

Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins

Supporting Information

*Kyle M. Lancaster, María-Eugenia Zaballa, Stephen Sproules, Mahesh Sundararajan,
Serena DeBeer, John H. Richards, Alejandro J. Vila, Frank Neese, and Harry B. Gray*

Table of Contents

Tables

Table S1. EPR Conditions	S2
--------------------------	----

Figures

Figure S1. QM/MM Partitioning	S3
Figure S2. Full MCD spectra	S4
Figure S3. QM/MM Optimized Active Sites	S5
Figure S4. Experimental and Calculated XAS	S6
Figure S5. SORCI MCD Spectra	S7

Input Coordinates (XYZ) for Calculations

Wild-type Azurin: X-ray Diffraction	S7
Wild-type Azurin: QM/MM	S9
C112D Azurin: X-ray Diffraction	S11
C112D Azurin: QM/MM Bidentate	S13
C112D Azurin: QM/MM Monodentate	S15
C112D Azurin: SORCI (QM/MM Bidentate)	S17
C112D/M121L Azurin: X-ray Diffraction	S17
C112D/M121L Azurin: QM/MM Bidentate	S19
C112D/M121L Azurin: QM/MM Monodentate	S21
C112D/M121L Azurin: SORCI (QM/MM Monodentate)	S23
C112D/M121F Azurin: X-ray Diffraction	S24
C112D/M121F Azurin: QM/MM Bidentate	S26
C112D/M121F Azurin: QM/MM Monodentate	S28
C112D/M121F Azurin: SORCI (QM/MM Monodentate)	S30

Tables

Table S1. Experimental conditions, linewidth (W_i , 10^{-4} cm $^{-1}$) and g - and A -strain coefficients ($\sigma_{g_i}/\sigma_{A_i}$) for frozen solution S-, X-, and Q-band EPR measurements

	frequency ^a	power ^b	modulation ^c	T^d	W_x	W_y	W_z	σ_{g_x}	σ_{g_y}	σ_{g_z}	σ_{A_x}	σ_{A_y}	σ_{A_z}
	3.6940	9.74	0.2	20	1	4	5	- 0.0024	0.001	0.0023	1	2	-8
C112D	9.3758	2.04	0.5	77	3.4	29	11	0.0	0.0026	0.0034	0	12	-9
	34.086	0.98	1.5	50	10	3	41	0.002	0.0043	0.0015	0	0	-15
	3.7190	9.69	0.2	20	9	80	10	0.009	0.010	0.008	10	10	-3
C112D/M121L	9.3750	6.42	0.5	77	22	10	14	0.013	0.015	0.006	12	15	-5
	34.109	2.02	1.5	50	0	26	44	0.0044	0.010	0.004	0	0	-7
	3.7150	9.74	0.2	20	8	9	5	0.017	0.008	0.004	10	10	-11
C112D/M121F	9.3749	6.45	0.5	77	8	8	7	0.014	0.008	0.007	3	3	-6
	34.092	2.02	1.5	50	18	24	50	0.0049	0.008	0.0024	0	0	-15

^aIn GHz. ^b In mW. ^cIn mT. ^d In K.

Figures

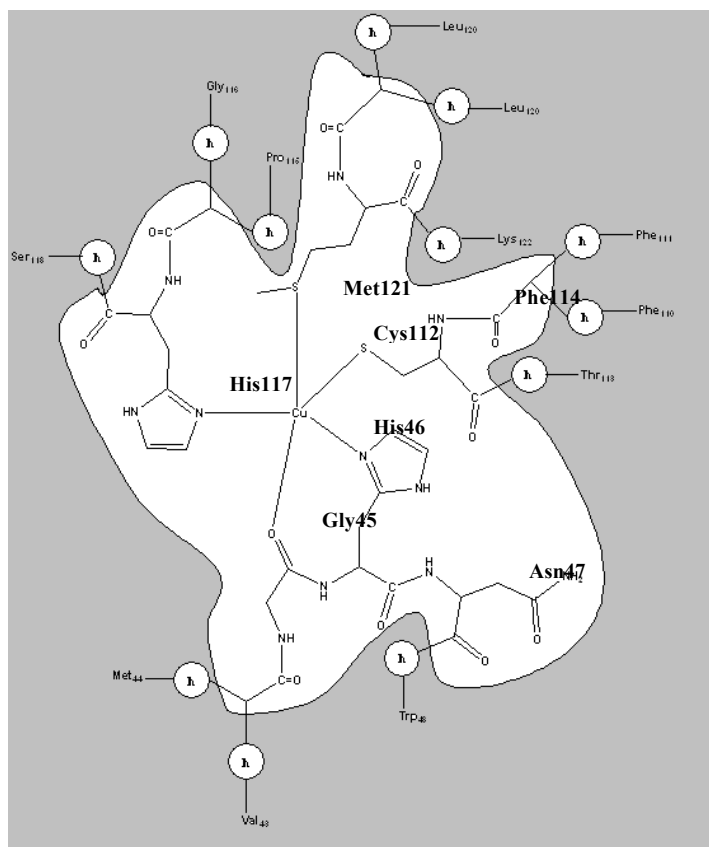


Figure S1. QM/MM partitioning for active site optimizations of wild-type azurin. The QM region is enveloped in white and included residues 45, 46, 47, 112, 114, 117, and 121. The surrounding gray area comprised the MM region. Analogous partitioning was employed for C112D and C112D/M121L,F azurins.

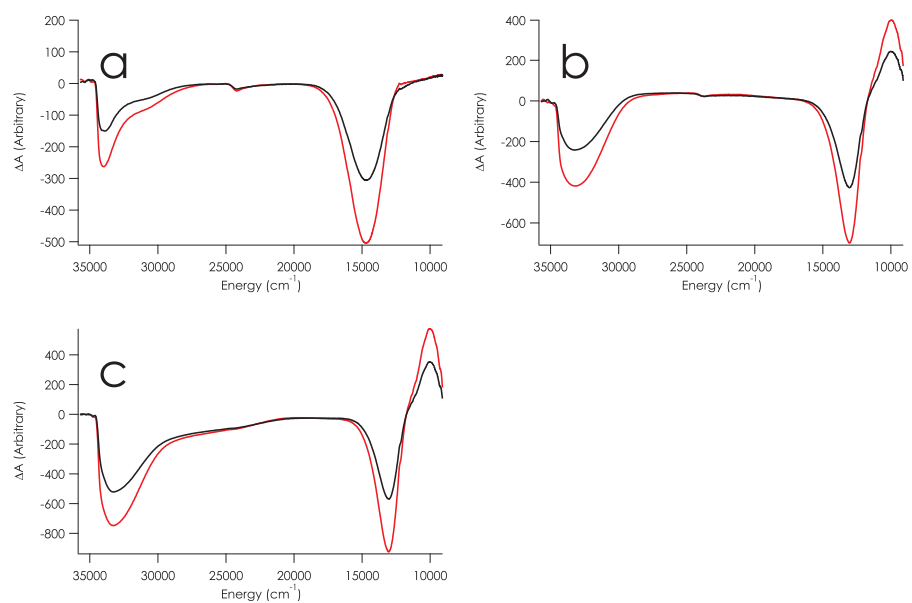


Figure S2. MCD spectra of (a) C112D, (b) C112D/M121L, and (c) C112D/M121F azurins. MCD spectra were recorded at a magnetic field strength of 7 T at 10 K (black) and 5.3 K (red) in 50 mM HEPES pH 7.0 containing 50% glycerol. Inverse temperature dependence of the circular dichroism indicates that all observed features are C-terms.

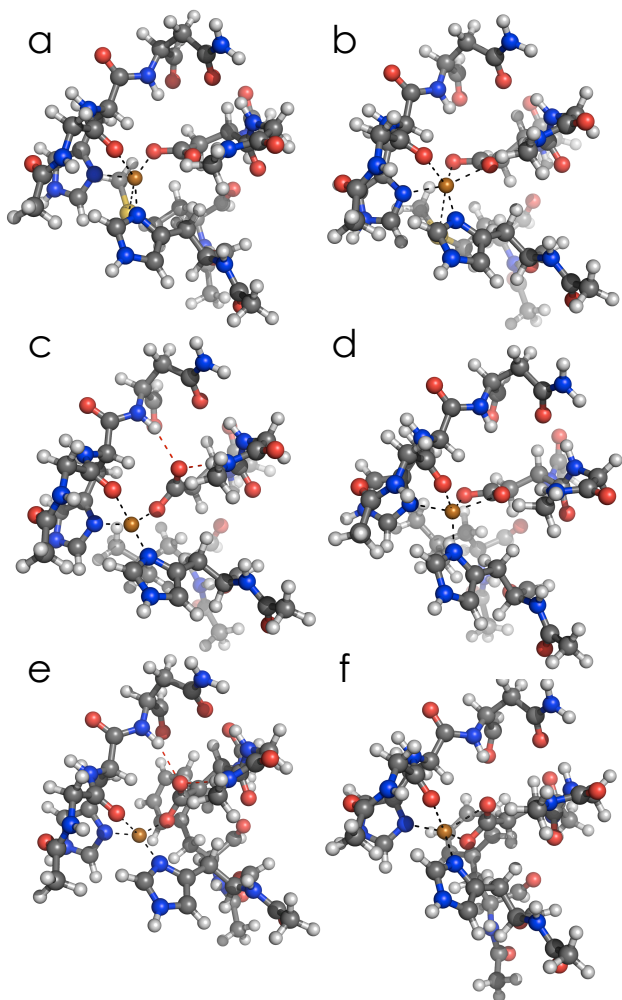


Figure S3. QM/MM optimized active sites. a) C112D monodentate, b) C112D bidentate, c) C112D/M121L monodentate, d) C112D/M121L bidentate, e) C112D/M121F monodentate, f) C112D/M121F bidentate. Inner-sphere coordination is indicated by black dashed lines, outer-sphere coordination is indicated by red dashed lines.

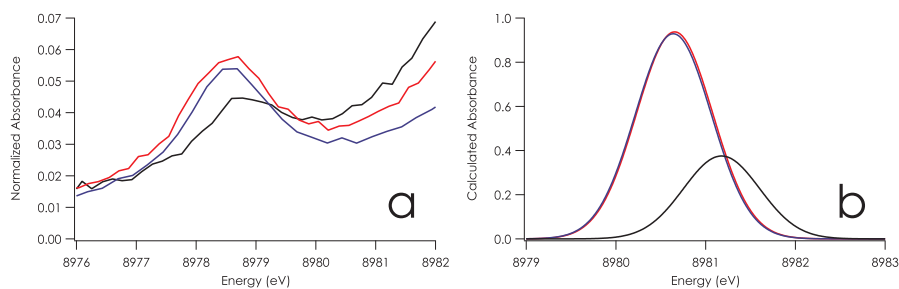


Figure S4. Experimental (a) and calculated (b) Cu K-edge XAS for C112D (black) and C112D/M121X (X = L, red; F, blue) from TDDFT calculations. Spectra were calculated using the B3LYP functional with the SV(P) basis set and ZORA. The ~8979 eV pre-edge feature in Cu K-edge XAS spectra arises from $1s \rightarrow 3d$ excitations that are formally forbidden in octahedral symmetry, but gain intensity upon tetrahedral site distortion. The intensity of this pre-edge feature has been used as a measure of 4p admixture into the $\psi_{x^2-y^2}$ SOMO. Integrated peak areas for the C112D/M121L and C112D/M121F pre-edge

features are 0.091 and 0.081, respectively. These data have been previously reported, though their discussion was primarily qualitative.¹¹ The corresponding LF peak in the C112D spectrum is far less intense, having an area of 0.025. Thus, C112D/M121F has a pre-edge feature with 0.9 times the absorbance of C112D/M121L, and C112D has a pre-edge feature with 0.27 times the absorbance of C112D/M121L. The pre-edge features are isoenergetic at 8978.5 eV in the type zero spectra. In the C112D spectrum the feature shifts to higher energy at 8978.7 eV. Calculated XAS spectra using the QM/MM bidentate C112D and crystallographic type zero coordinates are in agreement with experiment. Integrated areas are 1.00 and 0.99 for C112D/M121L and C112D/M121F, respectively. The lower intensity of the C112D protein is reproduced; it integrates to 0.40 units. Calculated absorbance areas require a scaling factor; for our purposes noting that the absorbance ratios trend in accord with experiment is satisfactory. The shift to higher energy is overestimated by 0.5 eV.

Unknown

Field Code Changed

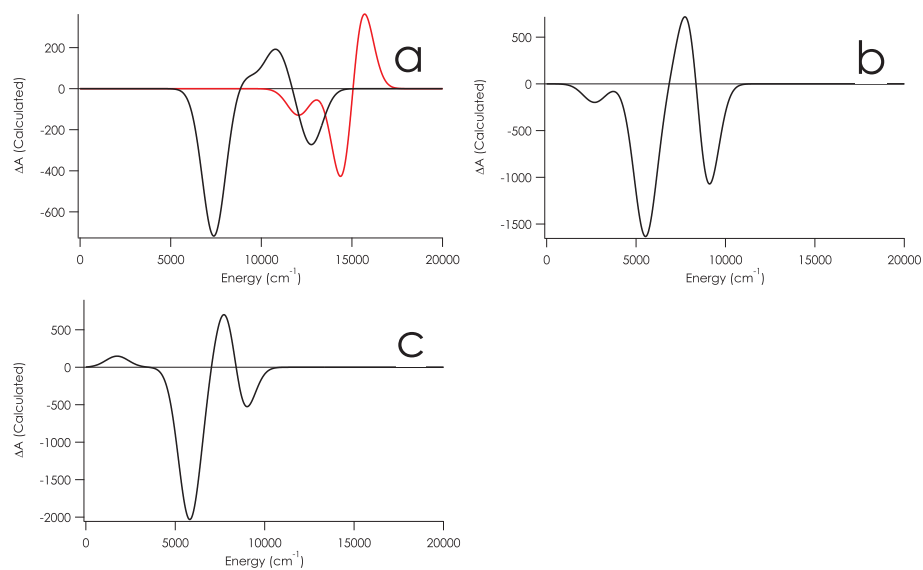


Figure S5. SORCI-MCD calculations of C112D (a, black = crystal, red = QM/MM), and C112D/M121X (X = L, b; F, c) azurins.

Input Coordinates (XYZ) for Calculations

Wild-type Azurin: X-ray Diffraction

```

C 2.542797 5.153864 5.697064
C 1.705299 5.714590 4.544079
O 0.475220 5.755975 4.624187
N 2.284791 6.219131 3.449127
C 1.483332 6.682889 2.315236
C 0.682409 5.547989 1.662478
O 1.110031 4.394232 1.676595
N -0.510372 5.826962 1.132444
C -1.318347 4.832033 0.445581
C -1.862794 5.456831 -0.831244
O -2.106413 6.660660 -0.886267
C -2.535673 4.372951 1.268053
C -2.198242 3.709077 2.597761
N -1.273827 2.778677 2.732068
C -2.748272 4.059624 3.793127
C -1.240612 2.543619 4.035258
N -2.117466 3.310579 4.654100
N -1.998626 4.653020 -1.870770
C -2.676995 5.059787 -3.087535
C -3.521102 3.846094 -3.415267
O -3.403878 2.795287 -2.732893
C -1.673371 5.367534 -4.218049
C -0.601607 4.332919 -4.500565
O -0.670317 3.203213 -4.032813
N 0.490687 4.663037 -5.176033

```

C	-3.493898	-2.413684	-4.529815
C	-2.850834	-1.070129	-4.242315
O	-3.112894	-0.073762	-4.934205
N	-2.012573	-1.039940	-3.210748
C	-1.256475	0.145730	-2.849058
C	0.177963	-0.132775	-3.255854
O	0.656350	-1.227300	-2.953743
C	-1.296668	0.393777	-1.341261
S	-0.167734	1.712744	-0.848403
N	0.909908	0.786173	-3.893992
C	2.262375	0.496601	-4.332839
C	3.327430	1.057828	-3.422489
O	4.514736	0.960222	-3.782587
N	2.981292	1.661456	-2.270159
C	4.022282	2.166309	-1.363316
C	6.005631	-3.294496	1.113475
C	4.523416	-3.349059	1.461474
O	4.088517	-4.331856	2.083865
N	3.696176	-2.382802	1.050209
C	2.292954	-2.441312	1.412266
C	1.448047	-3.388356	0.590344
O	0.465367	-3.972630	1.116209
C	1.659282	-1.087726	1.314863
C	2.100998	-0.125719	2.395492
N	1.427249	0.994052	2.591227
C	3.234512	-0.202565	3.149342
C	2.142262	1.657074	3.481259
N	3.205439	0.932877	3.795518
C	-1.242609	-6.667363	2.656781
C	-2.351663	-5.812387	2.066397
O	-3.533757	-6.017825	2.359713
N	-2.038601	-4.834819	1.214924
C	-3.059761	-3.927717	0.734565
C	-3.366578	-4.233911	-0.714434
O	-2.723023	-3.657334	-1.629293
C	-2.565655	-2.507327	0.902905
C	-2.308853	-2.173160	2.351849
S	-1.912017	-0.451717	2.669908
C	-3.490343	0.330317	2.523247
Cu	-0.106390	1.841380	1.413550
H	-3.362644	1.410603	2.731667
H	-4.216676	-0.081960	3.259820
H	-3.929864	0.236421	1.504863
H	-1.436652	-2.747053	2.733101
H	-3.174065	-2.457375	2.994685
H	-1.646300	-2.358501	0.297210
H	-3.323869	-1.813020	0.473187
H	-3.961865	-4.141717	1.350797
H	-4.105513	-5.045107	-0.953519
H	-1.065767	-4.668925	0.916901
H	-0.220944	-6.291160	2.437087
H	-1.341439	-7.702997	2.264990
H	-1.392922	-6.719353	3.755252
H	4.014580	-0.960690	3.251132
H	3.901716	1.232601	4.487377
H	1.938865	2.666194	3.859740
H	1.839111	-0.635751	0.308514
H	0.552544	-1.183964	1.387653
H	2.225784	-2.828686	2.451931
H	1.685547	-3.517592	-0.500594
H	4.029156	-1.612993	0.461773
H	6.227093	-4.128972	0.413927
H	6.347240	-2.342443	0.650181
H	6.587748	-3.485008	2.038892
H	-1.023985	-0.535915	-0.796287
H	-2.328871	0.673485	-1.037462
H	-1.699410	0.998682	-3.402366

H	-1.762630	-1.916385	-2.735687
H	-3.126109	-2.783882	-5.512304
H	-4.589571	-2.264297	-4.634899
H	-3.290792	-3.171836	-3.746835
H	0.465076	1.698403	-4.109515
H	2.441472	0.891107	-5.356012
H	2.383911	-0.606266	-4.362296
H	1.989771	1.686623	-1.977243
H	4.723855	2.826556	-1.916192
H	3.533430	2.735050	-0.545854
H	4.624934	1.334038	-0.932197
H	2.181576	7.113750	1.565649
H	0.798835	7.492642	2.650070
H	3.294090	6.130368	3.306088
H	2.068698	4.213252	6.045143
H	2.502279	5.871353	6.545545
H	3.611605	4.970682	5.448492
H	-4.215232	3.884440	-4.297099
H	1.179570	3.930595	-5.367816
H	0.627355	5.573429	-5.626244
H	-1.187734	6.340489	-3.975309
H	-2.236283	5.561021	-5.164566
H	-3.290847	5.965220	-2.894172
H	-1.780423	3.647611	-1.804906
H	-0.855197	6.792175	1.035227
H	-0.669016	3.965119	0.220520
H	-3.112607	3.663056	0.629274
H	-3.199596	5.242971	1.456779
H	-3.501084	4.809862	4.054367
H	-2.248216	3.321008	5.670855
H	-0.615029	1.799266	4.540942

Wild-Type Azurin: QM/MM

C	39.295166	30.687818	41.340846
H	39.629765	29.673798	41.050547
C	38.426742	31.285552	40.262502
O	37.186286	31.407371	40.337820
N	39.064987	31.730106	39.139735
H	40.069762	31.600774	39.023275
C	38.289248	32.206871	38.017280
H	37.608450	33.018624	38.335478
H	38.981270	32.617502	37.259524
C	37.474468	31.069356	37.381155
O	37.920823	29.918532	37.322065
N	36.258016	31.433129	36.876155
H	35.988700	32.425307	36.820127
C	35.481078	30.482115	36.106353
H	36.154662	29.635953	35.885851
C	34.242479	29.902914	36.854255
H	33.476450	30.696649	36.967748
H	33.797912	29.130439	36.193360
C	34.551655	29.327873	38.206896
N	35.532812	28.369328	38.435454
C	33.958622	29.628822	39.424150
H	33.142477	30.304330	39.686604
C	35.541145	28.120180	39.747665
H	36.209930	27.424266	40.255599
N	34.595468	28.857699	40.375410
H	34.421942	28.895876	41.401603
C	35.026358	31.136697	34.795145
O	34.765891	32.347412	34.752829
N	34.932199	30.276758	33.758184
H	35.117920	29.276205	33.927202
C	34.241486	30.539699	32.510335
H	33.629921	31.456340	32.642293

C	35.207111	30.802026	31.334181
H	34.628613	30.834902	30.385843
H	35.676988	31.797782	31.433438
C	36.251950	29.696409	31.217279
O	35.971567	28.529414	31.553713
N	37.451907	30.007346	30.692667
H	37.804915	30.948090	30.488100
H	38.109544	29.228584	30.497472
C	33.242194	29.359650	32.252147
O	33.247158	28.413789	33.041939
C	33.280557	23.122382	31.110555
H	32.907636	22.678101	32.053644
C	33.862263	24.474220	31.434534
O	33.594357	25.502195	30.803940
N	34.705718	24.498019	32.530474
H	34.895031	23.613244	33.011260
C	35.540231	25.638620	32.859061
H	35.156139	26.499041	32.283393
C	35.448222	25.922790	34.373617
H	34.410967	26.211382	34.619993
H	35.708958	25.014883	34.946278
S	36.572047	27.279949	34.933134
C	36.992087	25.305177	32.461302
O	37.491713	24.222580	32.815441
N	37.648252	26.243730	31.721261
H	37.145612	27.132068	31.505023
C	39.020534	26.051027	31.317043
H	39.222260	24.965378	31.312258
C	40.101084	26.689348	32.205072
O	41.289295	26.686753	31.867757
N	39.712308	27.177138	33.419314
H	38.732643	27.115338	33.735633
C	40.748880	27.641530	34.308958
H	41.376642	28.351095	33.760405
C	42.713588	22.224516	36.764702
H	43.138243	21.241378	36.488223
H	43.093509	22.468628	37.777966
C	41.205873	22.040964	36.843880
O	40.630169	20.970553	37.107507
N	40.429237	23.169759	36.645689
H	40.861831	24.046661	36.337505
C	39.030732	23.140183	37.045710
H	38.949600	22.797959	38.098405
C	38.362504	24.521316	36.925789
H	38.503497	24.929309	35.901547
H	37.268684	24.392445	37.052315
C	38.837693	25.511074	37.948991
N	38.196841	26.728459	38.160351
C	39.912352	25.431865	38.816607
H	40.630943	24.629328	38.976900
C	38.877070	27.372584	39.116961
H	38.666194	28.382577	39.469120
N	39.916446	26.609559	39.542589
H	40.626784	26.865630	40.250036
C	38.209823	22.120158	36.240773
O	37.245614	21.604217	36.837406
C	35.503890	18.870471	38.296228
H	35.104962	17.873592	38.573665
C	34.322768	19.665270	37.806917
O	33.156640	19.525788	38.211929
N	34.625552	20.636397	36.869121
H	35.612415	20.781726	36.613238
C	33.686578	21.644735	36.426453
H	32.757920	21.474579	37.009786
C	34.208781	23.074015	36.627107
H	35.128167	23.211908	36.028080
H	33.458444	23.776342	36.221804

C	34.489617	23.385948	38.099922
H	33.657852	23.064879	38.757458
H	35.400469	22.857929	38.438172
S	34.806630	25.169765	38.440305
C	33.149826	25.866306	38.073187
H	33.123050	26.888961	38.488067
H	32.951152	25.913934	36.988903
H	32.362195	25.259756	38.552788
C	33.390962	21.280883	34.940169
O	34.041809	21.805421	34.033501
H	40.190465	31.306637	41.507485
H	38.740781	30.631268	42.281582
H	32.516904	29.475388	31.542289
H	32.459833	23.204253	30.381188
H	34.014760	22.407800	30.728662
H	39.204376	26.404569	30.298842
H	40.344818	28.158945	35.183337
H	41.383370	26.783516	34.576143
H	43.030283	22.989221	36.038619
H	38.432815	21.920235	35.264226
H	36.367733	18.763516	37.621986
H	35.826941	19.283254	39.255797
H	32.644524	20.596007	34.809350
Cu	36.651041	27.392147	37.111032

C112D Azurin: X-ray Diffraction

C	4.558995	-6.459125	-2.391922
C	4.146389	-6.098535	-0.944458
O	3.119571	-6.543085	-0.461577
N	4.982515	-5.299096	-0.274945
C	4.736888	-4.878440	1.117528
C	3.526817	-3.967579	1.151749
O	3.335474	-3.117733	0.243612
N	2.664130	-4.127618	2.165852
C	1.525072	-3.160808	2.260105
C	1.490440	-2.625153	3.673624
O	1.900777	-3.324001	4.604840
C	0.165062	-3.810712	2.031888
C	-0.005268	-4.492468	0.705291
N	0.384323	-3.940272	-0.517300
C	-0.621249	-5.663248	0.415361
C	-0.019894	-4.744379	-1.496945
N	-0.637643	-5.781947	-0.955748
N	1.033378	-1.365352	3.841955
C	0.822724	-0.823639	5.178532
C	-0.460375	-0.036660	5.080657
O	-0.951979	0.227536	3.952784
C	1.997790	0.048001	5.667014
C	2.431387	1.145025	4.629927
O	1.793064	1.327960	3.585288
N	3.491416	1.877816	4.948310
C	-3.320727	4.633113	1.895931
C	-2.078539	3.803851	2.286778
O	-1.682198	3.749802	3.428610
N	-1.501772	3.158839	1.299995
C	-0.339675	2.364856	1.389899
C	0.861072	3.174547	0.774314
O	0.703699	3.803556	-0.303043
C	-0.683807	1.136601	0.571834
C	0.445249	0.122809	0.457539
O	1.591179	0.475039	0.322536
O	0.141360	-1.068232	0.472498
N	2.034261	3.174042	1.414968
C	3.141034	4.024627	0.902449
C	4.226893	3.164424	0.164313

O	5.290748	3.657844	-0.179533
N	3.975944	1.877605	-0.050835
C	4.952802	1.059382	-0.778900
C	3.325907	2.714876	-6.716852
C	1.949104	2.257249	-6.184881
O	0.922890	2.331828	-6.890508
N	1.914513	1.725082	-4.958375
C	0.679711	1.084515	-4.476619
C	-0.468301	2.051177	-4.227363
O	-1.657676	1.665741	-4.370183
C	0.972169	0.199318	-3.189545
C	1.790180	-0.992305	-3.510918
N	1.914520	-2.083078	-2.684989
C	2.486876	-1.297177	-4.634413
C	2.682433	-2.994471	-3.254081
N	3.037042	-2.543307	-4.446758
C	-5.027831	1.739569	-6.118317
C	-5.370377	1.556128	-4.633390
O	-6.558253	1.372677	-4.268214
N	-4.330136	1.565441	-3.812687
C	-4.450693	1.176114	-2.426020
C	-4.587555	2.443295	-1.575777
O	-3.587721	2.901954	-0.964603
C	-3.268505	0.315857	-2.045185
C	-3.356593	-1.031480	-2.752438
S	-1.993337	-2.015905	-2.178774
C	-2.614814	-2.600479	-0.578145
Cu	1.199082	-2.073956	-0.773769
H	-1.788486	-3.142410	-0.090164
H	-3.482095	-3.281622	-0.721164
H	-2.906722	-1.755683	0.081919
H	-3.234992	-0.915741	-3.850623
H	-4.324309	-1.549760	-2.570747
H	-2.319052	0.824429	-2.296263
H	-3.270371	0.168796	-0.943672
H	-5.417378	0.623685	-2.350877
H	-5.567990	2.989849	-1.592782
H	-3.388659	1.831896	-4.139059
H	-3.955580	1.960490	-6.305767
H	-5.654289	2.552880	-6.541734
H	-5.304084	0.805688	-6.654599
H	2.992069	-3.945692	-2.804968
H	3.619190	-3.033157	-5.132361
H	2.653828	-0.739959	-5.562199
H	1.444208	0.821779	-2.392451
H	-0.004966	-0.145911	-2.778507
H	0.304069	0.408103	-5.275322
H	-0.226477	3.096227	-3.895759
H	2.733962	1.750977	-4.344981
H	4.136263	2.696209	-5.956672
H	3.226458	3.743281	-7.121936
H	3.606180	2.054729	-7.566197
H	-1.586101	0.654657	0.997886
H	-0.929275	1.456796	-0.466739
H	-0.149749	2.117079	2.452990
H	-1.879133	3.295639	0.353834
H	-3.066710	5.712987	1.975094
H	-4.125879	4.428502	2.632256
H	-3.674206	4.406742	0.869005
H	2.136450	2.592446	2.268740
H	3.641306	4.569254	1.729925
H	2.702221	4.741197	0.180595
H	3.053931	1.464599	0.176097
H	5.967194	1.206862	-0.350687
H	4.654063	-0.005364	-0.690766
H	5.008158	1.345030	-1.855654
H	5.632052	-4.324448	1.469755

H	4.590516	-5.770693	1.764052
H	5.808473	-4.919511	-0.740882
H	4.940817	-7.503895	-2.404453
H	3.650748	-6.442295	-3.029401
H	5.342061	-5.799999	-2.827532
H	2.851864	-4.694363	3.001315
H	1.718811	-2.360097	1.527007
H	-0.601086	-3.008450	2.128446
H	-0.031283	-4.550731	2.837600
H	-1.071191	-6.427515	1.059942
H	-1.020783	-6.583991	-1.464848
H	0.107199	-4.573390	-2.571754
H	0.635274	-0.812459	3.073193
H	-0.931725	0.353424	6.022879
H	2.861829	-0.621004	5.878607
H	1.737824	0.543703	6.631613
H	4.019140	1.739786	5.814764
H	3.798105	2.624439	4.317033
H	0.712479	-1.671100	5.891957

C112D: QM/MM Bidentate

C	38.684659	20.256911	20.437416
H	38.477038	21.120986	19.775239
C	38.270020	20.624003	21.829176
O	37.276895	20.174859	22.437774
N	39.085024	21.531556	22.443644
H	39.882401	21.935954	21.952148
C	38.817228	21.958536	23.793870
H	38.670215	21.085844	24.451626
H	39.689503	22.530142	24.155245
C	37.585381	22.850057	23.847940
O	37.428275	23.741305	23.003034
N	36.727715	22.610050	24.874159
H	36.945326	21.884384	25.567996
C	35.593145	23.481216	25.094533
H	35.717388	24.317779	24.388678
C	34.233643	22.810352	24.799425
H	34.034933	22.012664	25.542692
H	33.452333	23.582303	24.949988
C	34.113325	22.249585	23.408077
N	34.540411	22.908261	22.261851
C	33.477996	21.086696	23.012055
H	33.032160	20.285116	23.594036
C	34.161080	22.173376	21.214786
H	34.326371	22.420613	20.166100
N	33.520233	21.054989	21.630894
H	32.937157	20.447033	21.033005
C	35.646481	24.036778	26.521919
O	36.032043	23.323887	27.455976
N	35.264248	25.331577	26.631576
H	34.764032	25.770908	25.846303
C	35.040860	25.997451	27.898165
H	34.971358	25.205538	28.671150
C	36.185342	26.939546	28.326807
H	35.825178	27.521956	29.202669
H	37.063523	26.349202	28.647595
C	36.610909	27.952151	27.262976
O	35.818400	28.279783	26.358134
N	37.846197	28.473969	27.377510
H	38.515376	28.218967	28.109276
H	38.143318	29.214462	26.714680
C	33.650263	26.699787	27.859435
O	33.030888	26.668309	26.794449
C	30.834551	31.368528	24.677546
H	30.211848	30.768479	23.993255

C	32.009106	30.524852	25.077846
O	32.282865	30.196485	26.237691
N	32.749959	30.095809	24.003045
H	32.380637	30.283327	23.069174
C	33.846100	29.162052	24.084769
H	34.039757	28.974766	25.154552
C	33.403309	27.870984	23.377765
H	32.511053	27.484009	23.887886
H	33.103383	28.149496	22.346288
C	34.365632	26.737813	23.210019
O	35.503575	26.865887	22.641227
O	33.964291	25.549834	23.495877
C	35.036803	29.842716	23.402336
O	34.934878	30.264048	22.235279
N	36.127440	30.004834	24.190639
H	36.145234	29.506455	25.105776
C	37.274567	30.736162	23.728337
H	36.919836	31.436565	22.949616
C	38.391505	29.904686	23.049876
O	39.456949	30.419657	22.725955
N	38.080930	28.591749	22.753237
H	37.128442	28.231141	22.880143
C	39.024958	27.813843	21.990791
H	40.020740	27.974345	22.421933
C	37.421754	29.428305	16.122679
H	37.308578	30.324013	15.481558
H	37.736173	28.622043	15.438087
C	36.055180	29.084445	16.663378
O	34.981996	29.280909	16.058068
N	36.018645	28.479908	17.901482
H	36.890588	28.333946	18.421060
C	34.807294	27.800478	18.330681
H	34.465091	27.131082	17.524183
C	35.047156	26.963062	19.592685
H	35.498793	27.577287	20.396884
H	34.062532	26.627797	19.980927
C	35.865173	25.727757	19.348203
N	35.995358	24.740901	20.320046
C	36.528761	25.296514	18.211700
H	36.656316	25.793081	17.248183
C	36.704858	23.742337	19.796743
H	37.014998	22.836465	20.318444
N	37.033104	24.038299	18.513385
H	37.528152	23.402868	17.888164
C	33.639510	28.777921	18.559324
O	32.498818	28.330847	18.356965
C	29.105960	28.464188	16.702586
H	28.223666	28.941533	16.235457
C	28.748550	28.374631	18.173941
O	27.593262	28.444236	18.636906
N	29.801824	28.174194	19.036247
H	30.766229	28.343707	18.720924
C	29.636515	27.830923	20.440488
H	28.661691	27.308402	20.536294
C	30.796039	26.957535	20.923147
H	31.735984	27.537510	20.885521
H	30.619692	26.696201	21.983557
C	30.898040	25.706952	20.059901
H	29.910905	25.224758	20.012620
H	31.194342	25.954943	19.025356
S	32.102814	24.456828	20.622700
C	31.354311	23.968345	22.222780
H	31.526686	22.887497	22.363904
H	31.807379	24.537838	23.051618
H	30.266710	24.146925	22.186460
C	29.519384	29.170318	21.209953
O	30.497425	29.638480	21.797982

H	39.771481	20.108895	20.341629
H	38.134403	19.388499	20.065120
H	33.242819	27.030354	28.735823
H	30.285946	31.707235	25.570058
H	31.103497	32.278893	24.134934
H	37.715382	31.330912	24.532998
H	38.804886	26.743027	22.011885
H	39.057376	28.199703	20.961124
H	38.235536	29.595624	16.845196
H	33.862983	29.725754	18.867562
H	29.994396	29.076363	16.483062
H	29.181190	27.477369	16.237772
H	28.614090	29.638309	21.140905
Cu	35.236177	24.778769	22.121062

C112D: QM/MM Monodentate

C	38.684659	20.256911	20.437416
H	38.477402	21.120869	19.775434
C	38.272257	20.621249	21.830087
O	37.278481	20.172916	22.438168
N	39.092913	21.522328	22.444638
H	39.885396	21.930820	21.948793
C	38.821146	21.960131	23.789954
H	38.670198	21.093081	24.454343
H	39.692489	22.533611	24.150289
C	37.589701	22.853164	23.827490
O	37.433561	23.729112	22.967267
N	36.733794	22.630002	24.858580
H	36.949776	21.913771	25.562203
C	35.605028	23.509988	25.072371
H	35.728936	24.343295	24.363187
C	34.240326	22.842610	24.785995
H	34.027461	22.075646	25.558011
H	33.467524	23.629404	24.901976
C	34.113296	22.222481	23.420424
N	34.534866	22.817908	22.241039
C	33.461951	21.050033	23.084512
H	33.022702	20.282203	23.712353
C	34.141154	22.040398	21.233209
H	34.301301	22.237939	20.172449
N	33.494490	20.948531	21.706414
H	32.886551	20.338565	21.134021
C	35.654782	24.053127	26.505290
O	36.017123	23.325174	27.438008
N	35.287813	25.351109	26.626623
H	34.848336	25.819422	25.825619
C	35.046347	26.006798	27.895531
H	34.973554	25.205224	28.658512
C	36.185222	26.946363	28.342417
H	35.817492	27.525698	29.216939
H	37.061357	26.354603	28.665937
C	36.614539	27.958434	27.280211
O	35.823491	28.275037	26.370570
N	37.845746	28.487557	27.397557
H	38.514417	28.235140	28.130530
H	38.144884	29.219388	26.725820
C	33.650263	26.699787	27.859435
O	33.019530	26.651657	26.801436
C	30.834551	31.368528	24.677546
H	30.211845	30.767680	23.993324
C	31.997764	30.522317	25.087034
O	32.268794	30.226508	26.258277
N	32.725021	30.043833	24.032461
H	32.410042	30.254871	23.084274
C	33.862688	29.172850	24.167760

H	34.086252	29.109800	25.245124
C	33.474318	27.775489	23.655863
H	32.867445	27.275613	24.427151
H	32.828820	27.885997	22.760402
C	34.583454	26.848736	23.237650
O	35.677925	27.265276	22.798354
O	34.263395	25.585639	23.270002
C	35.023952	29.856799	23.429475
O	34.884965	30.312473	22.279635
N	36.132316	30.009472	24.195726
H	36.168838	29.493167	25.097308
C	37.274567	30.736162	23.728337
H	36.916681	31.438450	22.952486
C	38.405064	29.918936	23.043789
O	39.458444	30.454716	22.708351
N	38.103259	28.606641	22.762309
H	37.149134	28.248391	22.911465
C	39.024958	27.813843	21.990791
H	40.028080	27.959182	22.411149
C	37.421754	29.428305	16.122679
H	37.311277	30.322219	15.478547
H	37.735098	28.619531	15.440653
C	36.055768	29.088829	16.664688
O	34.982223	29.281004	16.057792
N	36.018483	28.488738	17.904786
H	36.887739	28.351183	18.431719
C	34.808494	27.801515	18.324821
H	34.467274	27.151664	17.502195
C	35.058290	26.920989	19.558215
H	35.509675	27.506135	20.386497
H	34.077985	26.561580	19.935343
C	35.889541	25.705890	19.255566
N	36.023333	24.674420	20.180634
C	36.578129	25.340574	18.111634
H	36.714131	25.884640	17.175718
C	36.758352	23.714605	19.623507
H	37.075208	22.791168	20.108591
N	37.100639	24.077452	18.361647
H	37.614626	23.480240	17.714648
C	33.639510	28.777921	18.559324
O	32.498121	28.328879	18.359658
C	29.105960	28.464188	16.702586
H	28.222588	28.940983	16.237221
C	28.754982	28.379789	18.174564
O	27.605430	28.468796	18.648161
N	29.809586	28.165320	19.035875
H	30.776575	28.334710	18.722216
C	29.641258	27.827465	20.437261
H	28.663753	27.310840	20.536469
C	30.797321	26.950207	20.924543
H	31.753292	27.496513	20.826551
H	30.648428	26.735314	21.999209
C	30.816829	25.663480	20.106613
H	29.815912	25.209382	20.159298
H	31.037921	25.868455	19.044089
S	32.028457	24.401251	20.617088
C	31.388491	23.986796	22.279130
H	31.641124	22.932737	22.483806
H	31.846543	24.637372	23.043831
H	30.290686	24.094111	22.284383
C	29.519384	29.170319	21.209953
O	30.494914	29.640346	21.793209
H	39.771481	20.108896	20.341629
H	38.134403	19.388499	20.065120
H	33.242819	27.030354	28.735823
H	30.285946	31.707235	25.570058
H	31.103497	32.278893	24.134934

H	37.715382	31.330912	24.532998
H	38.804886	26.743027	22.011885
H	39.057376	28.199704	20.961124
H	38.235536	29.595624	16.845196
H	33.862983	29.725754	18.867562
H	29.994396	29.076363	16.483062
H	29.181190	27.477369	16.237772
H	28.614090	29.638309	21.140905
Cu	35.250059	24.636298	21.933422

C112D: SORCI (QM/MM Monodentate)

C	0.655978	-0.622665	3.372052
O	0.017874	0.077424	2.574832
N	1.047886	-1.899794	3.123738
H	1.531357	-2.420183	3.856805
C	0.638886	-2.563504	1.904331
C	1.801756	-2.817210	0.920075
H	2.515436	-3.545692	1.351408
H	1.369777	-3.285024	0.013668
C	2.560120	-1.576996	0.530800
N	1.961392	-0.366035	0.206471
C	3.919635	-1.444634	0.313999
H	4.737521	-2.155127	0.448733
C	2.926423	0.458557	-0.204719
H	2.785747	1.478861	-0.563232
N	4.130837	-0.158275	-0.145432
H	5.026696	0.249914	-0.412871
C	-2.327957	-1.919859	-2.314229
C	-1.622161	-1.368157	-1.116009
O	-2.081076	-0.399109	-0.419448
O	-0.424262	-1.769791	-0.875555
C	-0.699845	2.787869	-0.872698
N	0.017787	1.962071	-0.013403
C	-0.388121	4.100722	-0.560913
H	-0.726708	5.047359	-0.985357
C	0.745004	2.738706	0.788079
H	1.362504	2.391028	1.618016
N	0.535352	4.042598	0.474607
H	0.934787	4.845383	0.961647
C	1.063294	0.176781	-4.778194
S	1.681634	0.154596	-3.061169
C	2.178700	-1.602834	-2.907952
H	2.851677	-1.693033	-2.041101
H	1.297603	-2.248526	-2.745793
H	2.729524	-1.918833	-3.813357
Cu	0.007239	0.007268	-0.004794
H	0.717219	1.205979	-4.981580
H	0.214889	-0.518778	-4.916159
H	1.868394	-0.073855	-5.493874
H	0.959130	-0.247269	4.379186
H	0.169891	-3.535966	2.153490
H	-0.144677	-1.949842	1.438132
H	-1.386571	2.386716	-1.618968
H	-3.420738	-1.777112	-2.247022
H	-2.090857	-2.988496	-2.459221
H	-1.960347	-1.366393	-3.200075

C112D/M121L: X-ray Diffraction

C	4.021251	3.515018	6.183028
C	3.675357	4.113006	4.792927
O	2.581892	4.727589	4.583839
N	4.568547	3.919211	3.842002
C	4.366583	4.414127	2.472031
C	3.186012	3.651959	1.911191
O	3.019049	2.459817	2.260045

N	2.330354	4.336797	1.120263
C	1.306173	3.671723	0.298490
C	1.416323	4.180558	-1.152056
O	1.612051	5.318591	-1.341104
C	-0.119247	3.968070	0.704766
C	-0.417297	3.760302	2.174244
N	0.040269	2.679664	2.910200
C	-1.123119	4.517079	3.025761
C	-0.410346	2.774100	4.148657
N	-1.114001	3.897337	4.241398
N	1.258267	3.305219	-2.132799
C	0.931216	3.701166	-3.467997
C	-0.449503	3.076989	-3.875221
O	-1.047340	2.301872	-3.084426
C	2.096380	3.350276	-4.448654
C	2.525677	1.886055	-4.379969
O	1.756720	1.031103	-3.931515
N	3.719286	1.563894	-4.935571
C	-3.260176	-2.404561	-4.338301
C	-2.060171	-1.516228	-4.063159
O	-1.568722	-0.796910	-4.923067
N	-1.552837	-1.644172	-2.855557
C	-0.355173	-0.963954	-2.390544
C	0.819511	-1.967397	-2.466584
O	0.729367	-3.121661	-1.971404
C	-0.678864	-0.458683	-0.966669
C	0.523422	0.146376	-0.241695
O	1.639219	0.379229	-0.765063
O	0.307979	0.429756	0.927191
N	1.963500	-1.576499	-3.083819
C	3.109158	-2.533951	-3.126870
C	4.142728	-2.321073	-1.988359
O	5.178432	-3.008509	-1.981392
N	3.912867	-1.392544	-1.054101
C	4.824439	-1.250601	0.060204
C	3.379836	-6.400024	3.393154
C	2.026235	-5.664417	3.323792
O	1.115220	-6.107414	3.944307
N	1.904671	-4.531928	2.602316
C	0.694859	-3.698496	2.721205
C	-0.481290	-4.225518	1.918313
O	-1.656735	-4.035340	2.325414
C	1.049795	-2.265490	2.468548
C	1.827540	-1.654501	3.599959
N	1.922881	-0.294643	3.769912
C	2.486892	-2.214419	4.659501
C	2.606506	-0.026605	4.883989
N	2.971285	-1.177094	5.438779
C	-4.784855	-4.891762	3.627162
C	-5.230119	-3.731007	2.690270
O	-6.374004	-3.332553	2.727984
N	-4.318871	-3.160928	1.934833
C	-4.601368	-1.961355	1.184182
C	-4.730707	-2.494444	-0.226315
O	-3.728186	-2.511994	-0.986720
C	-3.428159	-0.973936	1.337349
C	-3.438687	-0.276759	2.699759
C	-2.236815	-0.500731	3.475229
C	-3.757982	1.207414	2.635233
Cu	1.119119	1.108443	2.532688
H	-1.343038	-0.031180	2.996677
H	-2.010405	-1.585778	3.594134
H	-2.314195	-0.076059	4.503972
H	-2.948184	1.769833	2.112759
H	-3.865055	1.636994	3.656586
H	-4.708789	1.410323	2.091889
H	-4.279398	-0.734210	3.280172

H	-2.481636	-1.529494	1.176253
H	-3.477543	-0.230755	0.510452
H	-5.570758	-1.562399	1.551688
H	-3.364489	-3.551792	1.883260
H	-5.696217	-2.983760	-0.526738
H	-3.748861	-5.246406	3.444056
H	-5.500477	-5.731503	3.509336
H	-4.866670	-4.526343	4.673307
H	2.860938	0.971102	5.260514
H	3.496705	-1.296829	6.309490
H	2.660931	-3.257905	4.943380
H	1.604933	-2.157786	1.505783
H	0.128232	-1.660940	2.331771
H	-0.275458	-4.779670	0.963011
H	0.341856	-3.805178	3.771965
H	2.676823	-4.192340	2.021518
H	4.194954	-5.966962	2.772319
H	3.212543	-7.453504	3.086784
H	3.700266	-6.414605	4.456633
H	-0.229918	2.075229	4.973459
H	-1.561119	4.262103	5.087271
H	-1.646010	5.469696	2.877856
H	-0.787410	3.324847	0.087507
H	-0.369492	5.022037	0.454259
H	1.513704	2.582733	0.359424
H	1.148665	2.300167	-1.916431
H	0.822066	4.809470	-3.479478
H	-0.863968	3.331214	-4.888186
H	2.951570	4.027170	-4.228582
H	1.792518	3.565007	-5.501472
H	4.357615	2.269066	-5.312158
H	4.000791	0.580537	-4.987524
H	5.280306	4.193431	1.881300
H	4.192337	5.511814	2.475481
H	5.421983	3.391564	4.035577
H	4.324340	4.336523	6.869156
H	3.101464	3.063589	6.608764
H	4.839873	2.763053	6.156142
H	-1.483993	0.302422	-1.034282
H	-1.063575	-1.295567	-0.348485
H	-0.167035	-0.115227	-3.076952
H	-2.011371	-2.279563	-2.190609
H	-2.922232	-3.292466	-4.917901
H	-3.985211	-1.854535	-4.973344
H	-3.754352	-2.745156	-3.404573
H	2.030509	-0.617682	-3.480927
H	5.850865	-0.993771	-0.286472
H	4.448234	-0.443753	0.722033
H	4.910357	-2.199338	0.638403
H	3.052485	-0.805834	-1.081380
H	3.645971	-2.447599	-4.094420
H	2.700277	-3.558148	-3.026480
H	2.532760	5.310137	0.855527

C112D/M121L: QM/MM Bidentate

C	38.029545	30.235725	44.457716
H	37.692668	29.184156	44.494452
C	37.683172	30.830806	43.107920
O	36.665030	31.498139	42.829094
N	38.602583	30.601039	42.118169
H	39.392407	29.977351	42.277457
C	38.336595	31.053612	40.774079
H	38.106994	32.133979	40.777865
H	39.240776	30.897190	40.159485
C	37.188125	30.277031	40.129899

O	37.077193	29.051050	40.322078
N	36.379502	30.990449	39.314683
H	36.487231	32.017060	39.232841
C	35.345394	30.344051	38.525217
H	35.589538	29.267717	38.510427
C	33.917673	30.565062	39.085094
H	33.662566	31.622176	38.905870
H	33.228010	29.949562	38.475154
C	33.690148	30.299321	40.549708
N	34.207441	29.248940	41.296494
C	32.866449	31.039952	41.379044
H	32.297923	31.941840	41.161242
C	33.720424	29.359426	42.534947
H	33.954497	28.697572	43.370609
N	32.899789	30.440517	42.624192
H	32.360070	30.751366	43.451279
C	35.390934	30.928151	37.101410
O	35.463341	32.151901	36.938199
N	35.323448	30.020074	36.097070
H	35.128271	29.043711	36.335345
C	34.952342	30.367069	34.736738
H	34.836537	31.471690	34.706394
C	36.033653	29.983018	33.694893
H	35.607488	30.047605	32.668991
H	36.872799	30.700832	33.704642
C	36.525264	28.553282	33.902433
O	35.753551	27.713120	34.412214
N	37.773194	28.227505	33.512964
H	38.474088	28.874204	33.138776
H	38.060363	27.237308	33.616884
C	33.530208	29.759864	34.420548
O	32.955402	29.139054	35.305415
C	30.753765	24.278980	33.953746
H	30.118882	24.387944	34.850182
C	31.955652	25.171274	34.150528
O	32.331340	26.022955	33.336700
N	32.579739	24.967241	35.355693
H	32.123475	24.324529	36.005926
C	33.702672	25.717936	35.882716
H	33.909490	26.548928	35.185976
C	33.256041	26.225769	37.262832
H	32.402924	26.910046	37.118361
H	32.854754	25.348681	37.814932
C	34.199466	26.869945	38.244386
O	35.443906	26.626193	38.361775
O	33.645643	27.635345	39.112410
C	34.881298	24.739141	35.959775
O	34.776969	23.695298	36.629002
N	35.967072	25.063612	35.210043
H	36.005833	26.004972	34.761539
C	37.105563	24.189937	35.168556
H	36.746046	23.156285	35.341309
C	38.179404	24.417549	36.250235
O	39.233918	23.776922	36.247494
N	37.861183	25.290197	37.259457
H	36.918119	25.693964	37.354729
C	38.777894	25.399904	38.361228
H	39.779890	25.591135	37.956455
C	37.342666	20.332872	41.663446
H	37.227397	19.233115	41.576106
H	37.638475	20.480949	42.723795
C	35.955723	20.930648	41.532252
O	34.910702	20.395211	41.951868
N	35.878475	22.183704	40.966135
H	36.730007	22.631839	40.610855
C	34.671636	22.979098	41.121004
H	34.294472	22.870971	42.160287

C	34.957511	24.461007	40.842361
H	35.462139	24.571300	39.860016
H	33.984653	24.975269	40.741630
C	35.743367	25.166504	41.915032
N	35.900991	26.550699	41.869212
C	36.388723	24.695453	43.048877
H	36.511467	23.686649	43.443202
C	36.619539	26.901894	42.941107
H	36.956420	27.911284	43.176585
N	36.926476	25.805418	43.680999
H	37.530523	25.791290	44.518887
C	33.509807	22.470506	40.230699
O	32.364564	22.778576	40.593643
C	29.212048	21.827166	41.920998
H	28.279079	21.277460	42.145694
C	28.745521	22.953433	41.028342
O	27.539083	23.236020	40.868629
N	29.707132	23.699336	40.381031
H	30.676251	23.354622	40.380075
C	29.382822	24.816720	39.505946
H	28.374826	25.163957	39.808290
C	30.402814	25.956760	39.561617
H	31.382563	25.567436	39.230825
H	30.111218	26.703885	38.801851
C	30.534819	26.633623	40.949239
H	29.688602	26.288876	41.572633
C	31.822487	26.185545	41.646715
H	31.921145	26.654664	42.640855
H	31.861306	25.087354	41.768925
H	32.697134	26.513004	41.055269
C	30.480223	28.167218	40.842422
H	30.560742	28.644258	41.840590
H	31.314639	28.538667	40.217396
H	29.533847	28.507451	40.384829
C	29.259534	24.189795	38.079870
O	30.256380	24.144537	37.356023
H	39.111145	30.291785	44.655877
H	37.516433	30.780990	45.254538
H	33.176608	29.990473	33.490426
H	30.243721	24.628068	33.042560
H	31.009132	23.218942	33.872308
H	37.608863	24.197127	34.197906
H	38.532620	26.212907	39.049988
H	38.836690	24.425812	38.869009
H	38.170062	20.673110	41.021634
H	33.732823	21.886049	39.423225
H	29.958479	21.126851	41.515207
H	29.536721	22.170452	42.907034
H	28.354010	23.790750	37.826630
Cu	35.152648	27.712794	40.425016

C112D/M121L: QM/MM Monodentate

C	38.029545	30.235725	44.457716
H	37.683376	29.187359	44.483737
C	37.677087	30.850638	43.118811
O	36.629399	31.473530	42.842431
N	38.618280	30.704188	42.136442
H	39.420004	30.089680	42.271174
C	38.307544	31.154131	40.800953
H	38.033516	32.222470	40.819662
H	39.202147	31.037814	40.163297
C	37.175765	30.325955	40.191213
O	37.108454	29.107255	40.440448
N	36.344096	30.979579	39.348272
H	36.443861	32.000431	39.209379

C	35.386531	30.266051	38.519256
H	35.683300	29.201584	38.527325
C	33.903030	30.419395	38.973443
H	33.555105	31.414756	38.648170
H	33.310550	29.675396	38.404195
C	33.607535	30.317598	40.442088
N	34.090382	29.341364	41.297176
C	32.767343	31.143214	41.171226
H	32.231635	32.037340	40.854803
C	33.567348	29.571449	42.505674
H	33.772324	28.996102	43.410657
N	32.757891	30.660287	42.468321
H	32.206952	31.022916	43.267528
C	35.453689	30.847049	37.094932
O	35.519421	32.074017	36.932863
N	35.358083	29.944374	36.089662
H	35.283402	28.945887	36.323528
C	34.970831	30.321053	34.741094
H	34.865197	31.427972	34.743360
C	36.041461	29.964790	33.679771
H	35.609530	30.050801	32.658175
H	36.879442	30.683687	33.704858
C	36.528158	28.530761	33.861225
O	35.732477	27.680647	34.310265
N	37.792582	28.214805	33.519953
H	38.508560	28.864680	33.180893
H	38.071194	27.220645	33.614289
C	33.530208	29.759864	34.420548
O	32.921448	29.184370	35.310620
C	30.753765	24.278979	33.953745
H	30.112378	24.379890	34.847044
C	31.953974	25.176500	34.177795
O	32.367073	25.985908	33.337505
N	32.526988	25.042156	35.419769
H	32.069789	24.406150	36.076644
C	33.704027	25.742059	35.906493
H	33.916841	26.574013	35.213814
C	33.375890	26.238935	37.326052
H	32.544613	26.966164	37.262023
H	32.991382	25.381953	37.911966
C	34.503357	26.865743	38.149381
O	35.644961	27.075570	37.673159
O	34.130593	27.155044	39.350323
C	34.871097	24.737476	35.941628
O	34.762156	23.691123	36.608744
N	35.958617	25.055722	35.193760
H	35.997115	25.996341	34.743758
C	37.105563	24.189937	35.168556
H	36.751116	23.154615	35.341776
C	38.175859	24.412999	36.253974
O	39.212245	23.741377	36.268574
N	37.865603	25.292630	37.254433
H	36.993472	25.849299	37.250221
C	38.777894	25.399904	38.361228
H	39.784799	25.593269	37.967647
C	37.342667	20.332872	41.663446
H	37.241333	19.230623	41.586027
H	37.636117	20.489397	42.723495
C	35.952499	20.912443	41.531394
O	34.913001	20.376470	41.963466
N	35.869897	22.157702	40.953196
H	36.721412	22.605819	40.597663
C	34.671935	22.959517	41.128554
H	34.294303	22.823716	42.164557
C	34.987578	24.442959	40.903959
H	35.501556	24.572626	39.927998
H	34.036353	24.994372	40.814155

C	35.798774	25.070096	42.006864
N	35.998024	26.447725	42.031433
C	36.440262	24.523306	43.109544
H	36.542313	23.492266	43.447458
C	36.731801	26.723040	43.117349
H	37.094415	27.708305	43.411677
N	37.011686	25.583819	43.794538
H	37.627547	25.534025	44.627599
C	33.509807	22.470506	40.230699
O	32.364252	22.781947	40.590848
C	29.212048	21.827166	41.920998
H	28.278353	21.278186	42.143919
C	28.750102	22.951917	41.024940
O	27.544576	23.231910	40.853260
N	29.714236	23.702163	40.382779
H	30.685779	23.361841	40.387197
C	29.385777	24.816827	39.509337
H	28.375131	25.157414	39.810056
C	30.396097	25.965819	39.556116
H	31.377275	25.594752	39.209854
H	30.081316	26.711528	38.804281
C	30.533763	26.640545	40.943811
H	29.682419	26.307367	41.566481
C	31.819830	26.183597	41.639378
H	31.927244	26.659577	42.630040
H	31.845288	25.086183	41.771447
H	32.691301	26.489940	41.032718
C	30.490215	28.174086	40.834587
H	30.582118	28.651651	41.831384
H	31.323084	28.543557	40.205465
H	29.543827	28.521960	40.382734
C	29.259534	24.189795	38.079870
O	30.251751	24.141672	37.353501
H	39.111145	30.291784	44.655877
H	37.516433	30.780990	45.254538
H	33.176608	29.990473	33.490426
H	30.243721	24.628068	33.042560
H	31.009132	23.218942	33.872309
H	37.608863	24.197127	34.197906
H	38.532620	26.212907	39.049988
H	38.836690	24.425812	38.869009
H	38.170062	20.673110	41.021634
H	33.732824	21.886049	39.423225
H	29.958479	21.126851	41.515207
H	29.536721	22.170452	42.907034
H	28.354010	23.790750	37.826630
Cu	35.206507	27.801843	40.869280

C112D/M121L: SORCI (QM/MM Monodentate)

C	0.924631	-0.300740	3.123839
O	0.000737	0.006085	2.346571
N	1.729160	-1.376515	2.966000
H	2.437702	-1.554671	3.680105
C	1.469616	-2.376965	1.943725
C	2.463230	-2.341862	0.742855
H	3.408550	-2.839127	1.035174
H	2.026137	-2.972467	-0.057494
C	2.831242	-0.999718	0.179094
N	1.944011	0.018192	-0.127516
C	4.101796	-0.577218	-0.176419
H	5.070595	-1.073973	-0.098276
C	2.652946	1.026948	-0.644033
H	2.249305	1.976639	-1.002605
N	3.969938	0.701809	-0.688728
H	4.722328	1.291440	-1.045767

C	-1.059267	-3.774979	-1.707907
C	-0.961407	-2.729156	-0.594976
O	-1.480152	-2.900884	0.534402
O	-0.283393	-1.692160	-0.955309
C	-2.342218	1.448629	-1.244693
N	-1.299950	1.428969	-0.321949
C	-2.906238	2.716706	-1.229066
H	-3.739553	3.144177	-1.789416
C	-1.234479	2.648058	0.228471
H	-0.549617	2.950739	1.023631
N	-2.186901	3.452640	-0.300944
H	-2.366315	4.422201	-0.037235
Cu	-0.000864	0.007940	0.000212
H	-2.608901	0.571751	-1.836526
H	1.517990	-3.381679	2.403641
H	0.426522	-2.240610	1.608954
H	-1.632623	-4.647089	-1.344882
H	-0.051149	-4.102115	-2.025319
H	-1.563025	-3.347769	-2.595348
H	1.150858	0.308265	4.029901

C112D/M121F: X-ray Diffraction

C	4.666106	6.640402	2.786158
C	4.167011	6.357741	1.336368
O	3.059386	6.768176	0.968836
N	4.954172	5.580671	0.571499
C	4.568199	5.267788	-0.814612
C	3.403818	4.266241	-0.836086
O	3.266432	3.433653	0.078808
N	2.559716	4.314472	-1.859209
C	1.551101	3.248167	-1.983193
C	1.613935	2.722302	-3.428845
O	1.912229	3.496938	-4.379238
C	0.085667	3.711090	-1.782830
C	-0.170516	4.560657	-0.557848
N	0.166038	4.177812	0.738363
C	-0.847894	5.730568	-0.445080
C	-0.253897	5.108518	1.586915
N	-0.853022	6.074736	0.887929
N	1.360173	1.421838	-3.587063
C	1.073249	0.848734	-4.908127
C	-0.226872	0.095987	-4.843605
O	-0.818684	-0.044324	-3.741951
C	2.230698	-0.031912	-5.517058
C	2.703358	-1.131896	-4.537195
O	2.000269	-1.373430	-3.573430
N	3.842487	-1.855407	-4.842634
C	-3.013206	-4.559746	-1.833222
C	-1.826706	-3.692044	-2.216181
O	-1.408064	-3.658890	-3.361958
N	-1.301341	-3.012191	-1.183304
C	-0.128114	-2.148497	-1.214245
C	1.051782	-2.956519	-0.652006
O	0.927934	-3.554752	0.485536
C	-0.443823	-1.044060	-0.284408
C	0.559573	0.084580	-0.276235
O	1.693455	-0.009291	-0.802853
O	0.166190	1.101941	0.341509
N	2.148215	-3.036747	-1.397508
C	3.285012	-3.844617	-0.883180
C	4.373739	-2.992986	-0.186976
O	5.434354	-3.532451	0.196281
N	4.155532	-1.689405	-0.013773
C	5.080850	-0.891517	0.803578
C	3.475780	-2.869154	6.582279
C	2.121900	-2.412260	6.084390

O	1.133247	-2.584882	6.764942
N	2.061508	-1.903674	4.845971
C	0.862817	-1.216988	4.402422
C	-0.215283	-2.218565	4.033767
O	-1.418489	-1.854722	3.974762
C	1.177724	-0.222717	3.229625
C	1.912053	0.990756	3.675601
N	2.078789	2.105980	2.884460
C	2.541580	1.272161	4.851117
C	2.779417	3.011904	3.524623
N	3.090724	2.526364	4.717589
C	-4.345353	-1.591736	6.320123
C	-4.941211	-1.417479	4.910848
O	-6.141372	-1.216757	4.801906
N	-4.128428	-1.484701	3.848967
C	-4.744139	-1.313644	2.511724
C	-4.726262	-2.534269	1.682170
O	-3.678111	-2.862223	1.067845
C	-4.119536	-0.223400	1.659565
C	-4.723471	-0.191099	0.235897
C	-4.004873	-0.637210	-0.853879
C	-6.029757	0.225934	0.031797
C	-4.544556	-0.611284	-2.154697
C	-6.602402	0.240813	-1.248985
C	-5.847825	-0.175267	-2.353749
Cu	1.242344	2.579274	1.143541
H	-3.000289	-1.049570	-0.715351
H	-3.921860	-0.945955	-3.001168
H	-6.287657	-0.158832	-3.365236
H	-7.642555	0.582871	-1.379647
H	-6.635370	0.575606	0.887765
H	-3.023891	-0.385862	1.585336
H	-4.275148	0.758700	2.160553
H	-5.801120	-1.059746	2.744252
H	-5.638022	-3.188704	1.623800
H	-3.135895	-1.749573	3.915800
H	-3.236275	-1.655441	6.331660
H	-4.769792	-2.515296	6.768811
H	-4.679236	-0.735615	6.942321
H	3.096306	3.985041	3.129514
H	3.620550	3.009389	5.449205
H	2.674420	0.690212	5.769664
H	1.735616	-0.756487	2.424186
H	0.213326	0.086283	2.771242
H	0.435800	-0.636316	5.251315
H	0.097120	-3.271525	3.803607
H	2.917305	-1.798486	4.294299
H	4.328257	-2.652318	5.901954
H	3.435858	-3.964804	6.762786
H	3.670364	-2.393743	7.567576
H	4.931184	7.716825	2.873439
H	3.819552	6.460288	3.480812
H	5.547190	6.035857	3.093698
H	5.846394	5.229777	0.922989
H	5.445506	4.818974	-1.327424
H	4.285761	6.201641	-1.346764
H	2.709026	4.887075	-2.700954
H	1.818826	2.444293	-1.269161
H	-0.230108	4.300125	-2.670308
H	-0.548746	2.798164	-1.745026
H	1.240016	0.800381	-2.769954
H	0.958592	1.712621	-5.604275
H	-0.632833	-0.348653	-5.793245
H	3.072561	0.635038	-5.807123
H	1.872913	-0.516414	-6.455454
H	-1.418332	-0.588388	-0.539455
H	-0.539305	-1.433875	0.754549

H	0.043700	-1.822277	-2.257584
H	2.210381	-2.490201	-2.281600
H	3.763152	-4.416492	-1.705876
H	2.877546	-4.554197	-0.136061
H	3.271864	-1.250625	-0.334086
H	6.110464	-0.939639	0.387718
H	4.725616	0.158852	0.805506
H	5.128514	-1.280611	1.846009
H	-1.687179	-3.201411	-0.249909
H	-2.681342	-5.621023	-1.779491
H	-3.776485	-4.496299	-2.636118
H	-3.463928	-4.268452	-0.860683
H	-1.297304	6.383535	-1.202652
H	-1.274072	6.924567	1.273649
H	-0.124035	5.109458	2.675637
H	4.431889	-1.626173	-5.646378
H	4.137485	-2.613435	-4.221159

C112D/M121F: QM/MM Bidentate

C	39.073276	39.559252	37.260771
H	38.975166	38.637549	37.864209
C	38.593933	39.236008	35.868875
O	37.571344	39.670679	35.323112
N	39.398861	38.368223	35.159441
H	40.205277	37.920192	35.591849
C	39.025813	38.007594	33.817409
H	38.803339	38.923742	33.246276
H	39.872684	37.488522	33.330949
C	37.805987	37.077336	33.758922
O	37.600043	36.285173	34.700762
N	37.072831	37.133876	32.621314
H	37.289944	37.873899	31.929707
C	36.003159	36.190225	32.328378
H	36.077574	35.380344	33.074965
C	34.584525	36.817409	32.366667
H	34.506843	37.555404	31.545339
H	33.870963	35.999677	32.127847
C	34.215278	37.469585	33.660890
N	34.449923	36.891352	34.904119
C	33.574566	38.683779	33.851755
H	33.248625	39.449383	33.147175
C	33.951013	37.736981	35.810166
H	33.908569	37.583390	36.881326
N	33.423649	38.829772	35.216301
H	33.058194	39.643420	35.727474
C	36.140264	35.610461	30.912946
O	36.293752	36.366440	29.948789
N	35.971245	34.264896	30.813014
H	35.775993	33.724914	31.664998
C	35.627301	33.639388	29.546899
H	35.523893	34.471705	28.815305
C	36.740149	32.733140	28.959411
H	36.325642	32.197926	28.075973
H	37.562384	33.358903	28.569610
C	37.236627	31.697467	29.963883
O	36.419750	31.210802	30.771953
N	38.534011	31.316857	29.921181
H	39.249309	31.716282	29.303038
H	38.834136	30.560176	30.562136
C	34.200804	32.990615	29.641828
O	33.581851	33.044663	30.703079
C	31.427470	28.336863	32.689449
H	30.762009	28.898755	33.375239
C	32.527983	29.279952	32.268942
O	32.619923	29.706936	31.112637

N	33.368089	29.697840	33.276288
H	33.138933	29.391891	34.224197
C	34.345508	30.783279	33.193534
H	34.531348	30.984358	32.124840
C	33.737363	32.007154	33.910943
H	32.995981	32.458973	33.224319
H	33.176982	31.650090	34.793767
C	34.601239	33.141222	34.406776
O	35.771726	33.403323	34.001671
O	34.041368	33.904891	35.286791
C	35.594821	30.243885	33.899039
O	35.626387	30.211154	35.147672
N	36.556379	29.738300	33.088089
H	36.582299	30.078384	32.100740
C	37.712749	29.056544	33.615798
H	37.406289	28.410240	34.459453
C	38.854014	29.983846	34.181265
O	39.983647	29.556090	34.342394
N	38.531567	31.279141	34.566484
H	37.567052	31.613801	34.532317
C	39.504120	32.041035	35.333324
H	40.489287	31.898085	34.874347
C	37.882658	30.059635	41.087238
H	37.850816	29.172615	41.754018
H	38.147056	30.909712	41.747486
C	36.494848	30.281712	40.526611
O	35.462224	29.769063	41.006036
N	36.458926	31.099234	39.427248
H	37.348864	31.403569	39.017392
C	35.233382	31.727669	38.954254
H	34.770912	32.323445	39.770659
C	35.487600	32.631550	37.740856
H	36.022121	32.059151	36.953820
H	34.512484	32.897629	37.293446
C	36.225961	33.880368	38.093570
N	36.457567	34.887571	37.167073
C	36.789202	34.248771	39.303781
H	36.820266	33.755492	40.275622
C	37.175430	35.827617	37.789273
H	37.586574	36.722818	37.317371
N	37.375448	35.479625	39.088386
H	37.899529	35.990245	39.804120
C	34.201401	30.695581	38.528707
O	33.012912	31.036197	38.539610
C	30.042792	31.345807	40.799365
H	29.178959	31.006759	41.383291
C	29.535640	31.197689	39.337249
O	28.549355	30.486268	39.069101
N	30.223812	31.779661	38.288788
H	31.195457	32.066048	38.431626
C	29.714626	31.780595	36.909429
H	28.663894	32.132529	36.951378
C	30.566207	32.748941	36.057912
H	30.555779	33.745585	36.542083
H	31.611381	32.386763	36.057258
C	30.041264	32.857405	34.638767
C	30.446932	31.980718	33.608991
H	31.189419	31.206831	33.817893
C	29.057248	33.818711	34.343375
H	28.747438	34.492846	35.148119
C	29.890366	32.066069	32.324935
H	30.255595	31.391771	31.538954
C	28.468703	33.892017	33.070852
H	27.676382	34.626753	32.875214
C	28.882770	33.007681	32.062875
H	28.395038	33.018868	31.084406
C	29.683124	30.365969	36.169644

O	30.744661	29.888890	35.767551
H	40.139010	39.830629	37.207535
H	38.510457	40.375699	37.721393
H	33.807889	32.690150	28.748140
H	30.887551	28.049072	31.774064
H	31.760065	27.451951	33.238844
H	38.205845	28.436651	32.862065
H	39.207436	33.093403	35.338194
H	39.529648	31.620195	36.349393
H	38.642656	29.955322	40.297435
H	34.498769	29.757729	38.254213
H	30.855036	30.603129	40.830292
H	30.431294	32.293045	41.183201
H	28.802806	29.849920	36.124111
Cu	35.506441	35.260055	35.417535

C112D/M121F: QM/MM Monodentate

C	39.073276	39.559252	37.260771
H	38.972637	38.636098	37.861590
C	38.594244	39.244462	35.868267
O	37.553351	39.656064	35.337907
N	39.421346	38.415219	35.143858
H	40.228079	37.966567	35.574747
C	39.022457	38.026337	33.817640
H	38.788071	38.929914	33.232773
H	39.859993	37.499263	33.323623
C	37.804111	37.095132	33.817071
O	37.600159	36.347261	34.792963
N	37.062148	37.099120	32.681802
H	37.269425	37.800897	31.951465
C	36.026040	36.109722	32.422558
H	36.168005	35.294792	33.156929
C	34.575777	36.669499	32.496931
H	34.425032	37.332999	31.623517
H	33.894698	35.803196	32.360477
C	34.209883	37.432167	33.730855
N	34.412092	36.974979	35.029112
C	33.576892	38.663886	33.796810
H	33.265775	39.361983	33.018585
C	33.902392	37.904386	35.845771
H	33.824991	37.851968	36.927682
N	33.402160	38.938109	35.137458
H	33.030627	39.796552	35.558788
C	36.149537	35.569927	30.985622
O	36.288284	36.359514	30.044277
N	35.986308	34.227728	30.845225
H	35.870271	33.647013	31.686617
C	35.634108	33.632557	29.566626
H	35.533676	34.482222	28.854706
C	36.741571	32.732601	28.959200
H	36.321081	32.204827	28.074013
H	37.561791	33.361704	28.570397
C	37.243680	31.690149	29.954092
O	36.429025	31.197480	30.759909
N	38.542151	31.313514	29.908972
H	39.257192	31.717271	29.293480
H	38.843562	30.556703	30.548860
C	34.200804	32.990615	29.641828
O	33.564514	33.051899	30.691584
C	31.427470	28.336863	32.689449
H	30.758771	28.894075	33.376555
C	32.520843	29.286735	32.272066
O	32.643080	29.672660	31.103549
N	33.311664	29.763124	33.290026
H	33.089629	29.463246	34.241732

C	34.349600	30.783284	33.176999
H	34.538079	30.952548	32.103925
C	33.852241	32.062267	33.879660
H	33.133876	32.569845	33.209042
H	33.298483	31.778350	34.792320
C	34.893046	33.094669	34.292774
O	36.058381	33.104837	33.834605
O	34.409835	33.960647	35.131423
C	35.570761	30.194972	33.890134
O	35.552892	30.095488	35.133534
N	36.558467	29.732726	33.085650
H	36.596835	30.096849	32.107683
C	37.712749	29.056544	33.615798
H	37.407968	28.413980	34.462421
C	38.848550	29.989909	34.183177
O	39.974378	29.554717	34.365727
N	38.525649	31.280780	34.569139
H	37.605236	31.694739	34.382450
C	39.504120	32.041035	35.333324
H	40.491699	31.899715	34.877583
C	37.882658	30.059635	41.087238
H	37.854460	29.175043	41.757299
H	38.144402	30.912455	41.744930
C	36.494891	30.277011	40.526917
O	35.461354	29.772751	41.012487
N	36.459030	31.085370	39.420458
H	37.348320	31.377620	38.999825
C	35.234817	31.723021	38.956137
H	34.775526	32.308157	39.782127
C	35.497166	32.650406	37.760474
H	36.042668	32.098128	36.966878
H	34.529130	32.927881	37.304920
C	36.240354	33.880944	38.166940
N	36.501652	34.928727	37.294645
C	36.793775	34.185096	39.398938
H	36.804184	33.645471	40.345912
C	37.229370	35.827418	37.970104
H	37.660617	36.737908	37.547152
N	37.404013	35.413479	39.251756
H	37.931008	35.873047	40.006945
C	34.201401	30.695580	38.528706
O	33.013890	31.040412	38.534124
C	30.042792	31.345807	40.799366
H	29.178802	31.006895	41.383133
C	29.534987	31.200221	39.338461
O	28.542207	30.498989	39.068962
N	30.231669	31.775428	38.291001
H	31.213930	32.025350	38.432011
C	29.727487	31.782765	36.910509
H	28.680627	32.146319	36.949142
C	30.597276	32.739796	36.064485
H	30.604679	33.733850	36.554242
H	31.634352	32.352988	36.062536
C	30.077238	32.862543	34.644902
C	30.511302	32.012086	33.605459
H	31.281085	31.262568	33.807114
C	29.067916	33.801347	34.361375
H	28.736996	34.457562	35.173226
C	29.950797	32.094340	32.322327
H	30.329954	31.436258	31.528901
C	28.480884	33.874419	33.088000
H	27.670087	34.590511	32.898745
C	28.918391	33.011884	32.070897
H	28.431359	33.025363	31.091850
C	29.683124	30.365969	36.169644
O	30.740240	29.884723	35.763815
H	40.139010	39.830629	37.207535

H	38.510457	40.375699	37.721393
H	33.807889	32.690150	28.748140
H	30.887551	28.049072	31.774064
H	31.760065	27.451951	33.238844
H	38.205845	28.436651	32.862065
H	39.207436	33.093403	35.338194
H	39.529648	31.620195	36.349393
H	38.642656	29.955322	40.297435
H	34.498769	29.757729	38.254213
H	30.855036	30.603129	40.830292
H	30.431295	32.293045	41.183200
H	28.802806	29.849920	36.124111
Cu	35.504826	35.473446	35.683932

C112D/M121F: SORCI (QM/MM Monodentate)

C	0.788936	-0.939710	3.264853
O	-0.029411	-0.329525	2.552748
N	1.391710	-2.041664	2.835931
C	0.945326	-2.630992	1.561915
C	1.987361	-2.571810	0.416227
C	2.638183	-1.224821	0.192564
N	1.930055	-0.046662	-0.032152
C	3.950241	-0.914320	0.043100
C	2.790601	0.938257	-0.260175
N	4.026747	0.439306	-0.196138
C	-2.171522	-2.563067	-2.383899
C	-1.648733	-2.066855	-1.056810
O	-2.161446	-2.390701	0.040493
O	-0.685642	-1.271389	-1.162039
C	-2.148873	2.155375	-0.620919
N	-1.118447	1.745368	0.196116
C	-2.391535	3.454603	-0.288578
C	-0.758206	2.723850	0.992474
N	-1.526819	3.771645	0.733266
Cu	-0.026702	0.084016	0.146605
H	-0.010489	2.670227	1.786719
H	-1.491416	4.676937	1.204560
H	-3.118623	4.177246	-0.664800
H	-2.602595	1.507745	-1.371492
H	2.010229	-2.568343	3.454784
H	0.698086	-3.695383	1.740897
H	-0.003992	-2.146550	1.287743
H	2.794699	-3.305809	0.601997
H	1.476981	-2.893017	-0.513178
H	4.849599	-1.529312	0.119124
H	4.890677	0.958871	-0.358332
H	2.546139	1.981537	-0.470931
H	-2.887641	-1.824912	-2.794932
H	-1.352121	-2.682214	-3.116217
H	-2.706306	-3.522691	-2.258873
H	1.053807	-0.605109	4.294681