

Supplementary material

Capturing and analyzing the excited state structure of a Cu(I) phenanthroline complex by time-resolved diffraction and theoretical calculations

Ivan I. Vorontsov,^{1,1} Tim Graber,² Andrey Yu. Kovalevsky,^{1,2} Irina V.
Novozhilova,¹³ Milan Gembicky,¹ Yu-Sheng Chen,^{3,4} and Philip
Coppens^{1*}

¹*Department of Chemistry, State University of New York at Buffalo,
New York, 14260, USA,* ²*University of Chicago, Illinois, 60637, USA,*
³*University of Toledo, Ohio, 43606, USA*

¹ current address: Department of Biochemistry and Molecular Biophysics , University of Arizona, Tucson, AZ 85721, USA

² current address: Bioscience Division, Group B-8, Los Alamos National Laboratory, Los Alamos, NM 87545

³ current address: Department of Chemistry, Box 68,, Middle Tennessee State University, Murfreesboro, TN 37132.

⁴ current address: ChemMatCARS, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439

Table S1. Final fractional atomic coordinates ($\times 10^4$) in ground and excited states.

	Ground-state reference structure			Excited-state structure		
	x	y	z	x	y	z
Cu(1)	249	7556	1063	290	7732	1059
N(1)	-438	7405	459	-487	7525	520
N(2)	783	6588	652	749	6730	609
C(1)	-1031	7828	364	-1087	7937	475
C(2)	-1439	7636	-80	-1561	7710	74
C(3)	-1230	7040	-446	-1414	7086	-302
C(4)	-591	6607	-365	-770	6663	-275
C(5)	-321	5989	-731	-564	6018	-656
C(6)	299	5607	-640	62	5647	-618
C(7)	693	5787	-174	526	5865	-193
C(8)	1337	5403	-58	1180	5494	-133
C(9)	1672	5606	395	1584	5734	284
C(10)	1390	6212	751	1364	6365	656
C(11)	434	6377	197	331	6482	192
C(12)	-219	6797	96	-329	6891	147
C(13)	-1245	8542	750	-1237	8680	868
C(14)	1771	6449	1245	1819	6643	1109
P(1)	742	9000	1255	757	9224	1264
P(2)	109	7290	1878	133	7511	1891
C(15)	950	8960	1944	943	9214	1956
C(16)	404	8425	2207	398	8668	2213
C(17)	1490	9357	965	1509	9600	986
C(18)	1884	10157	1120	1883	10420	1140
C(19)	2370	10496	827	2374	10768	853
C(20)	2463	10032	370	2490	10293	404
C(21)	2089	9214	218	2136	9457	254
C(22)	1606	8871	518	1648	9106	547
C(23)	229	10084	1127	227	10285	1117
C(24)	-152	10531	1476	-174	10728	1453
C(25)	-578	11297	1331	-611	11473	1293
C(26)	-639	11637	834	-662	11794	793

C(27)	-263	11192	483	-265	11352	455
C(28)	168	10428	627	176	10610	613
C(29)	649	6318	2137	684	6569	2170
C(30)	488	5368	1961	546	5607	2001
C(31)	908	4586	2098	976	4846	2153
C(32)	1487	4738	2412	1543	5030	2476
C(33)	1639	5665	2592	1672	5968	2649
C(34)	1225	6462	2456	1247	6745	2498
C(35)	-669	7029	2150	-650	7230	2151
C(36)	-1221	6717	1842	-1187	6887	1837
C(37)	-1823	6520	2045	-1793	6674	2030
C(38)	-1867	6675	2560	-1857	6843	2541
C(39)	-1316	6967	2872	-1321	7166	2859
C(40)	-715	7128	2671	-715	7344	2669
Cu(2)	4773	2585	3878	4783	2385	3860
N(3)	5629	2310	4345	5632	2061	4310
N(4)	4350	1790	4428	4345	1569	4384
C(1A)	6263	2551	4292	6269	2289	4262
C(2A)	6783	2274	4652	6785	1970	4615
C(3A)	6654	1791	5085	6649	1457	5037
C(4A)	5988	1572	5159	5981	1249	5107
C(5A)	5803	1092	5609	5789	739	5546
C(6A)	5162	864	5660	5145	524	5593
C(7A)	4650	1081	5262	4636	786	5201
C(8A)	3979	831	5296	3961	552	5230
C(9A)	3521	1047	4898	3507	811	4838
C(10A)	3715	1525	4465	3707	1318	4416
C(11A)	4811	1558	4820	4803	1294	4769
C(12A)	5499	1820	4775	5495	1541	4729
C(13A)	6411	3150	3840	6425	2920	3824
C(14A)	3205	1756	4039	3200	1596	3996
P(3)	4562	4206	3749	4573	4003	3683
P(4)	4680	2295	3037	4692	2026	3020
C(15A)	4636	4336	3060	4651	4068	2993
C(16A)	4318	3446	2773	4332	3155	2727
C(17A)	3746	4758	3814	3758	4569	3732
C(18A)	3664	5663	4045	3676	5495	3940
C(19A)	3029	6043	4079	3041	5884	3963

C(20A)	2469	5534	3880	2480	5362	3775
C(21A)	2544	4630	3652	2556	4436	3570
C(22A)	3179	4243	3622	3190	4041	3552
C(23A)	5140	5112	4042	5151	4930	3956
C(24A)	5244	6011	3815	5257	5805	3707
C(25A)	5652	6705	4064	5665	6518	3939
C(26A)	5961	6514	4544	5972	6369	4424
C(27A)	5858	5612	4769	5866	5491	4670
C(28A)	5455	4911	4518	5463	4770	4437
C(29A)	4131	1343	2754	4142	1054	2759
C(30A)	3962	559	3056	3971	301	3080
C(31A)	3557	-191	2852	3565	-464	2893
C(32A)	3330	-177	2342	3340	-495	2383
C(33A)	3498	602	2037	3512	253	2060
C(34A)	3892	1364	2241	3906	1029	2246
C(35A)	5429	2110	2709	5442	1803	2699
C(36A)	5918	1478	2922	5930	1187	2929
C(37A)	6485	1272	2682	6497	954	2696
C(38A)	6562	1708	2215	6577	1345	2219
C(39A)	6080	2334	1995	6097	1954	1982
C(40A)	5512	2538	2238	5528	2186	2219
P(5)	2881	1277	6444			
F(1)	1933	9749	3819			
F(2)	1178	8620	3495			
F(3)	2028	9077	3045			
F(4)	2019	7558	3390			
F(5)	2773	8681	3714			
F(6)	1925	8227	4163			
P(6)	1978	8676	3601			
F(7)	3013	161	6301			
F(8)	2815	1555	5847			
F(9)	2093	1076	6408			
F(10)	2756	2417	6568			
F(11)	2948	1028	7031			
F(12)	3670	1487	6469			

