	24.485407
H	2.071778	4.165011	22.099743	C	-0.060075	-7.250982	24.242063
H	0.596919	4.635017	20.110144	C	0.652361	-6.186100	23.477638
H	1.802680	5.778305	19.504206	N	1.651642	-6.432304	22.560608
H	4.406728	4.610704	18.902537	C	0.451136	-4.829953	23.406090
H	3.164091	0.602171	19.353075	C	2.020454	-5.273180	21.982282
H	3.226612	5.361577	21.508203	N	1.304882	-4.270857	22.471269
C	8.918495	3.455017	19.817419	H	-0.638472	-7.881101	23.554387
C	7.873624	2.564693	19.221324	H	-0.761893	-6.779857	24.935856
C	8.206786	1.382063	18.531673	H	2.055809	-7.340030	22.346806
C	6.519351	2.875708	19.367782	H	-0.248991	-4.235271	23.967392
C	7.234527	0.561902	18.008571	H	2.790775	-5.205193	21.234436
C	5.523811	2.078105	18.829640	C	-7.181160	-2.950888	29.433957
C	5.836478	0.863419	18.110806	N	-6.019054	-2.332987	30.042370
O	4.932029	0.125079	17.603526	C	-5.259537	-1.412390	29.449471
H	8.736283	4.502485	19.548570	N	-5.547293	-0.979140	28.228971
H	9.920471	3.174535	19.482015	N	-4.184282	-0.938314	30.100321
H	9.253799	1.111018	18.416302	H	-6.897176	-3.701704	28.689489
H	6.245278	3.761282	19.930732	H	-7.817502	-2.190766	28.977358
H	7.510069	-0.345194	17.478317	H	-5.641171	-2.765121	30.879455
C	-3.914069	1.669116	16.279901	H	-6.202794	-1.473067	27.625450
C	-2.596226	1.643351	16.963727	H	-5.027556	-0.194181	27.823256
N	-1.392296	1.551065	16.300880	H	-4.189637	-0.978416	31.114486
C	-2.256974	1.688264	18.287523	H	-3.670677	-0.153589	29.687676
C	-0.390611	1.560202	17.201222	Fe	1.551300	-2.202569	21.968447
N	-0.886543	1.642338	18.427087	C	-1.374191	-1.585892	23.583759
H	-4.233479	0.658063	15.999077	C	-0.088626	-2.313106	18.987092
H	-3.866668	2.276017	15.369118	C	4.488842	-2.915020	20.334944
H	-1.270095	1.507652	15.292681	C	3.255158	-1.862725	24.868646
H	-2.907170	1.760173	19.141847	N	1.033889	-1.802816	23.851150
H	0.653208	1.523338	16.934559	C	-0.221381	-1.549350	24.334932
C	-4.845831	3.986349	21.544202	C	-0.167686	-1.241151	25.746098
C	-3.503765	3.364720	21.662795	C	1.150655	-1.310020	26.106446
N	-3.250434	2.313244	22.515234	C	1.883597	-1.670217	24.909689
C	-2.340970	3.535119	20.956567	C	1.766206	-1.061810	27.439215
C	-1.997264	1.877425	22.300122	O	-2.933159	-1.997187	17.817470
N	-1.410036	2.591891	21.348574	C	-1.337921	-0.864458	26.593171
H	-4.785268	4.903065	20.952272	C	-1.730456	0.621324	26.449998
H	-5.268329	4.228154	22.524745	C	-2.835787	0.981802	27.435421
H	-3.900030	1.939976	23.223956	O	-2.531860	1.053110	28.650085
H	-2.133739	4.245304	20.170512	O	-4.024700	1.134812	26.976704
H	-1.557635	1.043688	22.813259	N	2.086186	-2.632743	20.053042
C	-8.456632	-3.832993	17.609375	C	1.263420	-2.572427	18.961514
C	-8.005691	-3.033519	18.784729	C	2.007426	-2.807300	17.744320
O	-8.090024	-1.719641	18.582280	C	3.304919	-3.018386	18.119217
O	-7.584136	-3.551407	19.822622	C	3.341758	-2.875878	19.563304
H	-7.564004	-4.177082	17.073018	C	1.403306	-2.799780	16.381588
H	-9.070826	-3.238669	16.930499	N	3.491506	-2.399979	22.505042
C	-10.883834	-3.395514	22.655914	C	4.558272	-2.683416	21.696576
C	-10.980186	-2.097342	23.373784	C	5.789888	-2.682317	22.453256

C	5.444958	-2.382156	23.749581	O	-5.069008	1.223109	24.486305
C	3.999017	-2.211118	23.756909	H	-4.629464	1.177040	25.385284
C	7.138449	-2.967466	21.892761	H	-5.351356	0.308541	24.299539
C	6.278668	-2.269356	24.933692	O	-5.760137	3.038859	28.278040
C	7.564349	-1.888777	24.984964	H	-5.123139	2.386438	27.901146
N	-0.373216	-2.050652	21.398150	H	-5.178463	3.675354	28.738157
C	-0.846791	-2.079669	20.120480	O	1.185418	2.276048	24.291695
C	-2.262847	-1.801638	20.114010	H	1.285631	3.247943	24.146200
C	-2.633832	-1.619410	21.434258	H	0.235136	2.187400	24.487661
C	-1.445368	-1.779722	22.211885	H	-7.341092	-2.976789	21.372164
C	-3.167303	-1.698259	18.987859	H	-2.049435	0.835982	25.427957
C	-3.979725	-1.285078	21.973740	H	-0.857143	1.241154	26.674283
C	-4.983981	-2.440797	21.923100	H	-1.101725	-1.059659	27.643524
C	-6.212657	-2.129802	22.728951	H	-2.201566	-1.496876	26.349093
O	-7.379379	-2.613707	22.311982	H	2.419424	-1.891101	27.735118
O	-6.181912	-1.479451	23.769119	H	2.374761	-0.149209	27.424373
C	4.448445	-3.353571	17.199974	H	1.003263	-0.941552	28.211594
O	5.627716	-2.578407	17.458550	H	-2.302127	-1.418815	24.110399
C	4.841131	-4.825231	17.260092	H	3.791698	-1.713204	25.794768
H	5.645019	-5.014617	16.538643	H	5.790828	-2.514997	25.876520
Cu	0.154389	1.890399	20.175862	H	8.083093	-1.855524	25.940477
H	8.891071	3.392425	20.913367	H	8.123170	-1.583884	24.106267
H	-4.673317	2.104938	16.938341	H	7.785819	-3.412186	22.653816
H	-5.531461	3.294705	21.032081	H	7.086249	-3.658463	21.047084
H	-9.006487	-4.710143	17.956796	H	7.619779	-2.043944	21.542675
H	-10.071117	-4.017670	23.050776	H	5.415167	-3.084750	19.810190
H	0.595659	-7.919073	24.825698	H	4.107804	-3.143635	16.177650
H	-7.746919	-3.426172	30.227401	H	3.980999	-5.453794	17.005353
O	1.930251	-0.476115	21.658234	H	5.190882	-5.099299	18.261138
O	0.818120	0.474544	21.919433	H	2.164066	-2.879794	15.602338
O	-7.095148	0.021771	20.443099	H	0.704345	-3.636626	16.257109
H	-7.038195	0.822499	19.882230	H	0.842689	-1.873829	16.209551
H	-7.734472	-1.189324	19.362221	H	-0.617279	-2.284449	18.047236
O	-7.489242	-2.203801	26.201232	H	-4.165274	-1.303611	19.253248
H	-7.102824	-1.985078	25.327198	H	-4.396256	-0.427795	21.435204
H	-7.394087	-3.175491	26.245853	H	-3.883372	-0.975148	23.011002
O	1.883544	2.877279	27.272857	H	-4.546611	-3.340772	22.381037
H	1.674876	2.642410	26.343925	H	-5.245800	-2.708450	20.897894
H	1.068594	2.631687	27.751515	H	5.354243	-1.625178	17.478451
O	-7.715455	2.453537	24.371113	H	1.200510	1.001002	22.661644
H	-6.810431	2.074982	24.448514	H	-7.832264	0.243309	21.047158
H	-7.793032	2.667324	23.422000				

OLYP-Fe<sup>3+</sup>-(O-OH)<sup>-</sup>-Cu<sup>2+</sup>-Y237<sup>-</sup>-Prop-A-H.2:

204

C	0.705000	7.351000	24.202000	N	2.078710	2.444975	19.676593
C	1.299240	6.117349	23.589030	C	3.756550	3.804461	19.099649
O	1.654342	5.158816	24.302474	C	3.118004	1.700157	19.337029
H	1.458551	7.803730	24.857014	N	4.173940	2.490510	18.986561
H	-0.144834	7.057316	24.827221	H	1.220964	6.994672	21.763994
H	0.377401	8.089810	23.466804	H	2.100891	4.183143	22.078837
N	1.427199	6.125897	22.248279	H	0.605474	4.666554	20.098254
C	2.174779	5.118256	21.524093	H	1.812689	5.806931	19.491170
C	1.673405	4.900738	20.091466	H	4.410243	4.631863	18.876644
C	2.465546	3.771923	19.532387	H	3.163704	0.626163	19.346189

H	3.235736	5.400270	21.490202	N	1.326474	-4.266892	22.463328
C	8.913918	3.472750	19.818480	H	-0.634262	-7.861658	23.551104
C	7.871985	2.583062	19.217758	H	-0.747670	-6.763815	24.935058
C	8.206673	1.396038	18.535370	H	2.073284	-7.338534	22.350217
C	6.518312	2.896777	19.355737	H	-0.227127	-4.224817	23.959634
C	7.235691	0.575267	18.011577	H	2.810222	-5.208765	21.229388
C	5.524088	2.097376	18.818153	C	-7.218740	-2.931190	29.417722
C	5.837173	0.878763	18.106646	N	-6.036753	-2.326692	30.000005
O	4.933922	0.138531	17.599964	C	-5.268996	-1.423986	29.392068
H	8.722039	4.522760	19.567778	N	-5.561757	-0.997171	28.168909
H	9.916197	3.204897	19.473850	N	-4.176763	-0.966771	30.020819
H	9.253578	1.122693	18.425884	H	-6.962200	-3.664785	28.645226
H	6.242698	3.785336	19.913642	H	-7.876502	-2.162385	29.004845
H	7.513217	-0.334816	17.488168	H	-5.661018	-2.749109	30.842958
C	-3.912335	1.660267	16.288203	H	-6.299487	-1.423353	27.622194
C	-2.593774	1.657741	16.970484	H	-5.046530	-0.210240	27.757847
N	-1.390062	1.588469	16.304858	H	-4.147760	-1.040323	31.032687
C	-2.253174	1.698285	18.294123	H	-3.664843	-0.175921	29.618185
C	-0.386600	1.605909	17.202744	Fe	1.572492	-2.191100	21.947886
N	-0.881532	1.670898	18.430455	C	-1.364341	-1.568571	23.543576
H	-4.225804	0.641037	16.031270	C	-0.049114	-2.330894	18.961016
H	-3.870587	2.246696	15.364090	C	4.523242	-2.893680	20.332985
H	-1.270034	1.556857	15.296069	C	3.262008	-1.813432	24.852434
H	-2.903002	1.750987	19.149891	N	1.043751	-1.783559	23.825501
H	0.656919	1.587833	16.933345	C	-0.216048	-1.538623	24.302513
C	-4.846430	3.998794	21.527341	C	-0.171828	-1.231535	25.713558
C	-3.500648	3.385466	21.654697	C	1.145341	-1.284307	26.079714
N	-3.241925	2.341461	22.514575	C	1.887522	-1.639932	24.887665
C	-2.337008	3.557818	20.950915	C	1.750122	-1.014039	27.413299
C	-1.985862	1.910239	22.305127	O	-2.873878	-1.977314	17.761836
N	-1.401331	2.621663	21.349632	C	-1.348057	-0.864887	26.557145
H	-4.789269	4.905234	20.919402	C	-1.729961	0.626305	26.436760
H	-5.266074	4.258476	22.504798	C	-2.821874	0.982299	27.436717
H	-3.890072	1.972553	23.222516	O	-2.504550	1.066801	28.645779
H	-2.132256	4.265118	20.161587	O	-4.021861	1.115410	26.995824
H	-1.543987	1.081327	22.823796	N	2.119477	-2.638240	20.040171
C	-8.459694	-3.794582	17.710688	C	1.301216	-2.598066	18.944556
C	-8.125556	-3.035319	18.952983	C	2.051015	-2.848485	17.733388
O	-8.124503	-1.813396	19.047260	C	3.348851	-3.041507	18.115911
O	-7.804074	-3.852548	19.971422	C	3.378536	-2.878850	19.558098
H	-7.519573	-4.085607	17.225133	C	1.451636	-2.870813	16.368480
H	-9.033535	-3.166880	17.027055	N	3.512048	-2.376774	22.496690
C	-10.885230	-3.391094	22.667614	C	4.585725	-2.644512	21.691537
C	-10.923175	-2.072980	23.352059	C	5.816854	-2.602634	22.446929
N	-9.850480	-1.211714	23.360532	C	5.464833	-2.293341	23.739398
C	-11.897176	-1.408345	24.056254	C	4.014827	-2.159089	23.745723
C	-10.198030	-0.093230	24.045807	C	7.171642	-2.859192	21.887298
N	-11.441523	-0.177266	24.489456	C	6.298331	-2.137034	24.918595
H	-10.734084	-3.270077	21.588540	C	7.569387	-1.708457	24.956807
H	-11.830695	-3.917317	22.823422	N	-0.349594	-2.042961	21.368543
H	-8.948349	-1.416069	22.938945	C	-0.812196	-2.075446	20.086451
H	-12.902003	-1.748668	24.273889	C	-2.225416	-1.782128	20.064719
H	-9.519083	0.734732	24.194641	C	-2.605154	-1.585989	21.379976
C	-0.049308	-7.240032	24.241119	C	-1.425917	-1.756081	22.170686
C	0.672140	-6.178938	23.478145	C	-3.121532	-1.678571	18.930225
N	1.670723	-6.429439	22.561121	C	-3.959694	-1.271509	21.909616
C	0.473255	-4.822258	23.401091	C	-4.884238	-2.500437	21.934085
C	2.040149	-5.272742	21.977814	C	-6.122621	-2.293627	22.751659

O	-7.258801	-2.573759	22.375555	H	1.344511	3.300289	24.205844
O	-5.862946	-1.796497	23.960112	H	0.204593	2.313158	24.450014
C	4.502281	-3.367056	17.205161	H	-7.580999	-3.308918	20.778819
O	5.664788	-2.565783	17.460193	H	-2.056356	0.854951	25.420106
C	4.924769	-4.829522	17.282328	H	-0.847902	1.232904	26.658820
H	5.735340	-5.009300	16.565831	H	-1.120419	-1.079502	27.605754
Cu	0.161919	1.926701	20.174238	H	-2.212199	-1.489246	26.295943
H	8.891071	3.392425	20.913367	H	2.434931	-1.816392	27.710596
H	-4.673317	2.104938	16.938341	H	2.321273	-0.076993	27.398891
H	-5.531461	3.294705	21.032081	H	0.981861	-0.923900	28.184312
H	-9.006487	-4.710143	17.956796	H	-2.294177	-1.397095	24.065127
H	-10.071117	-4.017670	23.050776	H	3.793660	-1.648443	25.778732
H	0.595659	-7.919073	24.825698	H	5.824226	-2.387592	25.867179
H	-7.746919	-3.426172	30.227401	H	8.093263	-1.645488	25.907959
O	1.943617	-0.464799	21.623533	H	8.110397	-1.394136	24.070344
O	0.839397	0.486803	21.918845	H	7.837639	-3.259774	22.656539
O	-6.788819	0.516043	20.553988	H	7.137974	-3.576156	21.062337
H	-6.649516	1.098918	19.783343	H	7.620183	-1.930911	21.507330
H	-7.207751	-0.269972	20.148609	H	5.453455	-3.052080	19.811404
O	-7.635411	-1.999089	25.886462	H	4.161891	-3.175481	16.179341
H	-8.527996	-1.608660	25.795557	H	4.078709	-5.477884	17.029981
H	-7.814403	-2.957115	25.986236	H	5.276123	-5.086146	18.287420
O	1.591528	3.060097	27.444505	H	2.214333	-2.971849	15.593764
H	1.435465	2.809354	26.511034	H	0.750846	-3.708537	16.262440
H	0.723968	2.902816	27.865562	H	0.894167	-1.947818	16.172317
O	-7.621800	2.616662	24.460833	H	-0.572167	-2.310712	18.017828
H	-6.743825	2.174266	24.510448	H	-4.122357	-1.285344	19.184900
H	-7.757389	2.746809	23.502789	H	-4.434981	-0.478020	21.324928
O	-5.074092	1.232635	24.537316	H	-3.861674	-0.888417	22.922110
H	-4.622786	1.193024	25.433723	H	-4.354412	-3.347625	22.392389
H	-5.325529	0.311033	24.357691	H	-5.168277	-2.801140	20.925073
O	-5.795429	2.913071	28.389360	H	5.372571	-1.618565	17.475292
H	-5.137098	2.315674	27.962969	H	1.233464	0.991307	22.668969
H	-5.251795	3.671348	28.677727	H	-6.667506	-1.874115	24.576354
O	1.174450	2.341708	24.361623				

OLYP-Fe<sup>4+</sup>=O<sup>2-</sup>...HO<sup>-</sup>-Cu<sup>2+</sup>-Y237\*-Prop-A-H.1:

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C	0.705000	7.351000	24.202000	H	0.943780	6.810055	21.713449
C	1.446854	6.198870	23.591446	H	1.938569	4.081877	22.063342
O	2.078003	5.395420	24.304486	H	0.655450	4.743347	19.973050
H	1.394710	7.909903	24.842256	H	1.996871	5.803655	19.526648
H	-0.092015	6.948554	24.837140	H	4.476775	4.517270	18.918731
H	0.263666	8.025782	23.463232	H	3.081761	0.559401	19.435818
N	1.381877	6.070299	22.253055	H	3.198706	5.238713	21.621386
C	2.122566	5.031868	21.558114	C	8.944399	3.249867	19.822410
C	1.733608	4.896636	20.081565	C	7.869444	2.337849	19.333820
C	2.495981	3.730902	19.552165	C	8.167191	1.077395	18.765220
N	2.059608	2.420226	19.691961	C	6.521943	2.729738	19.429645
C	3.795120	3.716236	19.144668	C	7.178087	0.271233	18.275134
C	3.074494	1.635229	19.393890	C	5.503070	1.943319	18.937560
N	4.169735	2.385133	19.054595	C	5.789903	0.670051	18.283990



O	4.888097	-0.019708	17.742089	H	1.682165	-7.621904	22.118391
H	8.819804	4.243081	19.373048	H	-0.199647	-4.351070	23.942336
H	9.935708	2.867160	19.569373	H	2.457835	-5.545595	20.917105
H	9.203916	0.751051	18.712824	C	-7.236580	-2.848121	29.460790
H	6.290677	3.668129	19.917573	N	-6.110895	-2.177724	30.088225
H	7.413417	-0.689099	17.827356	C	-5.357960	-1.251074	29.489071
C	-3.887700	1.420565	16.582511	N	-5.638188	-0.841881	28.256224
C	-2.589291	1.594212	17.299538	N	-4.330744	-0.709357	30.147893
N	-1.380079	1.681392	16.642714	H	-6.909319	-3.527146	28.666217
C	-2.256026	1.660694	18.627567	H	-7.939590	-2.114024	29.060164
C	-0.388881	1.808680	17.541561	H	-5.727278	-2.597382	30.928738
N	-0.887985	1.804448	18.770507	H	-6.279029	-1.349930	27.649299
H	-4.256175	0.394432	16.694415	H	-5.100702	-0.076129	27.841742
H	-3.750976	1.605911	15.512628	H	-4.216412	-0.873617	31.140612
H	-1.249394	1.657824	15.634211	H	-3.680575	-0.073016	29.672303
H	-2.908642	1.623761	19.480782	Fe	1.584416	-2.426134	21.806832
H	0.650451	1.910618	17.274641	C	-1.312814	-1.615774	23.425235
C	-4.944297	4.050954	21.564779	C	-0.115822	-2.651347	18.861197
C	-3.578004	3.512898	21.750459	C	4.465464	-3.271835	20.201649
N	-3.291738	2.513611	22.655037	C	3.284809	-2.147160	24.733376
C	-2.424614	3.691209	21.035140	N	1.073675	-1.997478	23.711703
C	-2.019508	2.119563	22.472990	C	-0.166613	-1.663098	24.183537
N	-1.467526	2.813371	21.488002	C	-0.105440	-1.356097	25.597650
H	-4.920447	4.955722	20.952690	C	1.207203	-1.478088	25.959882
H	-5.434456	4.276697	22.515932	C	1.924396	-1.890745	24.769760
H	-3.937046	2.121742	23.357537	C	1.838899	-1.230061	27.285154
H	-2.243442	4.360054	20.206648	O	-2.955122	-2.206536	17.693093
H	-1.516648	1.357544	23.035950	C	-1.268594	-0.988283	26.461527
C	-8.401068	-3.845183	17.673540	C	-1.750952	0.465392	26.293178
C	-8.091377	-3.052610	18.900352	C	-2.751122	0.857746	27.376660
O	-8.536754	-1.800031	18.837938	O	-2.373936	0.807376	28.570519
O	-7.484257	-3.526081	19.864512	O	-3.934421	1.200178	27.011222
H	-7.461264	-4.219505	17.255350	N	2.064312	-2.979928	19.917485
H	-8.928996	-3.250408	16.925750	C	1.227647	-2.954125	18.837175
C	-10.884047	-3.413640	22.628896	C	1.960494	-3.243328	17.623408
C	-10.976353	-2.078553	23.276861	C	3.266589	-3.419630	17.993328
N	-9.875934	-1.274821	23.478059	C	3.315504	-3.233898	19.432578
C	-12.026660	-1.336374	23.758623	C	1.338764	-3.317839	16.271360
C	-10.282596	-0.121565	24.064946	N	3.494352	-2.757379	22.383522
N	-11.591565	-0.117659	24.245866	C	4.549162	-3.040598	21.562964
H	-10.701196	-3.314654	21.551545	C	5.787562	-3.032186	22.309141
H	-11.824457	-3.954775	22.763114	C	5.454396	-2.719726	23.607112
H	-8.921788	-1.555262	23.287959	C	4.010799	-2.544018	23.625754
H	-13.073621	-1.612840	23.784414	C	7.130809	-3.323389	21.739996
H	-9.594762	0.668553	24.331856	C	6.295619	-2.600494	24.786150
C	-0.152411	-7.362826	24.249455	C	7.579116	-2.213360	24.829503
C	0.490866	-6.359395	23.365852	N	-0.364528	-2.215732	21.248647
N	1.372196	-6.683862	22.362046	C	-0.850519	-2.296129	19.980234
C	0.389763	-4.994570	23.311569	C	-2.247808	-1.936616	19.972525
C	1.768456	-5.557179	21.739887	C	-2.589802	-1.645786	21.281569
N	1.185332	-4.503873	22.297878	C	-1.401409	-1.829321	22.056689
H	-0.739267	-8.081738	23.665933	C	-3.165220	-1.855381	18.854578
H	-0.821896	-6.857652	24.950046	C	-3.921542	-1.252256	21.820547

C	-4.910423	-2.423219	21.881776	O	0.835450	2.778829	24.800159
C	-6.091159	-2.138238	22.765689	H	1.256410	3.637057	24.593645
O	-7.264936	-2.666981	22.422058	H	0.846587	2.307475	23.920805
O	-6.008514	-1.495248	23.806084	H	-7.264946	-3.006796	21.474276
C	4.410019	-3.749698	17.074907	H	-2.193464	0.615093	25.308395
O	5.570668	-2.930408	17.312143	H	-0.889850	1.135674	26.367358
C	4.850238	-5.204783	17.164650	H	-0.989611	-1.132180	27.508392
H	5.660672	-5.382605	16.447615	H	-2.104307	-1.675351	26.268430
Cu	0.183548	2.028420	20.558916	H	2.445555	-2.084693	27.605208
H	8.891071	3.392426	20.913366	H	2.495346	-0.352140	27.237412
H	-4.673317	2.104936	16.938341	H	1.086705	-1.039377	28.053332
H	-5.531461	3.294704	21.032081	H	-2.226059	-1.371839	23.946254
H	-9.006489	-4.710142	17.956797	H	3.830810	-1.993411	25.652948
H	-10.071115	-4.017670	23.050778	H	5.813027	-2.846296	25.731585
H	0.595660	-7.919073	24.825699	H	8.103253	-2.174432	25.781328
H	-7.746918	-3.426168	30.227401	H	8.131762	-1.907401	23.946997
O	1.935243	-0.846327	21.469010	H	7.782494	-3.766450	22.497961
O	0.924192	1.669261	22.296829	H	7.070628	-4.018596	20.898677
O	-7.802525	-0.002095	20.750258	H	7.610861	-2.402651	21.382571
H	-7.738615	0.808451	20.202811	H	5.388955	-3.446673	19.672847
H	-8.249302	-1.244893	19.625924	H	4.064731	-3.567322	16.049939
O	-7.532139	-2.019332	26.173219	H	4.009346	-5.861835	16.918465
H	-7.055526	-1.872157	25.327254	H	5.204707	-5.451065	18.170987
H	-7.563721	-2.993361	26.238075	H	2.084968	-3.477240	15.490887
O	1.337864	2.789140	27.697815	H	0.617998	-4.143581	16.221467
H	1.151580	2.680216	26.740074	H	0.798932	-2.392736	16.037883
H	0.453945	2.727783	28.103587	H	-0.652776	-2.668352	17.924927
O	-7.708198	2.486071	24.109207	H	-4.149369	-1.426682	19.115335
H	-6.823316	2.115545	24.321425	H	-4.354465	-0.445772	21.218366
H	-7.747974	2.435863	23.137577	H	-3.804340	-0.850429	22.824525
O	-5.054300	1.270620	24.562999	H	-4.421567	-3.300934	22.330651
H	-4.601054	1.230369	25.457973	H	-5.232997	-2.726783	20.883977
H	-5.282660	0.346911	24.354013	H	5.264228	-1.999964	17.363325
O	-5.101071	3.357723	28.489335	H	1.342626	0.792088	22.180910
H	-4.678453	2.597295	28.019745	H	-8.608512	0.158382	21.279187
H	-4.837594	4.123600	27.950251				

OLYP-Fe<sup>4+</sup>=O<sup>2-</sup>...HO<sup>-</sup>-Cu<sup>2+</sup>-Y237\*-Prop-A-H.2:

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C	0.705000	7.351000	24.202000	N	2.053742	2.399144	19.705098
C	1.429916	6.185447	23.594993	C	3.788867	3.694826	19.158272
O	2.048025	5.374903	24.311773	C	3.069743	1.613962	19.412132
H	1.411527	7.912777	24.820474	N	4.166002	2.365635	19.073228
H	-0.083430	6.965040	24.856923	H	0.944812	6.799697	21.713365
H	0.261306	8.021375	23.460890	H	1.905484	4.060010	22.071962
N	1.368276	6.054342	22.256649	H	0.646745	4.723539	19.971735
C	2.102645	5.007724	21.567664	H	1.992788	5.783108	19.535925
C	1.724101	4.875479	20.087885	H	4.469517	4.498719	18.932338
C	2.489609	3.711139	19.562469	H	3.076747	0.539488	19.458078

H	3.180240	5.203445	21.639925	C	-0.143618	-7.346977	24.253981
C	8.938831	3.252992	19.821649	C	0.507638	-6.345928	23.373730
C	7.866244	2.333863	19.343123	N	1.391625	-6.673295	22.370286
C	8.168318	1.062985	18.796595	C	0.405220	-4.981594	23.313840
C	6.518676	2.723060	19.432510	C	1.786622	-5.546200	21.747615
C	7.178569	0.242783	18.329632	N	1.202726	-4.493984	22.298658
C	5.500456	1.924402	18.962644	H	-0.741431	-8.054066	23.666843
C	5.789946	0.635843	18.339276	H	-0.805645	-6.836914	24.958619
O	4.885892	-0.069750	17.822113	H	1.703419	-7.610586	22.131950
H	8.803669	4.246659	19.376133	H	-0.185170	-4.336155	23.941537
H	9.930912	2.877398	19.561298	H	2.480537	-5.536818	20.925741
H	9.205217	0.740885	18.746740	C	-7.265158	-2.849650	29.441443
H	6.287513	3.671447	19.902578	N	-6.133197	-2.171170	30.045847
H	7.415747	-0.726060	17.901055	C	-5.391560	-1.247013	29.432805
C	-3.894447	1.405740	16.594764	N	-5.683388	-0.855010	28.195807
C	-2.594408	1.578294	17.309197	N	-4.367426	-0.687364	30.078704
N	-1.387137	1.673125	16.649532	H	-6.951749	-3.529787	28.641179
C	-2.258736	1.635668	18.636759	H	-7.984982	-2.122419	29.055736
C	-0.393123	1.795659	17.547505	H	-5.751692	-2.567125	30.898752
N	-0.891046	1.781302	18.777423	H	-6.338790	-1.366821	27.618831
H	-4.273436	0.385609	16.723477	H	-5.141493	-0.101116	27.759732
H	-3.756587	1.571587	15.521795	H	-4.227460	-0.869366	31.065131
H	-1.258830	1.658191	15.641177	H	-3.713869	-0.058549	29.596227
H	-2.909304	1.588290	19.491393	Fe	1.603418	-2.415124	21.801124
H	0.644673	1.902157	17.279437	C	-1.298731	-1.617477	23.416110
C	-4.943714	4.055364	21.556046	C	-0.091972	-2.632150	18.850756
C	-3.579424	3.513184	21.741428	C	4.485067	-3.257942	20.199817
N	-3.298543	2.513918	22.647380	C	3.300038	-2.125395	24.729470
C	-2.425191	3.684651	21.026308	N	1.089887	-1.981373	23.704943
C	-2.030033	2.111678	22.465440	C	-0.152864	-1.655141	24.176271
N	-1.473465	2.800563	21.482102	C	-0.094206	-1.344206	25.589111
H	-4.917384	4.958512	20.941643	C	1.219484	-1.456358	25.952475
H	-5.429040	4.285610	22.508941	C	1.939954	-1.868806	24.764063
H	-3.947075	2.121973	23.344636	C	1.848831	-1.200519	27.277274
H	-2.239275	4.351109	20.197837	O	-2.939015	-2.195048	17.680758
H	-1.531233	1.346688	23.031288	C	-1.260459	-0.987688	26.454308
C	-8.242053	-3.971746	17.701789	C	-1.787605	0.447254	26.261604
C	-7.928836	-3.145043	18.905129	C	-2.787100	0.827671	27.348012
O	-7.831327	-1.924374	18.916734	O	-2.398691	0.810230	28.539621
O	-7.756432	-3.908503	19.999559	O	-3.986765	1.120882	26.990643
H	-7.338958	-4.519013	17.406041	N	2.084258	-2.971229	19.912396
H	-8.573654	-3.338065	16.878703	C	1.251145	-2.938793	18.829506
C	-10.892459	-3.400214	22.669275	C	1.986306	-3.223956	17.616552
C	-10.926949	-2.072438	23.334978	C	3.289607	-3.403384	17.988502
N	-9.845927	-1.221863	23.342758	C	3.336581	-3.222572	19.428827
C	-11.902557	-1.387040	24.017103	C	1.366651	-3.291794	16.262851
C	-10.190075	-0.089514	24.006750	N	3.509993	-2.744007	22.381259
N	-11.439548	-0.154188	24.436380	C	4.565932	-3.027733	21.561595
H	-10.753453	-3.294107	21.586834	C	5.803244	-3.019736	22.308415
H	-11.834045	-3.927708	22.842885	C	5.469651	-2.706908	23.605957
H	-8.940140	-1.439006	22.934463	C	4.026080	-2.529085	23.624414
H	-12.914391	-1.712155	24.226289	C	7.146245	-3.313385	21.739755
H	-9.503702	0.733541	24.145195	C	6.310091	-2.587744	24.785150

C	7.597558	-2.212190	24.827770	H	-5.247137	0.310919	24.331107
N	-0.343957	-2.206412	21.238779	O	-5.187422	3.331343	28.399508
C	-0.828157	-2.281412	19.969758	H	-4.747317	2.565476	27.959664
C	-2.227094	-1.924701	19.959673	H	-4.766084	4.101178	27.978752
C	-2.569964	-1.641740	21.269550	O	0.754963	2.811332	24.783503
C	-1.383805	-1.826713	22.046760	H	1.198133	3.661455	24.582566
C	-3.146889	-1.846115	18.843318	H	0.804411	2.316195	23.919780
C	-3.907857	-1.273940	21.810478	H	-7.545975	-3.325902	20.782243
C	-4.850401	-2.489296	21.882230	H	-2.248178	0.562378	25.280930
C	-6.078298	-2.253287	22.708850	H	-0.948596	1.146702	26.307260
O	-7.222474	-2.517427	22.345932	H	-0.969964	-1.101822	27.501496
O	-5.797962	-1.753418	23.911579	H	-2.078321	-1.701800	26.283307
C	4.436654	-3.730884	17.074149	H	2.472834	-2.043918	27.593076
O	5.591841	-2.904507	17.311268	H	2.487164	-0.309563	27.231762
C	4.881466	-5.184324	17.170991	H	1.095108	-1.028522	28.048235
H	5.695648	-5.362952	16.458666	H	-2.214205	-1.383631	23.936963
Cu	0.174094	2.002975	20.563430	H	3.845887	-1.967823	25.648591
H	8.891071	3.392426	20.913366	H	5.824948	-2.824059	25.731532
H	-4.673317	2.104936	16.938341	H	8.121364	-2.173880	25.780115
H	-5.531461	3.294704	21.032081	H	8.153466	-1.915608	23.944298
H	-9.006486	-4.710145	17.956797	H	7.794056	-3.765680	22.495970
H	-10.071115	-4.017670	23.050778	H	7.084332	-4.002036	20.893018
H	0.595660	-7.919073	24.825699	H	7.631935	-2.392505	21.390123
H	-7.746918	-3.426168	30.227401	H	5.409310	-3.428936	19.672510
O	1.952602	-0.837562	21.451515	H	4.092672	-3.554860	16.047401
O	0.902182	1.644417	22.307281	H	4.043440	-5.844777	16.923325
O	-6.628430	0.538371	20.302060	H	5.231022	-5.426315	18.179988
H	-6.431938	1.043391	19.488647	H	2.115064	-3.440220	15.482194
H	-7.021960	-0.283861	19.948657	H	0.651199	-4.121704	16.204893
O	-7.572639	-1.989236	25.832417	H	0.821180	-2.368610	16.035278
H	-8.468407	-1.607212	25.745164	H	-0.626189	-2.643127	17.913229
H	-7.738887	-2.951045	25.917695	H	-4.130963	-1.420580	19.108926
O	1.306776	2.775671	27.602619	H	-4.377437	-0.491662	21.206337
H	1.125629	2.677097	26.638710	H	-3.786896	-0.858829	22.808261
H	0.473983	2.479682	28.016857	H	-4.325184	-3.330759	22.355717
O	-7.661516	2.495255	24.084905	H	-5.149310	-2.812482	20.884978
H	-6.785798	2.097879	24.291708	H	5.277530	-1.977320	17.394648
H	-7.665535	2.547064	23.110162	H	1.337521	0.774614	22.186648
O	-5.055967	1.238949	24.548543	H	-6.598262	-1.825211	24.536590
H	-4.616788	1.196965	25.453773				