Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary material

for

Angle isomerism, as exemplified in a five coordinate, dimeric copper(II) Schiff base complex. Observation of Ostwald ripening

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Coordinates of the optimised geometries of 1a and 1b at BP86/LanL2DZ level

1a at LanL2DZ/BP86
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.536155	-0.296692	1.722354
2	29	0	-1.405487	0.649020	0.722637
3	6	0	0.323260	3.117944	1.169286
4	1	0	1.102814	2.389272	1.412240
5	6	0	0.550083	4.511572	1.148182
6	1	0	1.539977	4.904693	1.396566
7	6	0	-0.525150	5.373759	0.807032
8	1	0	-0.375016	6.458476	0.776360
9	6	0	-1.789796	4.831763	0.506523
10	1	0	-2.644958	5.455425	0.232818
11	6	0	-1.963697	3.422414	0.558651
12	6	0	-4.253759	0.700656	0.194797
13	6	0	-3.898476	-0.681094	0.508533
14	6	0	-5.545395	1.180030	-0.369279
15	6	0	-6.211902	2.316365	0.169695
16	1	0	-5.771171	2.847675	1.018577
17	6	0	-7.430829	2.762904	-0.387697
18	1	0	-7.935760	3.636024	0.041925
19	6	0	-7.996016	2.093787	-1.500914
20	1	0	-8.938721	2.445811	-1.936156
21	6	0	-7.330011	0.973465	-2.055893
22	1	0	-7.751968	0.458154	-2.926536
23	6	0	-6.114489	0.520670	-1.496726
24	1	0	-5.595882	-0.338227	-1.937643
25	6	0	-4.874630	-1.801652	0.638601

26	6	0	-6.244401	-1.605182	0.978973
27	1	0	-6.638602	-0.594765	1.118093
28	6	0	-7.096437	-2.715825	1.165269
29	1	0	-8.145655	-2.552867	1.436508
30	6	0	-6.600260	-4.033432	1.011363
31	1	0	-7.267161	-4.892086	1.152730
32	6	0	-5.235017	-4.237397	0.688314
33	1	0	-4.842579	-5.255595	0.585099
34	6	0	-4.377872	-3.131805	0.514062
35	1	0	-3.312578	-3.270063	0.302880
36	7	0	-0.898384	2.590906	0.887065
37	7	0	-3.220958	2.858377	0.291596
38	7	0	-3.186662	1.528459	0.411510
39	8	0	-2.635906	-0.975513	0.758424
40	17	0	-0.536293	0.295946	-1.722281
41	29	0	1.405485	-0.649449	-0.722625
42	6	0	-0.322885	-3.118725	-1.168695
43	1	0	-1.102551	-2.390224	-1.411810
44	6	0	-0.549504	-4.512381	-1.147228
45	1	0	-1.539348	-4.905717	-1.395467
46	6	0	0.525867	-5.374324	-0.805900
47	1	0	0.375891	-6.459054	-0.774950
48	6	0	1.790445	-4.832069	-0.505567
49	1	0	2.645703	-5.455540	-0.231724
50	6	0	1.964135	-3.422710	-0.558049
51	6	0	4.253753	-0.700490	-0.194786
52	6	0	3.898235	0.681123	-0.508846
53	6	0	5.545476	-1.179486	0.369408
54	6	0	6.212108	-2.315957	-0.169120
55	1	0	5.771396	-2.847687	-1.017748
56	6	0	7.431132	-2.762085	0.388391
57	1	0	7.936162	-3.635315	-0.040889
58	6	0	7.996295	-2.092410	1.501284
59	1	0	8.939078	-2.444116	1.936614
60	6	0	7.330157	-0.971954	2.055838
61	1	0	7.752091	-0.456220	2.926242
62	6	0	6.114536	-0.519577	1.496557
63	1	0	5.595825	0.339429	1.937138
64	6	0	4.874202	1.801797	-0.639302
65	6	0	6.244005	1.605448	-0.979606
66	1	0	6.638384	0.595051	-1.118381
67	6	0	7.095851	2.716175	-1.166275
68	1	0	8.145097	2.553303	-1.437456
69	6	0	6.599448	4.033748	-1.012812
70	1	0	7.266202	4.892469	-1.154472
71	6	0	5.234169	4.237589	-0.689832
72	1	0	4.841551	5.255753	-0.586965
73	6	0	4.377215	3.131910	-0.515201
74	1	0	3.311898	3.270053	-0.304061
75	7	0	0.898695	-2.591447	-0.886659
76	7	0	3.221317	-2.858412	-0.291139
77	7	0	3.186796	-1.528527	-0.411318
78	8	0	2.635599	0.975277	-0.758756

1b at LanL2DZ/BP86
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.470459	-0.721068	0.403031
2	17	0	0.345522	0.003529	1.790263
3	7	0	-1.004382	-2.669548	0.321795
4	6	0	0.230664	-3.232022	0.417690
5	1	0	1.060891	-2.540656	0.590480
6	6	0	0.414846	-4.626593	0.286881
7	1	0	1.420335	-5.047230	0.373596
8	6	0	-0.717383	-5.447838	0.046222
9	1	0	-0.601667	-6.532631	-0.054072
10	6	0	-1.995104	-4.864958	-0.069187
11	1	0	-2.894732	-5.456397	-0.259206
12	6	0	-2.121427	-3.456856	0.066743
13	7	0	-3.381017	-2.846176	-0.055686
14	7	0	-3.286984	-1.520464	0.078716
15	6	0	-4.355025	-0.663093	0.088569
16	6	0	-3.906643	0.712806	0.260673
17	8	0	-2.638754	0.948255	0.548896
18	6	0	-4.780076	1.910327	0.101591
19	6	0	-5.852461	1.956812	-0.833953
20	1	0	-6.086723	1.078263	-1.442761
21	6	0	-6.599989	3.143899	-0.996003
22	1	0	-7.416376	3.174564	-1.726395
23	6	0	-6.297356	4.291047	-0.221517
24	1	0	-6.887380	5.207027	-0.343769
25	6	0	-5.227337	4.252630	0.707888
26	1	0	-4.990973	5.137561	1.310040
27	6	0	-4.465511	3.074772	0.859898
28	1	0	-3.625786	3.032004	1.562013
29	6	0	-5.769213	-1.124785	0.041218
30	6	0	-6.713099	-0.626913	0.985532
31	1	0	-6.389759	0.094030	1.744957
32	6	0	-6.199869	-2.088233	-0.914487
33	1	0	-5.479102	-2.498561	-1.628087
34	6	0	-7.544963	-2.518852	-0.941246
35	1	0	-7.862834	-3.256119	-1.687745
36	6	0	-8.479294	-2.008449	-0.006518
37	1	0	-9.521490	-2.348281	-0.026283
38	6	0	-8.055866	-1.063863	0.960133
39	1	0	-8.767685	-0.673184	1.696600
40	29	0	1.470396	0.721110	-0.402578
41	17	0	-0.345630	-0.003436	-1.789832
42	7	0	1.004394	2.669605	-0.321393
43	6	0	-0.230666	3.232097	-0.416980
44	1	0	-1.060981	2.540732	-0.589354
45	6	0	-0.414756	4.626700	-0.286387
46	1	0	-1.420261	5.047354	-0.372840
47	6	0	0.717583	5.447957	-0.046285
48	1	0	0.601937	6.532774	0.053825
49	6	0	1.995324	4.865059	0.068801
50	1	0	2.895036	5.456507	0.258391
51	6	0	2.121554	3.456926	-0.066884

52	7	0	3.381160	2.846223	0.055279
53	7	0	3.287034	1.520487	-0.078836
54	6	0	4.355039	0.663070	-0.088786
55	6	0	3.906560	-0.712844	-0.260501
56	8	0	2.638575	-0.948317	-0.548270
57	6	0	4.779988	-1.910361	-0.101362
58	6	0	5.852605	-1.956664	0.833923
59	1	0	6.087051	-1.077978	1.442464
60	6	0	6.600142	-3.143735	0.996052
61	1	0	7.416715	-3.174255	1.726242
62	6	0	6.297278	-4.291049	0.221903
63	1	0	6.887306	-5.207019	0.344215
64	6	0	5.227028	-4.252811	-0.707243
65	1	0	4.990487	-5.137873	-1.309134
66	6	0	4.465197	-3.074967	-0.859327
67	1	0	3.625294	-3.032334	-1.561237
68	6	0	5.769261	1.124706	-0.041836
69	6	0	6.712911	0.626650	-0.986288
70	1	0	6.389370	-0.094395	-1.745531
71	6	0	6.200180	2.088281	0.913622
72	1	0	5.479596	2.498751	1.627325
73	6	0	7.545298	2.518848	0.940007
74	1	0	7.863371	3.256216	1.686321
75	6	0	8.479392	2.008268	0.005140
76	1	0	9.521607	2.348062	0.024611
77	6	0	8.055701	1.063553	-0.961268
78	1	0	8.767332	0.672731	-1.697842