Supplementary Information for

Solid, solution and gas phase behaviour of mono- and dinuclear 2,6-diacetylpyridine (dap) hydrazone copper complexes probed by X-ray, mass spectrometry and theoretical calculations

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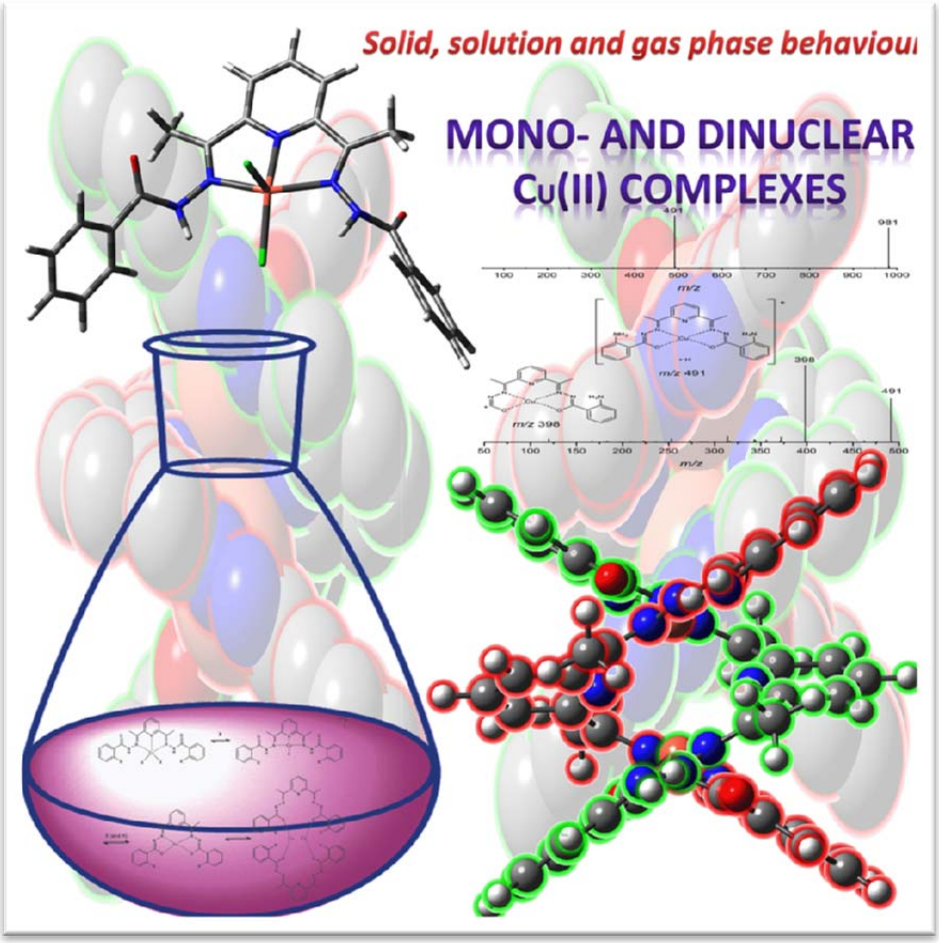

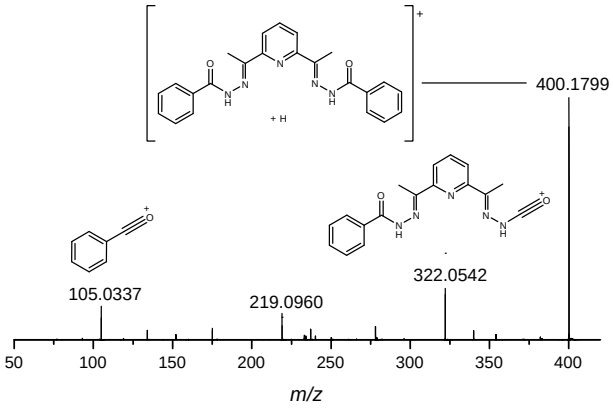

Figure S1. ESI(+)-MS/MS of **dapBH**.

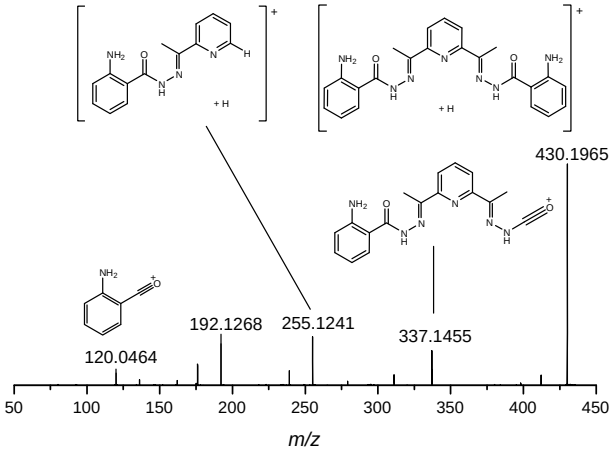

Figure S2. ESI(+)-MS/MS of **dapAH**.

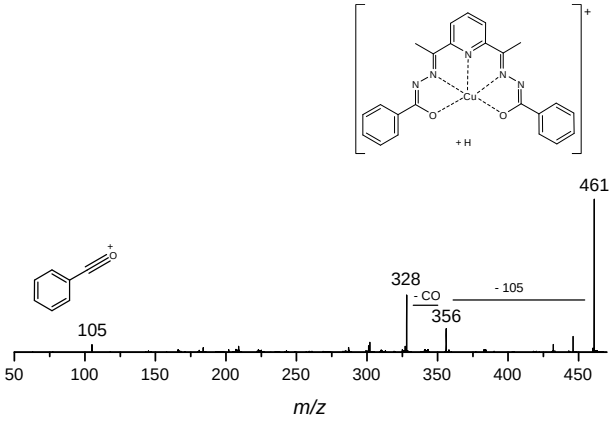

Figure S3. ESI(+)-MS/MS of the ion of *m/z* 461.

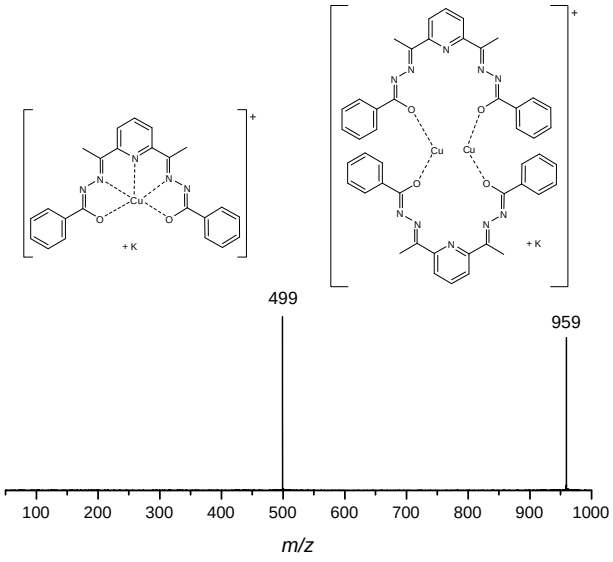

Figure S4. ESI(+)-MS/MS of the ion of *m/z* 959.

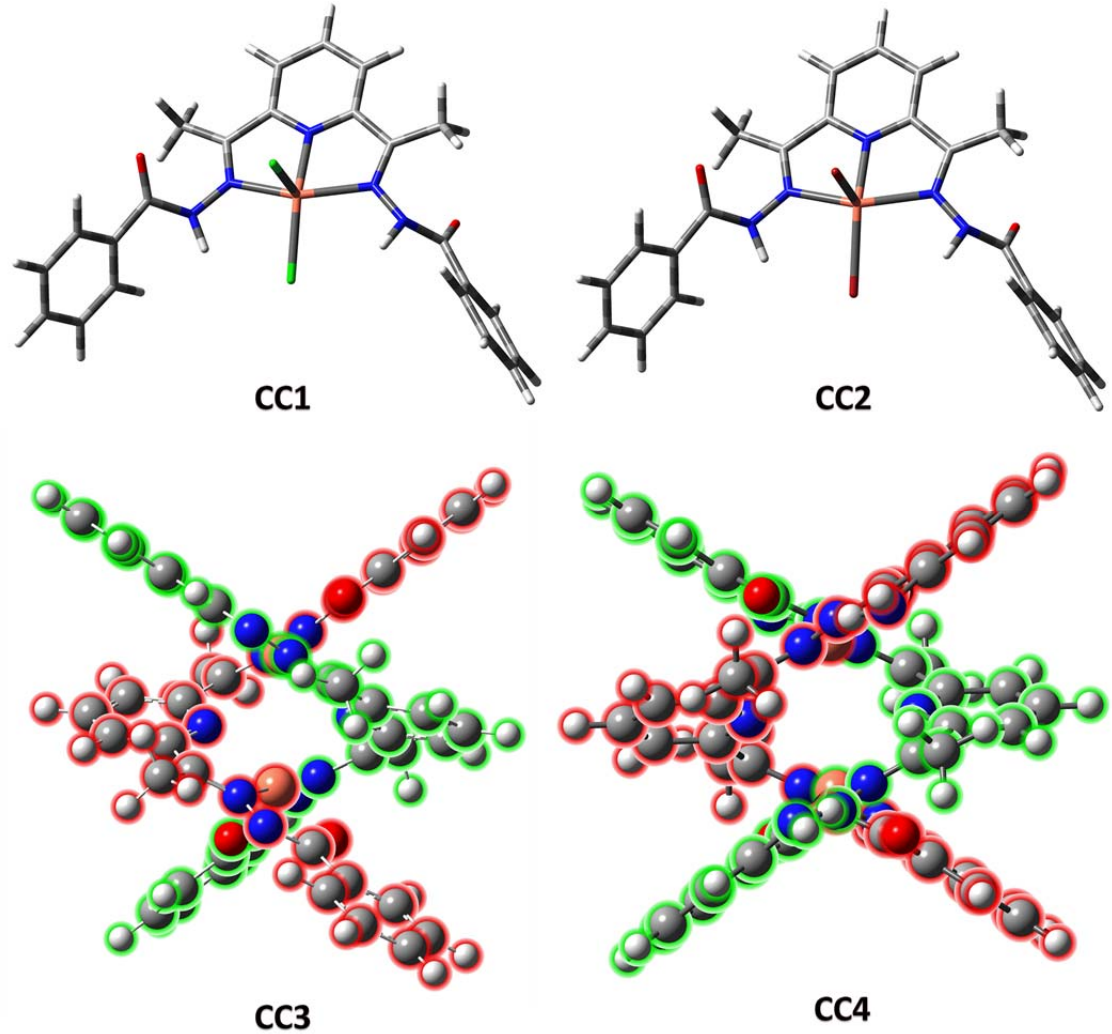

Figure S5. Optimized geometries **CC1**, **CC2**, **CC3** and **CC4** at the B3LYP/6-31G(d,p)/Lanl2dz level of theory considering water as the solvent.

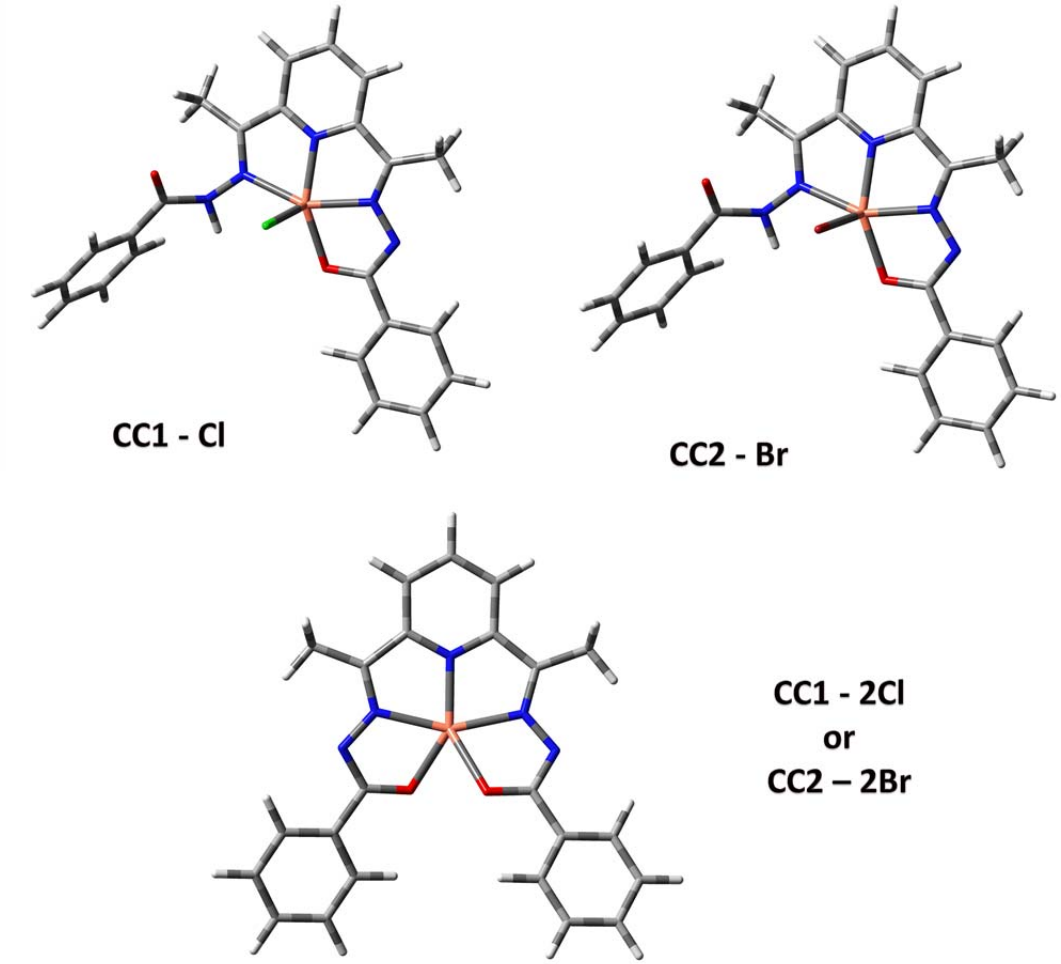

Figure S6. Optimized geometries for detected intermediates at the B3LYP/6-31G(d,p)/Lanl2dz level of theory considering water as the solvent.

Cartesian coordinates, energy and thermal corrections for all the calculated structures

CC1

```
E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)=    -2429.87609767 hartree
Zero-point correction =                           0.393300 hartree
Thermal correction to Energy at 298.15 K =        0.426056 hartree
Thermal correction to Enthalpy at 298.15 K =      0.427000 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.324421 hartree
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.017838	0.374029	0.152859
2	17	0	0.098366	-1.845873	-0.509167
3	17	0	-0.600921	0.281469	2.590791
4	7	0	-1.928736	0.788036	-0.598427

5	7	0	0.046590	2.336448	-0.146363
6	7	0	2.994809	-0.151376	0.545167
7	7	0	2.031017	0.814887	0.377402
8	7	0	-2.863704	-0.202746	-0.754875
9	6	0	4.053596	-0.262317	-0.375566
10	6	0	-5.483962	-3.528937	-1.205908
11	1	0	-5.396223	-4.206721	-2.049110
12	6	0	-2.216096	2.038633	-0.805581
13	6	0	1.254351	4.367169	-0.023998
14	1	0	2.175354	4.907887	0.153203
15	6	0	2.340170	2.076382	0.414501
16	6	0	-4.823253	-1.486369	-0.082554
17	6	0	4.871037	-1.500561	-0.233519
18	6	0	-6.505176	-2.924128	0.905487
19	1	0	-7.202695	-3.138918	1.709054
20	6	0	-1.077457	2.955630	-0.527574
21	6	0	-1.090873	4.349067	-0.651416
22	1	0	-1.989789	4.877295	-0.942834
23	6	0	-3.507661	2.556257	-1.346195
24	1	0	-4.015596	1.774070	-1.913656
25	1	0	-3.330542	3.411587	-2.001249
26	1	0	-4.170022	2.863201	-0.531390
27	6	0	0.089260	5.047187	-0.387806
28	1	0	0.104715	6.127683	-0.477563
29	6	0	-4.032648	-0.227015	0.025463
30	6	0	-4.706012	-2.372154	-1.165759
31	1	0	-4.037624	-2.150747	-1.991700
32	6	0	1.198728	2.975100	0.089519
33	6	0	3.674987	2.636084	0.779769
34	1	0	4.236674	1.910309	1.370579
35	1	0	3.553925	3.552201	1.362029
36	1	0	4.256678	2.862176	-0.118702
37	6	0	-5.735529	-1.764585	0.947086
38	1	0	-5.824062	-1.066261	1.772191
39	6	0	6.460475	-3.796715	-0.092939
40	1	0	7.075975	-4.689578	-0.038404
41	6	0	4.915678	-2.254290	0.950330
42	1	0	4.361674	-1.937969	1.828474
43	6	0	-6.379029	-3.808744	-0.170166
44	1	0	-6.981310	-4.711590	-0.203788
45	6	0	5.639592	-1.895917	-1.339391
46	1	0	5.604509	-1.297640	-2.243354
47	6	0	6.425778	-3.042964	-1.270316
48	1	0	7.011448	-3.349540	-2.131364
49	6	0	5.710053	-3.398674	1.016403
50	1	0	5.748518	-3.974097	1.935879
51	8	0	-4.356640	0.720931	0.726936
52	8	0	4.268158	0.602232	-1.213277
53	1	0	-2.391800	-1.095165	-0.888752
54	1	0	2.562881	-1.031027	0.811125

CC2

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -6657.82294460 hartree
Zero-point correction = 0.408784 hartree
Thermal correction to Energy at 298.15 K = 0.440898 hartree
Thermal correction to Enthalpy at 298.15 K = 0.441842 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.339407 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.171232	-1.894422	-0.608464
2	29	0	0.007010	0.460288	0.026858
3	35	0	-0.632876	0.533558	2.575496
4	7	0	0.070584	2.410392	-0.375243
5	6	0	0.100643	5.111117	-0.723707
6	1	0	0.110836	6.187336	-0.855654
7	6	0	1.263991	4.453307	-0.316435
8	1	0	2.179110	5.006441	-0.146999
9	6	0	-1.050931	3.007609	-0.797133
10	6	0	2.358789	2.189935	0.222523
11	6	0	1.215428	3.066164	-0.149975
12	6	0	3.684447	2.774958	0.583197
13	1	0	4.247674	2.074836	1.202642
14	1	0	3.547050	3.707157	1.135810
15	1	0	4.273279	2.980097	-0.315571
16	6	0	-3.465150	2.564171	-1.635664
17	1	0	-3.962640	1.755758	-2.175008
18	1	0	-3.278994	3.388980	-2.326332
19	1	0	-4.140937	2.906358	-0.846313
20	6	0	-1.070747	4.395023	-0.977198
21	1	0	-1.968246	4.905122	-1.303347
22	6	0	-2.181242	2.075248	-1.051222
23	7	0	2.059793	0.925273	0.229940
24	7	0	-1.896547	0.835816	-0.780353
25	7	0	3.029240	-0.026716	0.440564
26	7	0	-2.832220	-0.159062	-0.907619
27	6	0	4.103965	-0.154713	-0.459952
28	6	0	-4.011581	-0.149180	-0.144230
29	8	0	4.324984	0.684718	-1.321081
30	8	0	-4.345445	0.827387	0.512244
31	6	0	4.929791	-1.380246	-0.265187
32	6	0	-4.803170	-1.410952	-0.211935
33	6	0	5.718832	-1.805379	-1.345234
34	1	0	5.692789	-1.238154	-2.269308
35	6	0	-4.668669	-2.342947	-1.253535
36	1	0	-3.984351	-2.159404	-2.075693
37	6	0	-5.735430	-1.642582	0.811313
38	1	0	-5.837201	-0.908916	1.603569
39	6	0	4.962189	-2.093726	0.943747
40	1	0	4.390943	-1.753132	1.801447
41	6	0	6.513640	-2.942323	-1.225558
42	1	0	7.115274	-3.272293	-2.066718
43	6	0	-6.508004	-2.800966	0.805108
44	1	0	-7.221262	-2.979172	1.603795
45	6	0	6.536502	-3.655904	-0.023090
46	1	0	7.158789	-4.540736	0.070875
47	6	0	-5.449418	-3.498533	-1.258596
48	1	0	-5.347993	-4.212203	-2.070073
49	6	0	5.765318	-3.227903	1.060547
50	1	0	5.794214	-3.771914	1.999310
51	6	0	-6.364796	-3.731324	-0.229011
52	1	0	-6.969407	-4.633210	-0.235267
53	1	0	2.596646	-0.905602	0.711042
54	1	0	-2.359977	-1.057350	-1.000143

CC3

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p))= -3016.29560938 hartree
Zero-point correction = 0.731219 hartree
Thermal correction to Energy at 298.15 K = 0.789622 hartree
Thermal correction to Enthalpy at 298.15 K = 0.790566 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.631846 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.122447	-1.558405	-0.380596
2	29	0	-0.109983	1.557630	0.380179
3	7	0	-0.180253	-0.195473	1.825728
4	7	0	-2.860550	2.373931	0.266252
5	7	0	-2.002670	1.566877	0.930506
6	8	0	-0.953696	3.029906	-0.883031
7	6	0	-2.210742	3.096473	-0.657595
8	6	0	0.839032	-1.178228	3.773588
9	1	0	1.695606	-1.663203	4.225044
10	6	0	-2.388511	0.792701	1.902747
11	6	0	-1.310663	0.026176	2.550384
12	6	0	-1.426844	-0.394833	3.879687
13	1	0	-2.346144	-0.224536	4.426109
14	6	0	0.869557	-0.817181	2.416983
15	6	0	-0.327351	-0.980473	4.502106
16	1	0	-0.383908	-1.286278	5.541359
17	6	0	-3.806167	0.717041	2.389176
18	1	0	-4.474978	1.136612	1.638994
19	1	0	-3.931727	1.292277	3.314632
20	1	0	-4.089118	-0.318385	2.597214
21	7	0	-0.176943	0.197008	-1.825656
22	7	0	-2.014769	-1.550797	-0.932485
23	7	0	-2.880378	-2.350334	-0.269046
24	8	0	-0.980527	-3.022252	0.882650
25	6	0	-2.237806	-3.078197	0.655708
26	6	0	-1.308279	-0.015798	-2.551477
27	6	0	0.878761	0.809310	-2.416307
28	6	0	-2.393258	-0.772728	-1.904492
29	6	0	-0.314296	0.980637	-4.503004
30	1	0	-0.367019	1.285860	-5.542631
31	6	0	-3.072159	-4.015120	1.463701
32	6	0	-1.419402	0.404879	-3.881323
33	1	0	-2.339478	0.241665	-4.428613
34	6	0	0.852854	1.169271	-3.773287
35	1	0	1.713994	1.646579	-4.224212
36	6	0	2.019006	1.196251	-1.570888
37	6	0	2.007533	-1.212980	1.572551
38	7	0	1.734132	-1.556984	0.341951
39	7	0	1.747236	1.542480	-0.340529
40	7	0	2.736042	-1.931282	-0.476506
41	7	0	2.751103	1.908936	0.478952
42	6	0	2.280130	-2.523614	-1.605618
43	8	0	1.060102	-2.637797	-1.923782
44	8	0	1.079282	2.627918	1.924770
45	6	0	-2.412457	4.822375	-2.450874
46	1	0	-1.343226	4.721055	-2.599418
47	6	0	-3.036140	4.040640	-1.466298

48	6	0	-4.421735	4.164723	-1.267574
49	1	0	-4.903259	3.561653	-0.506544
50	6	0	3.405653	-1.300197	2.115898
51	1	0	3.762629	-2.335648	2.115231
52	1	0	3.471863	-0.896938	3.126352
53	1	0	4.073809	-0.728166	1.466029
54	6	0	3.334840	-3.052017	-2.523127
55	6	0	2.946112	-3.665203	-3.724279
56	1	0	1.888843	-3.738884	-3.954166
57	6	0	-5.164926	5.054646	-2.041010
58	1	0	-6.235371	5.144055	-1.880637
59	6	0	4.702422	-2.954650	-2.215597
60	1	0	5.002801	-2.483002	-1.287268
61	6	0	5.658629	-3.458231	-3.095971
62	1	0	6.713510	-3.377398	-2.850283
63	6	0	5.262800	-4.066931	-4.291106
64	1	0	6.009563	-4.459228	-4.975424
65	6	0	2.971369	3.640864	3.727169
66	1	0	1.914495	3.722103	3.956342
67	6	0	4.723601	2.918173	2.219484
68	1	0	5.021280	2.444670	1.291229
69	6	0	3.356529	3.025280	2.526083
70	6	0	-4.458160	-4.129153	1.261812
71	1	0	-4.933363	-3.523576	0.498802
72	6	0	-2.456693	-4.800198	2.450780
73	1	0	-1.387090	-4.706699	2.601768
74	6	0	-4.589223	-5.791724	3.016137
75	1	0	-5.177154	-6.479456	3.617061
76	6	0	-5.209785	-5.012536	2.034606
77	1	0	-6.280474	-5.094221	1.871740
78	6	0	-3.211061	-5.683444	3.221875
79	1	0	-2.725090	-6.286826	3.982985
80	6	0	3.903947	-4.169710	-4.602617
81	1	0	3.592088	-4.642299	-5.529453
82	6	0	5.682782	3.414554	3.100711
83	1	0	6.737228	3.326210	2.855745
84	6	0	3.932195	4.138136	4.606364
85	1	0	3.623094	4.612630	5.533150
86	6	0	5.290494	4.025655	4.295786
87	1	0	6.039575	4.412302	4.980784
88	6	0	-4.536197	5.830502	-3.019980
89	1	0	-5.117529	6.523388	-3.621403
90	6	0	-3.158385	5.712242	-3.222564
91	1	0	-2.666134	6.313006	-3.981707
92	6	0	-3.810011	-0.684068	-2.391341
93	1	0	-4.483063	-1.094360	-1.639805
94	1	0	-3.941444	-1.261121	-3.314860
95	1	0	-4.082367	0.353479	-2.602790
96	6	0	2.298686	2.504732	1.607709
97	6	0	3.418217	1.272507	-2.113058
98	1	0	3.782896	2.305274	-2.113259
99	1	0	3.482302	0.867642	-3.123004
100	1	0	4.081477	0.696232	-1.461959

CC4

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -3237.70457329 hartree
Zero-point correction = 0.795288 hartree

Thermal correction to Energy at 298.15 K = 0.858750 hartree
Thermal correction to Enthalpy at 298.15 K = 0.859694 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.692814 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.050552	-2.832862	-1.426343
2	7	0	2.819658	2.175674	-0.086852
3	8	0	1.050713	2.831982	-1.427679
4	7	0	1.868793	1.571564	0.660348
5	6	0	2.202613	0.982039	1.775432
6	6	0	2.302034	2.783866	-1.176347
7	6	0	3.627678	0.920513	2.242965
8	1	0	4.068715	1.921670	2.279996
9	1	0	4.217333	0.327753	1.534896
10	1	0	3.713339	0.449678	3.221808
11	6	0	3.252375	3.445510	-2.107191
12	6	0	2.694767	4.239963	-3.129995
13	1	0	1.613360	4.307358	-3.171285
14	6	0	4.675041	3.331076	-2.026568
15	7	0	5.307765	2.526882	-1.109665
16	1	0	4.737357	2.232089	-0.322043
17	1	0	6.283401	2.717189	-0.931807
18	6	0	5.456286	4.040179	-2.970762
19	1	0	6.538438	3.956113	-2.910536
20	6	0	3.476545	4.923807	-4.048375
21	1	0	3.015855	5.533261	-4.819137
22	6	0	4.873124	4.818217	-3.957577
23	1	0	5.508288	5.348016	-4.662452
24	29	0	0.000143	-1.658206	0.000405
25	7	0	-1.868831	-1.571078	0.660816
26	7	0	-0.000117	0.000602	1.876907
27	6	0	-2.301903	-2.784501	-1.175213
28	7	0	-2.819642	-2.175482	-0.086231
29	6	0	-2.202801	-0.980974	1.775549
30	6	0	-3.252164	-3.446407	-2.105966
31	6	0	-1.090830	-0.415691	2.559882
32	6	0	-4.674851	-3.331952	-2.025595
33	7	0	-5.307746	-2.527474	-1.109067
34	1	0	-4.737438	-2.232350	-0.321497
35	1	0	-6.283400	-2.717746	-0.931278
36	6	0	1.090525	0.417134	2.559868
37	6	0	-2.694414	-4.241180	-3.128442
38	1	0	-1.613000	-4.308563	-3.169562
39	6	0	1.130633	0.403650	3.962958
40	1	0	2.008081	0.756322	4.490514
41	6	0	-1.131152	-0.401608	3.962964
42	1	0	-2.008681	-0.754062	4.490533
43	6	0	-3.627925	-0.919212	2.242877
44	1	0	-4.068951	-1.920356	2.280415
45	1	0	-4.217507	-0.326858	1.534411
46	1	0	-3.713707	-0.447834	3.221450
47	6	0	-5.455951	-4.041414	-2.969646
48	1	0	-6.538114	-3.957361	-2.909591
49	6	0	-4.872642	-4.819789	-3.956105
50	1	0	-5.507701	-5.349851	-4.660876
51	6	0	-0.000317	0.001178	4.665968
52	1	0	-0.000398	0.001418	5.750797

53	6	0	-3.476048	-4.925364	-4.046689
54	1	0	-3.015236	-5.535056	-4.817189
55	8	0	-1.051020	2.832776	1.426371
56	7	0	2.819927	-2.175388	0.086945
57	8	0	1.051011	-2.831782	1.427777
58	7	0	1.869029	-1.571327	-0.660245
59	6	0	2.202812	-0.981738	-1.775305
60	6	0	2.302330	-2.783604	1.176440
61	6	0	3.627879	-0.920062	-2.242810
62	1	0	4.068994	-1.921182	-2.279926
63	1	0	4.217480	-0.327325	-1.534679
64	1	0	3.713519	-0.449129	-3.221609
65	6	0	3.252727	-3.445174	2.107264
66	6	0	2.695238	-4.239626	3.130134
67	1	0	1.613839	-4.307101	3.171495
68	6	0	4.675371	-3.330628	2.026548
69	7	0	5.307937	-2.526473	1.109508
70	1	0	4.737436	-2.231840	0.321897
71	1	0	6.283584	-2.716671	0.931605
72	6	0	5.456738	-4.039613	2.970732
73	1	0	6.538879	-3.955466	2.910430
74	6	0	3.477130	-4.923360	4.048500
75	1	0	3.016539	-5.532817	4.819318
76	6	0	4.873698	-4.817651	3.957617
77	1	0	5.508946	-5.347365	4.662479
78	29	0	-0.000086	1.658267	-0.000353
79	7	0	-1.869032	1.570871	-0.660822
80	7	0	-0.000056	-0.000614	-1.876818
81	6	0	-2.302346	2.784265	1.175164
82	7	0	-2.819953	2.175189	0.086150
83	6	0	-2.202893	0.980633	-1.775515
84	6	0	-3.252754	3.446064	2.105843
85	6	0	-1.090815	0.415516	-2.559817
86	6	0	-4.675416	3.331426	2.025350
87	7	0	-5.308116	2.526915	1.108717
88	1	0	-4.737701	2.231962	0.321160
89	1	0	-6.283784	2.717054	0.930862
90	6	0	1.090674	-0.416961	-2.559757
91	6	0	-2.695190	4.240901	3.128370
92	1	0	-1.613788	4.308423	3.169582
93	6	0	1.130820	-0.403436	-3.962846
94	1	0	2.008338	-0.755960	-4.490385
95	6	0	-1.131093	0.401461	-3.962901
96	1	0	-2.008662	0.753796	-4.490484
97	6	0	-3.628002	0.918579	-2.242847
98	1	0	-4.069163	1.919655	-2.280635
99	1	0	-4.217514	0.326321	-1.534244
100	1	0	-3.713700	0.446952	-3.221308
101	6	0	-5.456691	4.040763	2.969350
102	1	0	-6.538838	3.956573	2.909200
103	6	0	-4.873565	4.819200	3.955868
104	1	0	-5.508752	5.349169	4.660594
105	6	0	-0.000171	-0.001124	-4.665879
106	1	0	-0.000216	-0.001332	-5.750708
107	6	0	-3.476992	4.924966	4.046563
108	1	0	-3.016325	5.534714	4.817105

CC1-HCl

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -1969.02613408 hartree
Zero-point correction = 0.379618 hartree
Thermal correction to Energy at 298.15 K = 0.410029 hartree
Thermal correction to Enthalpy at 298.15 K = 0.410973 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.314321 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.581914	-0.539626	0.050115
2	17	0	0.005101	-0.218954	2.458794
3	7	0	-2.545288	-0.961564	-0.006469
4	7	0	-0.554361	-2.508367	-0.197927
5	7	0	2.456979	-0.023307	-0.740968
6	7	0	1.457656	-0.964254	-0.601292
7	7	0	-3.377992	0.090856	-0.022725
8	6	0	3.536834	0.050735	0.146906
9	6	0	-5.508780	3.730217	-0.132159
10	1	0	-6.591066	3.738826	-0.043861
11	6	0	-2.894803	-2.216216	0.052070
12	6	0	0.615597	-4.536178	-0.524790
13	1	0	1.532721	-5.078413	-0.715097
14	6	0	1.754423	-2.229061	-0.679187
15	6	0	-3.420820	2.497297	-0.212159
16	6	0	4.386098	1.268708	-0.011140
17	6	0	-3.414982	4.917518	-0.390441
18	1	0	-2.868141	5.848935	-0.502835
19	6	0	-1.739900	-3.131883	-0.069791
20	6	0	-1.782997	-4.530977	-0.124799
21	1	0	-2.719832	-5.063221	-0.012115
22	6	0	-4.304747	-2.704476	0.162644
23	1	0	-4.986376	-1.857642	0.234760
24	1	0	-4.425949	-3.337820	1.048129
25	1	0	-4.577658	-3.305285	-0.712166
26	6	0	-0.589528	-5.221922	-0.340156
27	1	0	-0.598428	-6.305746	-0.382565
28	6	0	-2.662055	1.220841	-0.176718
29	6	0	-4.821806	2.518672	-0.099146
30	1	0	-5.358481	1.583986	0.014551
31	6	0	0.594867	-3.139198	-0.455231
32	6	0	3.091426	-2.788019	-1.043563
33	1	0	3.660605	-2.054233	-1.617408
34	1	0	2.976012	-3.692715	-1.643304
35	1	0	3.666307	-3.029300	-0.144764
36	6	0	-2.724143	3.707476	-0.358425
37	1	0	-1.643710	3.683620	-0.444490
38	6	0	6.038759	3.518967	-0.184320
39	1	0	6.678749	4.393589	-0.251498
40	6	0	4.447010	2.008076	-1.203097
41	1	0	3.881813	1.697210	-2.076260
42	6	0	-4.808133	4.931866	-0.277458
43	1	0	-5.346094	5.875073	-0.302004
44	6	0	5.170809	1.654875	1.086150
45	1	0	5.124406	1.066974	1.996440
46	6	0	5.988210	2.779170	1.001210
47	1	0	6.586183	3.078503	1.856389

48	6	0	5.272652	3.129318	-1.285758
49	1	0	5.323265	3.692635	-2.212210
50	8	0	-1.382129	1.262773	-0.299936
51	8	0	3.756101	-0.822160	0.976499
52	1	0	2.079788	0.863110	-1.053242

CC2-HBr

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -4083.00005701 hartree
Zero-point correction = 0.379378 hartree
Thermal correction to Energy at 298.15 K = 0.409941 hartree
Thermal correction to Enthalpy at 298.15 K = 0.410885 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.313121 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.583512	-0.524656	-0.088940
2	7	0	-2.549617	-0.935108	-0.187455
3	7	0	-0.566125	-2.486517	-0.394123
4	7	0	2.449154	-0.001919	-0.910460
5	7	0	1.450509	-0.943930	-0.774554
6	7	0	-3.376479	0.121691	-0.201726
7	6	0	3.547988	0.051986	-0.045212
8	6	0	-5.489280	3.771770	-0.332784
9	1	0	-6.573484	3.784398	-0.273081
10	6	0	-2.906125	-2.188869	-0.152499
11	6	0	0.593472	-4.512378	-0.767966
12	1	0	1.507709	-5.054566	-0.971891
13	6	0	1.741441	-2.208034	-0.883038
14	6	0	-3.405382	2.530056	-0.372134
15	6	0	4.393784	1.273768	-0.194072
16	6	0	-3.384312	4.952075	-0.522932
17	1	0	-2.830616	5.882098	-0.610694
18	6	0	-1.755317	-3.107257	-0.283392
19	6	0	-1.804841	-4.504642	-0.367807
20	1	0	-2.744608	-5.034513	-0.268903
21	6	0	-4.319683	-2.671187	-0.063049
22	1	0	-4.997160	-1.821981	0.019893
23	1	0	-4.451807	-3.320899	0.808902
24	1	0	-4.588761	-3.253119	-0.951702
25	6	0	-0.614407	-5.196588	-0.596222
26	1	0	-0.628174	-6.279249	-0.661092
27	6	0	-2.653293	1.249668	-0.333960
28	6	0	-4.808681	2.556729	-0.295457
29	1	0	-5.352294	1.623305	-0.207066
30	6	0	0.579623	-3.117007	-0.668967
31	6	0	3.071668	-2.764417	-1.275792
32	1	0	3.634003	-2.022601	-1.846191
33	1	0	2.945355	-3.658805	-1.888581
34	1	0	3.659690	-3.020925	-0.389824
35	6	0	-2.699860	3.738512	-0.486822
36	1	0	-1.617691	3.710487	-0.545720
37	6	0	6.042178	3.528388	-0.351155
38	1	0	6.680482	4.404704	-0.412013
39	6	0	4.432228	2.037776	-1.371275

40	1	0	3.851090	1.744478	-2.240031
41	6	0	-4.779851	4.971703	-0.446112
42	1	0	-5.312864	5.917616	-0.474263
43	6	0	5.198796	1.637569	0.896125
44	1	0	5.169650	1.030851	1.794709
45	6	0	6.014083	2.763979	0.819413
46	1	0	6.627786	3.045868	1.669367
47	6	0	5.255823	3.161122	-1.445981
48	1	0	5.289002	3.743568	-2.361327
49	8	0	-1.371436	1.286453	-0.435379
50	8	0	3.785784	-0.838766	0.759875
51	1	0	2.067714	0.891509	-1.196529
52	35	0	-0.002296	-0.248187	2.443259

CC1-2HCl or CC2-2HBr

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -1508.10867148 hartree
Zero-point correction = 0.365272 hartree
Thermal correction to Energy at 298.15 K = 0.392804 hartree
Thermal correction to Enthalpy at 298.15 K = 0.393748 hartree
Thermal correction to Gibbs Free Energy at 298.15 K = 0.304127 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.227216	1.995385	0.329011
2	6	0	2.493415	2.291098	0.509216
3	7	0	0.252947	2.891527	0.298335
4	6	0	3.386196	1.147205	0.302984
5	6	0	3.000588	3.677514	0.772833
6	6	0	-0.859485	2.327631	-0.265557
7	7	0	2.757610	-0.004626	0.000054
8	6	0	4.790288	1.165800	0.324221
9	1	0	3.648975	4.026710	-0.040089
10	1	0	3.584693	3.716617	1.700017
11	1	0	2.154423	4.359085	0.859248
12	8	0	-0.887929	1.170637	-0.767083
13	6	0	-2.075648	3.183110	-0.300583
14	6	0	3.382282	-1.158578	-0.302982
15	1	0	5.327193	2.073228	0.573661
16	6	0	5.472080	-0.009229	-0.000055
17	6	0	-3.250469	2.665223	-0.865654
18	6	0	-2.075864	4.486410	0.220781
19	6	0	2.485612	-2.299416	-0.509241
20	6	0	4.786293	-1.181942	-0.324324
21	1	0	6.558309	-0.011060	-0.000092
22	1	0	-3.230938	1.655771	-1.261420
23	6	0	-4.408160	3.438609	-0.907979
24	1	0	-1.163341	4.878291	0.654906
25	6	0	-3.235626	5.257154	0.175903
26	7	0	1.220422	-1.999442	-0.329040
27	6	0	2.988115	-3.687564	-0.772761
28	1	0	5.320040	-2.091204	-0.573861
29	6	0	-4.403274	4.735897	-0.388148
30	1	0	-5.315228	3.031453	-1.345720
31	1	0	-3.230497	6.265312	0.580718
32	29	0	0.774975	-0.001348	-0.000008

33	7	0	0.243152	-2.892318	-0.298329
34	1	0	2.139681	-4.366317	-0.859081
35	1	0	3.635376	-4.038824	0.040178
36	1	0	3.572073	-3.728666	-1.699943
37	1	0	-5.306567	5.338937	-0.422278
38	6	0	-0.867333	-2.324742	0.265682
39	8	0	-0.891834	-1.167728	0.767371
40	6	0	-2.086382	-3.176120	0.300650
41	6	0	-3.259381	-2.654415	0.865990
42	6	0	-2.091086	-4.479247	-0.221105
43	1	0	-3.236386	-1.645148	1.262057
44	6	0	-4.419699	-3.423865	0.908202
45	1	0	-1.179965	-4.874116	-0.655462
46	6	0	-3.253461	-5.246052	-0.176342
47	6	0	-4.419284	-4.720996	0.387964
48	1	0	-5.325328	-3.013751	1.346161
49	1	0	-3.251800	-6.254104	-0.581452
50	1	0	-5.324620	-5.320972	0.421983

HCl

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -460.80112182 hartree
Zero-point correction = 0.006413 hartree
Thermal correction to Energy at 298.15 K = 0.008774 hartree
Thermal correction to Enthalpy at 298.15 K = 0.009718 hartree
Thermal correction to Gibbs Free Energy at 298.15 K =-0.011478 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000000	0.000000	0.071572
2	1	0	0.000000	0.000000	-1.216723

HBr

E(M06-2X/6-311+g(2d,p)// B3LYP/6-31G(d,p)/)= -2574.76644147 hartree
Zero-point correction = 0.005801 hartree
Thermal correction to Energy at 298.15 K = 0.008161 hartree
Thermal correction to Enthalpy at 298.15 K = 0.009106 hartree
Thermal correction to Gibbs Free Energy at 298.15 K =-0.013418 hartree

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.039412
2	1	0	0.000000	0.000000	-1.379432