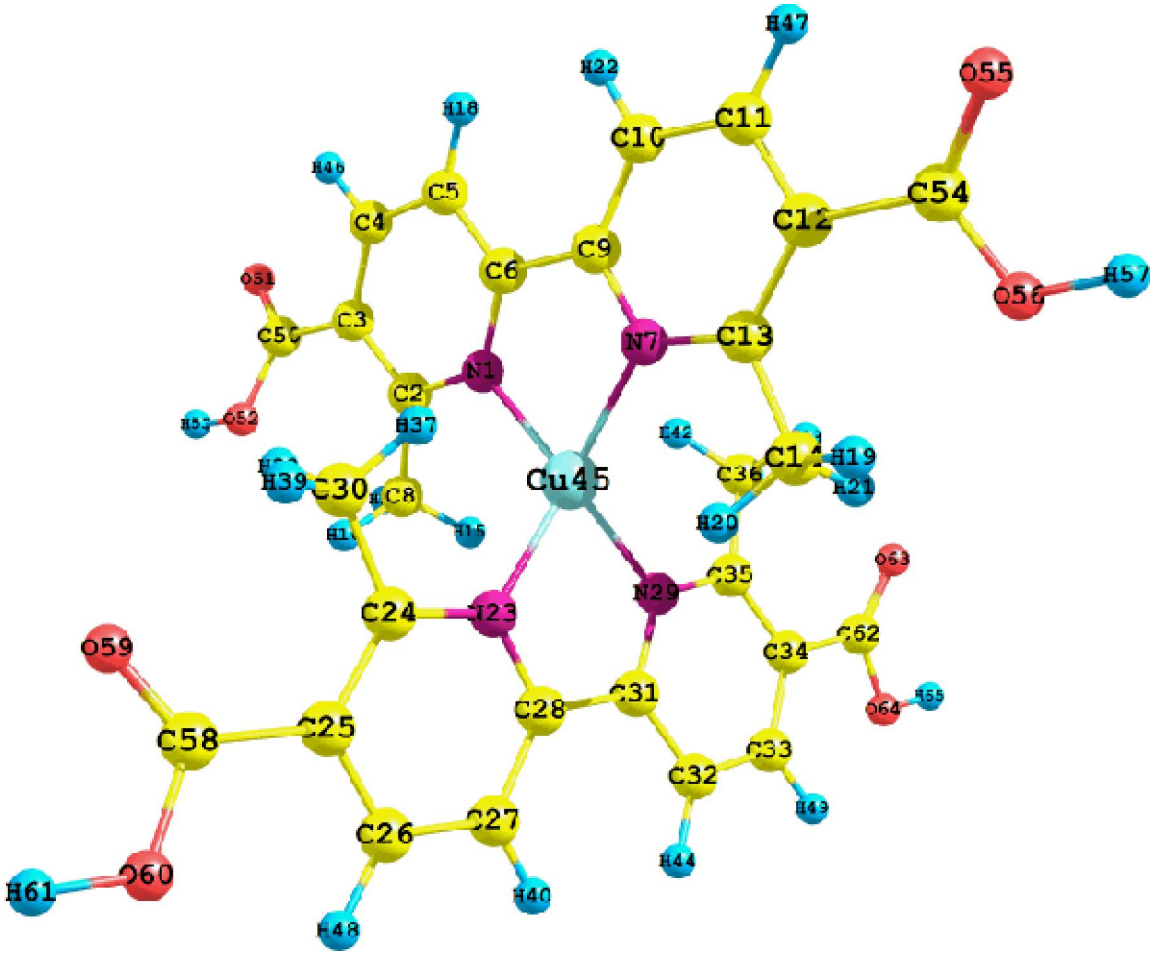
SUPPLEMENTARY DATA

Optimized molecular structure, total energy and Infrared (IR) spectra for the copper complexes in presence of solvent (CuL4 and CuL6 in MeOH solution; CuL7, CuL8 and CuL9 in Chloroform Solution).

1 Molecular system: CuL4

Optimized molecular structure



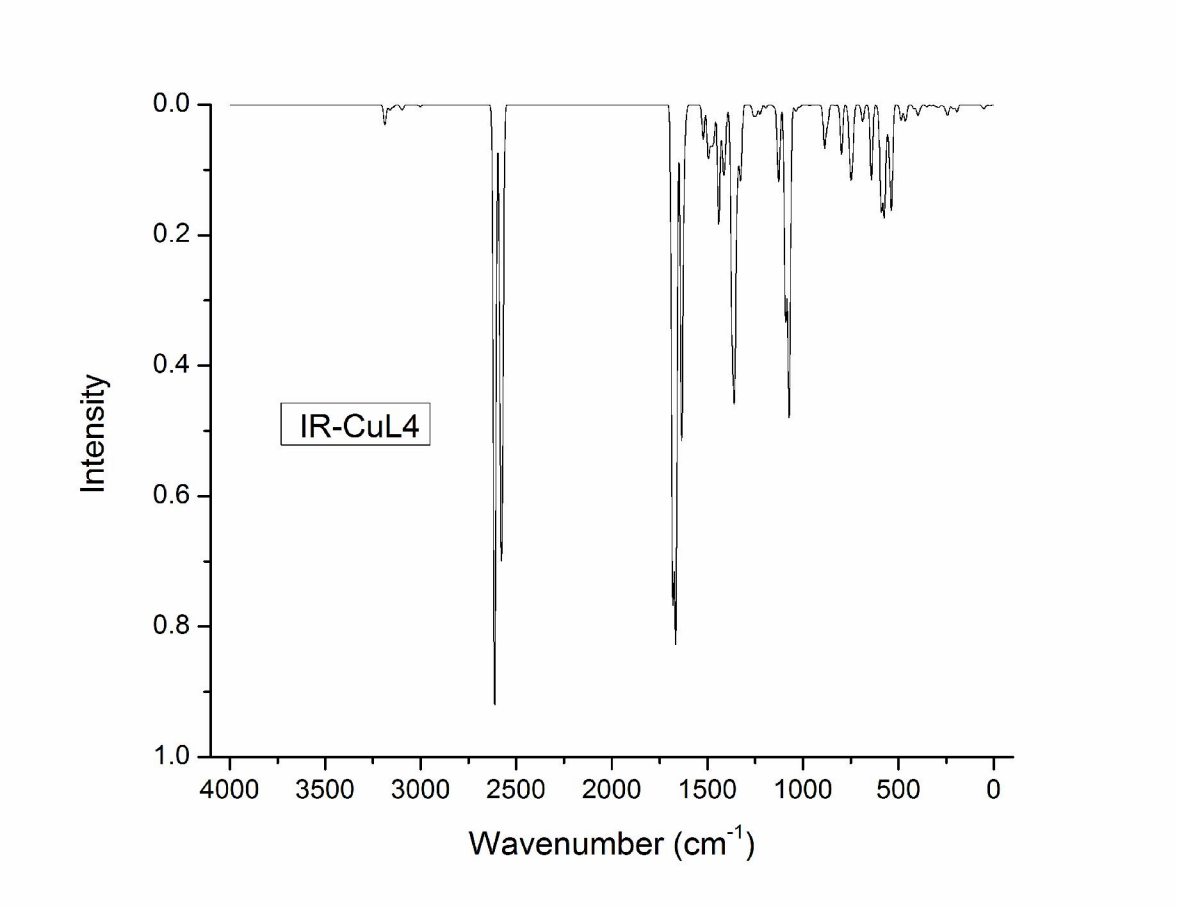
Geometrical parameters

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.135542	1.454239	-0.941666
2	6	-2.199826	1.205754	-1.746820
3	6	-3.049182	2.274319	-2.123579
4	6	-2.739847	3.576222	-1.693208
5	6	-1.637339	3.805514	-0.872356
6	6	-0.853563	2.709434	-0.496254
7	7	0.879882	1.657803	0.803759
8	6	-2.358079	-0.217542	-2.189376
9	6	0.314456	2.829513	0.403228

10	6	0.817458	4.062084	0.833785
11	6	1.938872	4.064080	1.661673
12	6	2.543874	2.853579	2.040523
13	6	1.970412	1.632418	1.610510
14	6	2.457911	0.270709	2.005257
15	1	-1.385826	-0.723297	-2.122194
16	1	-3.064414	-0.745233	-1.532032
17	1	-2.748545	-0.287690	-3.208236
18	1	-1.406549	4.810950	-0.528212
19	1	2.856671	0.258164	3.023575
20	1	1.630697	-0.445654	1.917709
21	1	3.265133	-0.056249	1.333927
22	1	0.357369	4.998696	0.527505
23	7	-0.884063	-1.556258	0.871863
24	6	-1.996578	-1.476462	1.643173
25	6	-2.597985	-2.665504	2.124531
26	6	-2.005443	-3.902777	1.819515
27	6	-0.861467	-3.956815	1.023827
28	6	-0.325573	-2.755086	0.548117
29	7	1.169100	-1.469949	-0.839065
30	6	-2.494357	-0.094905	1.939792
31	6	0.864918	-2.696200	-0.328639
32	6	1.643149	-3.819155	-0.627215
33	6	2.755386	-3.654820	-1.451520
34	6	3.077390	-2.386283	-1.964339
35	6	2.243276	-1.284673	-1.647070
36	6	2.447102	0.108285	-2.159816
37	1	-1.680662	0.623650	1.779337
38	1	-3.322528	0.167873	1.265082
39	1	-2.873457	-0.009709	2.962809
40	1	-0.411554	-4.915176	0.775535
41	1	2.719619	0.112366	-3.220227
42	1	1.526802	0.686742	-2.009276
43	1	3.264691	0.605494	-1.618758
44	1	1.400336	-4.798695	-0.222052
45	29	0.014934	0.021161	-0.064294
46	1	-3.380193	4.402584	-1.998624
47	1	2.364668	5.003945	2.011115
48	1	-2.453181	-4.819607	2.196539
49	1	3.385219	-4.507753	-1.693061
50	6	-4.264536	2.134637	-2.968113
51	8	-4.752402	3.083170	-3.614251
52	8	-4.827909	0.907149	-2.943999
53	1	-5.673944	0.854593	-3.531639
54	6	3.759583	2.960728	2.889054
55	8	3.989332	3.941634	3.623504
56	8	4.623814	1.930478	2.760556
57	1	5.461852	2.049633	3.350540
58	6	-3.849328	-2.640580	2.922309
59	8	-4.664018	-1.699096	2.956020
60	8	-4.039552	-3.788145	3.620176
61	1	-4.927056	-3.783160	4.141836
62	6	4.289019	-2.232434	-2.808162
63	8	4.846333	-1.153516	-3.084936
64	8	4.762091	-3.422877	-3.256352
65	1	5.616406	-3.311602	-3.819589

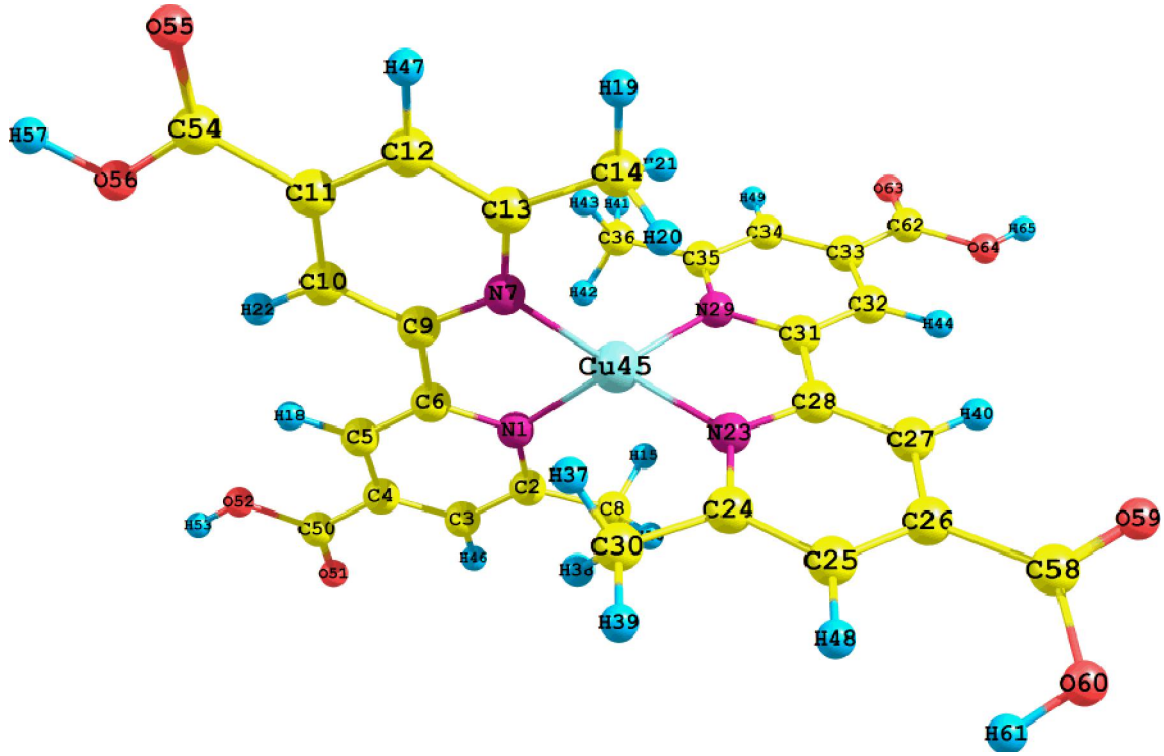
Total Energy: -3540.882399 Hartree

Infrared (IR) spectrum



2 Molecular system: CuL6

Optimized molecular structure



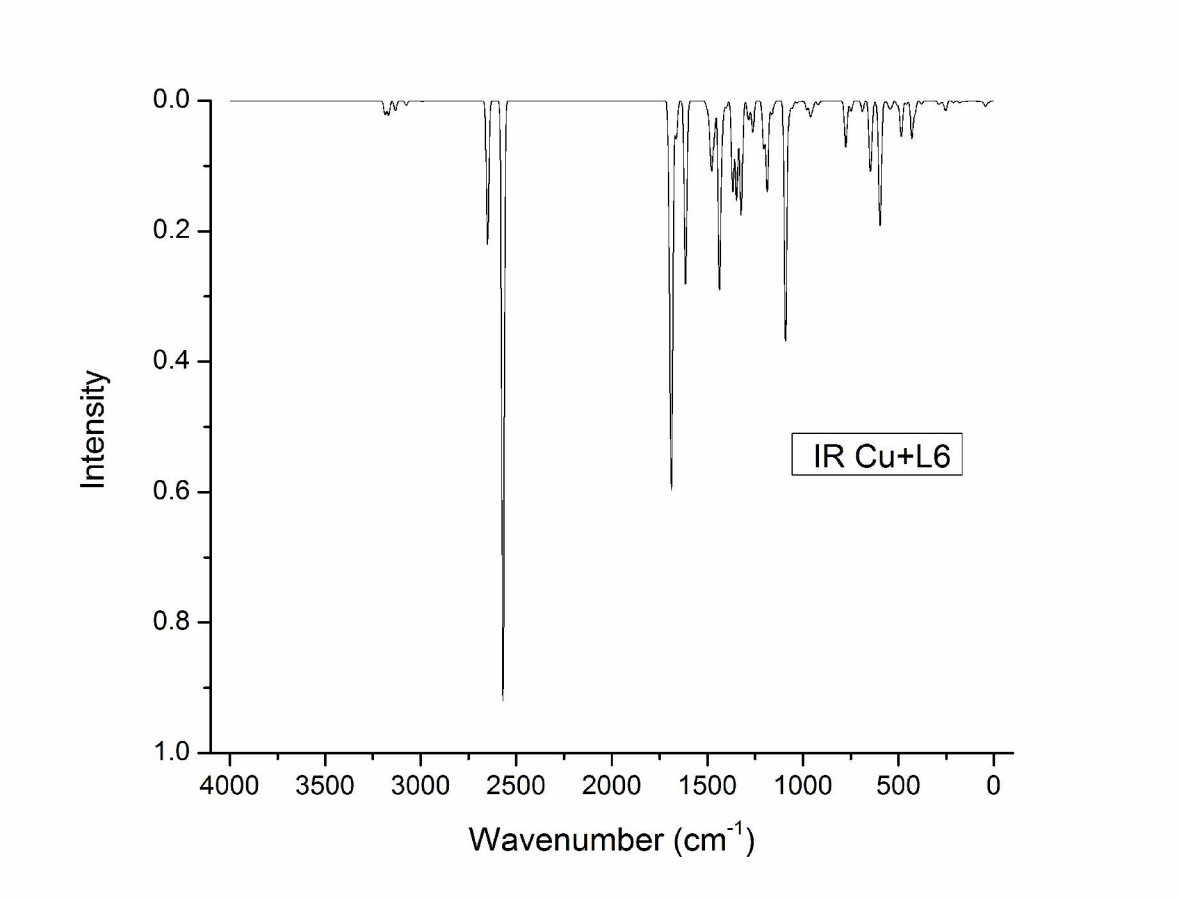
Geometrical parameters

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.537505	0.867040	1.006772
2	6	1.426742	1.746022	2.033760
3	6	2.576004	2.263340	2.649756
4	6	3.838081	1.863833	2.191915
5	6	3.938650	0.957914	1.128609
6	6	2.759835	0.473022	0.553143
7	7	1.510672	-0.855928	-1.014585
8	6	0.043180	2.125378	2.459031
9	6	2.744694	-0.486016	-0.573070
10	6	3.908227	-0.990860	-1.162446
11	6	3.779753	-1.889179	-2.229323
12	6	2.505640	-2.262439	-2.675879
13	6	1.372684	-1.728111	-2.044042
14	6	-0.022297	-2.081669	-2.454077
15	1	-0.484761	2.621006	1.630497
16	1	-0.533192	1.225232	2.719066
17	1	0.061444	2.799784	3.321376
18	1	4.917061	0.645650	0.769752
19	1	-0.026366	-2.750537	-3.320895
20	1	-0.547497	-2.574229	-1.621952
21	1	-0.587117	-1.170512	-2.700747
22	1	4.895558	-0.698126	-0.811934
23	7	-1.534935	-0.997723	0.861759
24	6	-1.410551	-2.047086	1.709112
25	6	-2.550728	-2.701857	2.201804
26	6	-3.821664	-2.261933	1.809050

27	6	-3.931217	-1.174989	0.930669
28	6	-2.764390	-0.557332	0.473737
29	7	-1.537234	1.041571	-0.836200
30	6	-0.021980	-2.461545	2.081395
31	6	-2.765743	0.594395	-0.454622
32	6	-3.936825	1.199859	-0.921106
33	6	-3.821480	2.288256	-1.795222
34	6	-2.553239	2.738135	-2.183977
35	6	-1.412293	2.090393	-1.686875
36	6	-0.023008	2.504307	-2.057611
37	1	0.550794	-2.718525	1.178049
38	1	0.501805	-1.627234	2.571527
39	1	-0.028640	-3.323451	2.756594
40	1	-4.917228	-0.836043	0.616538
41	1	-0.029882	3.367502	-2.731117
42	1	0.550388	2.759294	-1.154110
43	1	0.500499	1.671107	-2.550108
44	1	-4.920035	0.848003	-0.616180
45	29	-0.005594	0.020084	0.007085
46	1	2.484616	2.967830	3.475351
47	1	2.392650	-2.960450	-3.504341
48	1	-2.415903	-3.552352	2.872169
49	1	-2.450754	3.582292	-2.864517
50	6	5.050997	2.419187	2.852542
51	8	5.013587	3.217331	3.806442
52	8	6.200803	1.966596	2.307898
53	1	7.038361	2.352122	2.770101
54	6	4.974861	-2.463241	-2.906379
55	8	4.911977	-3.248186	-3.869892
56	8	6.138707	-2.043934	-2.364909
57	1	6.964077	-2.441077	-2.839122
58	6	-5.090734	-2.920678	2.254311
59	8	-6.179106	-2.690666	1.700998
60	8	-5.057380	-3.798860	3.281284
61	1	-4.175727	-3.921855	3.790213
62	6	-5.024608	2.985937	-2.326489
63	8	-4.972318	3.965419	-3.092231
64	8	-6.182312	2.444532	-1.891046
65	1	-7.013182	2.931306	-2.260537

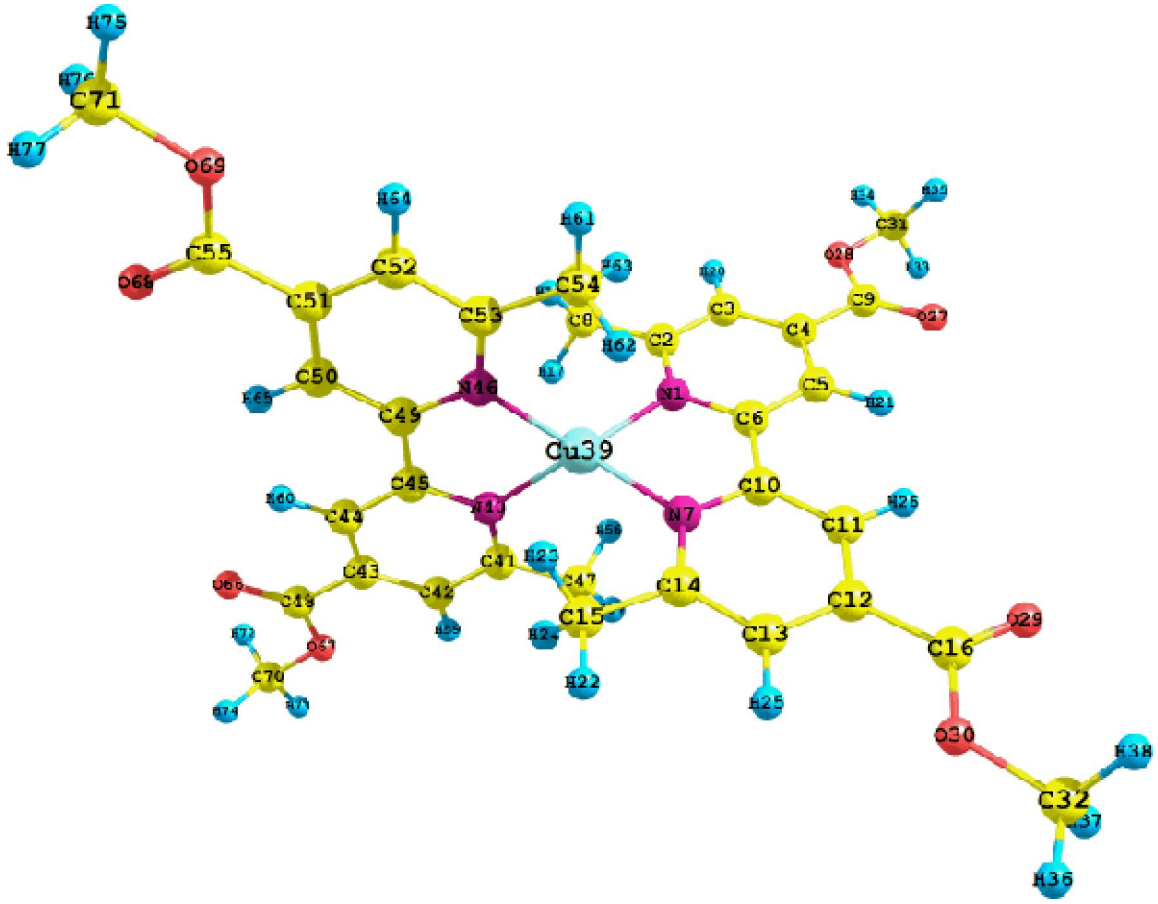
Total Energy: -3541.0450193 Hartree

Infrared (IR) spectrum



3 Molecular system: CuL7

Optimized molecular structure



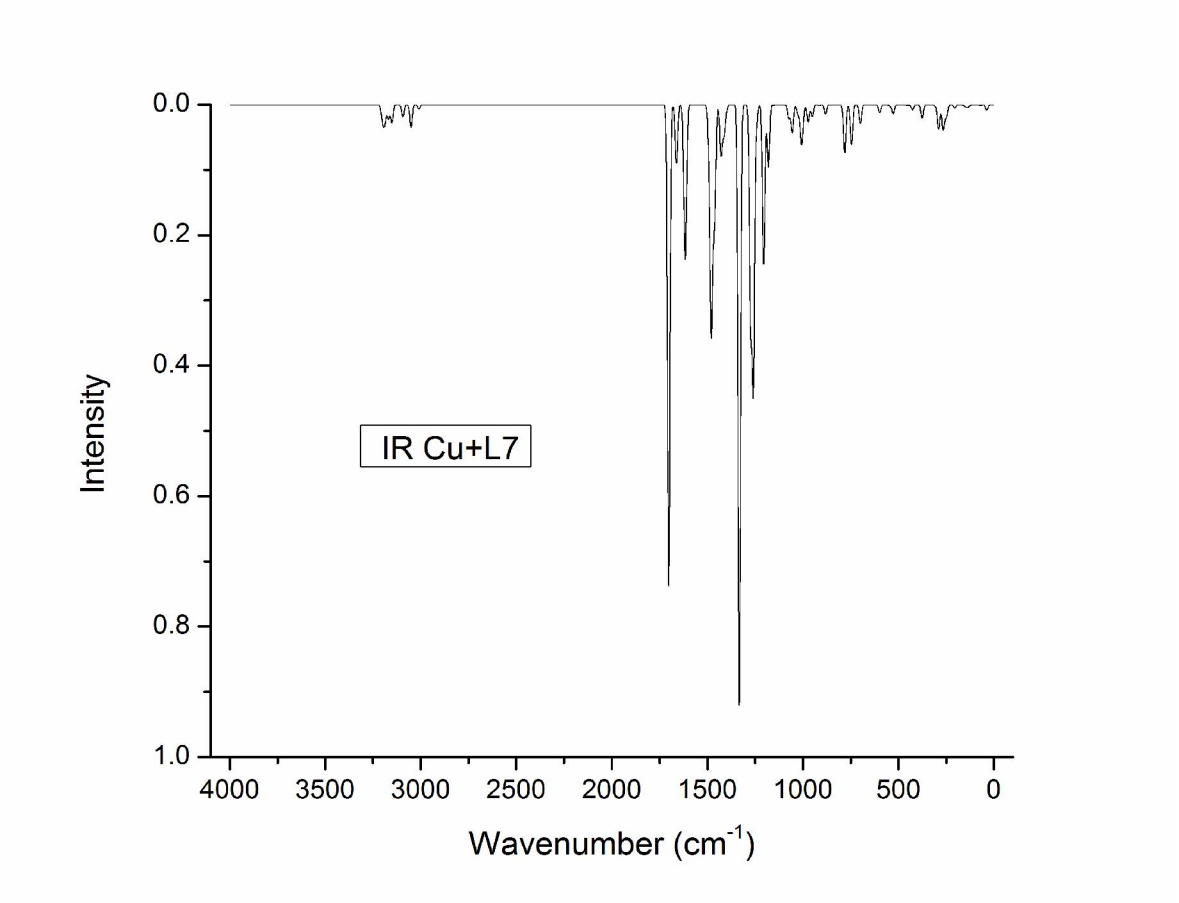
Geometrical parameters

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	-1.531527	0.950631	0.931062
2	6	-1.411984	1.926229	1.865364
3	6	-2.553431	2.530965	2.414258
4	6	-3.819614	2.114967	1.984162
5	6	-3.929115	1.105398	1.019840
6	6	-2.759346	0.536452	0.509039
7	7	-1.531726	-0.950819	-0.930907
8	6	-0.023348	2.312812	2.269052
9	6	-5.074852	2.711132	2.520040
10	6	-2.759460	-0.536486	-0.508781
11	6	-3.929344	-1.105280	-1.019491
12	6	-3.820045	-2.114851	-1.983834
13	6	-2.553948	-2.530994	-2.414049
14	6	-1.412380	-1.926412	-1.865240
15	6	-0.023825	-2.313142	-2.269059
16	6	-5.075394	-2.710879	-2.519604
17	1	0.522381	1.432365	2.637162
18	1	0.531347	2.695678	1.400486
19	1	-0.030901	3.079361	3.049740
20	1	-2.450377	3.311736	3.163037

21	1	-4.916337	0.787310	0.690271
22	1	-0.031534	-3.079780	-3.049659
23	1	0.521919	-1.432775	-2.637343
24	1	0.530955	-2.695942	-1.400519
25	1	-2.451053	-3.311766	-3.162850
26	1	-4.916494	-0.787073	-0.689827
27	8	-6.211611	2.363508	2.164314
28	8	-4.838170	3.678460	3.439637
29	8	-6.212088	-2.363119	-2.163801
30	8	-4.838892	-3.678228	-3.439224
31	6	-6.001642	4.344468	4.036229
32	6	-6.002489	-4.344103	-4.035720
33	1	-6.627490	3.607824	4.549951
34	1	-5.588482	5.066743	4.740229
35	1	-6.582196	4.844376	3.254344
36	1	-5.589469	-5.066425	-4.739755
37	1	-6.583036	-4.843945	-3.253787
38	1	-6.628296	-3.607387	-4.549389
39	29	0.000001	-0.000217	-0.000031
40	7	1.531706	-0.950795	0.930924
41	6	1.412338	-1.926372	1.865271
42	6	2.553893	-2.530989	2.414071
43	6	3.819998	-2.114896	1.983833
44	6	3.929319	-1.105348	1.019468
45	6	2.759448	-0.536518	0.508769
46	7	1.531549	0.950563	-0.931140
47	6	0.023775	-2.313039	2.269124
48	6	5.075335	-2.710937	2.519617
49	6	2.759359	0.536406	-0.509065
50	6	3.929140	1.105370	-1.019820
51	6	3.819660	2.114938	-1.984146
52	6	2.553487	2.530917	-2.414292
53	6	1.412028	1.926161	-1.865445
54	6	0.023402	2.312720	-2.269189
55	6	5.074909	2.711125	-2.519973
56	1	-0.521938	-1.432633	2.637358
57	1	-0.531025	-2.695879	1.400615
58	1	0.031469	-3.079628	3.049772
59	1	2.450980	-3.311748	3.162882
60	1	4.916476	-0.787180	0.689784
61	1	0.030975	3.079197	-3.049948
62	1	-0.522329	1.432243	-2.637225
63	1	-0.531303	2.695675	-1.400670
64	1	2.450450	3.311690	-3.163071
65	1	4.916353	0.787299	-0.690209
66	8	6.212035	-2.363267	2.163746
67	8	4.838815	-3.678204	3.439321
68	8	6.211662	2.363491	-2.164237
69	8	4.838246	3.678398	-3.439634
70	6	6.002394	-4.344094	4.035832
71	6	6.001730	4.344386	-4.036224
72	1	6.628167	-3.607392	4.549564
73	1	5.589353	-5.066449	4.739819
74	1	6.582984	-4.843893	3.253903
75	1	5.588583	5.066681	-4.740210
76	1	6.582307	4.844265	-3.254337
77	1	6.627552	3.607733	-4.549965

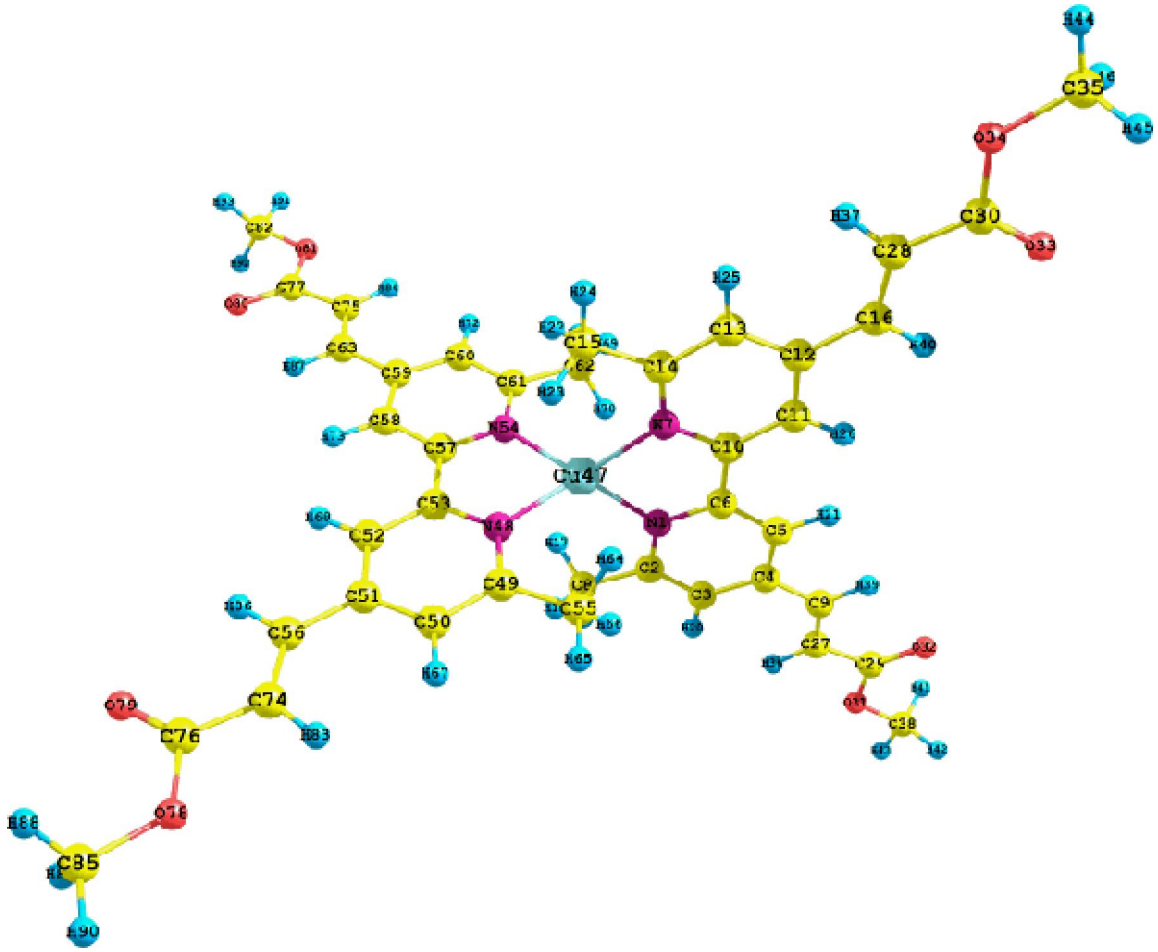
Total Energy: -3698.0339625 Hartree

Infrared (IR) spectrum



4 Molecular system: CuL8

Optimized molecular structure



Geometrical parameters

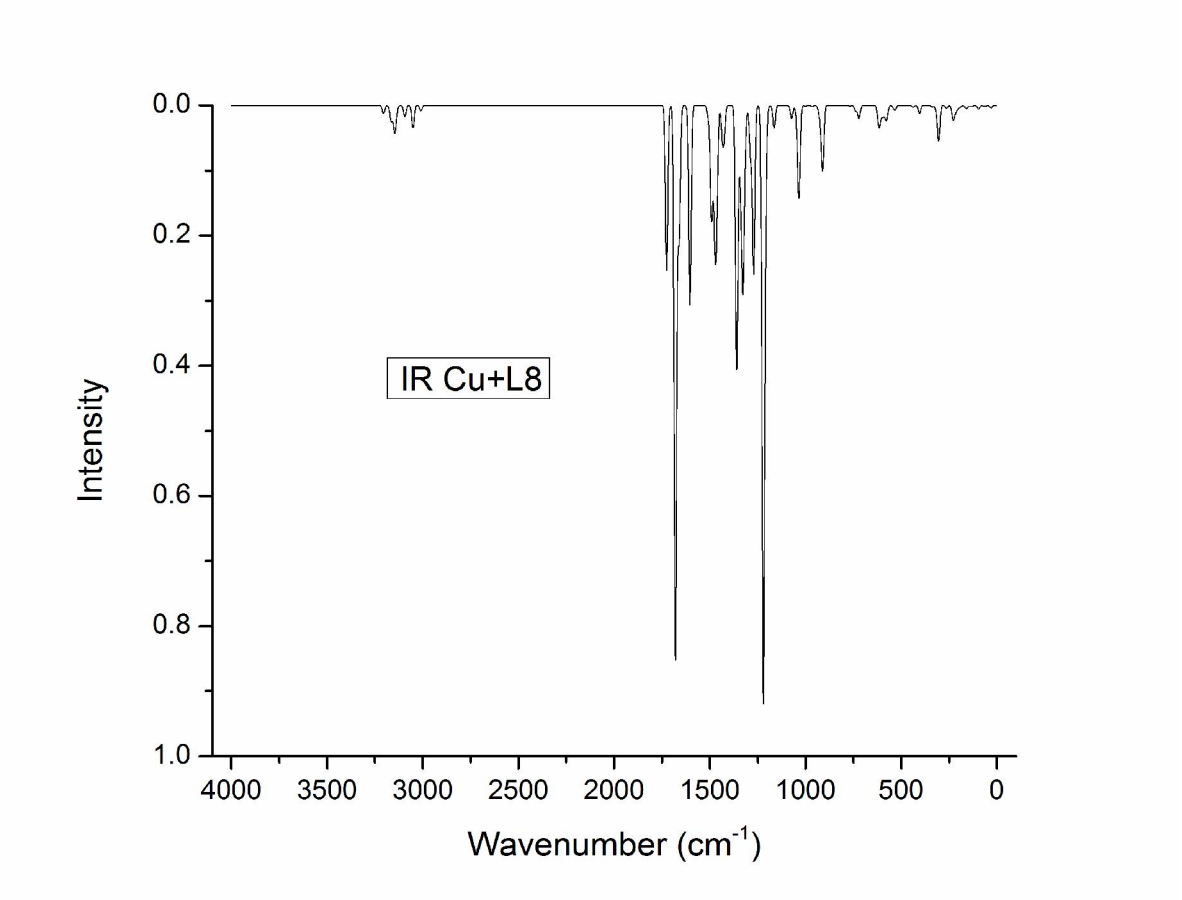
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.535054	0.949089	0.928709
2	6	1.422520	1.928953	1.863740
3	6	2.560679	2.533539	2.407960
4	6	3.842425	2.128187	1.986554
5	6	3.931817	1.109767	1.020451
6	6	2.763314	0.537501	0.509082
7	7	1.535423	-0.949713	-0.928370
8	6	0.033275	2.314581	2.268757
9	6	5.079458	2.714060	2.506843
10	6	2.763527	-0.537779	-0.508616
11	6	3.932245	-1.109692	-1.019892
12	6	3.843228	-2.128093	-1.986050
13	6	2.561639	-2.533754	-2.407639
14	6	1.423255	-1.929531	-1.863496
15	6	0.034160	-2.315461	-2.268727
16	6	5.080470	-2.713640	-2.506211
17	1	-0.510211	1.433819	2.639392
18	1	0.039819	3.083413	3.047429
19	1	-0.523362	2.693154	1.399580

20	1	2.435071	3.313623	3.156061
21	1	4.911767	0.780221	0.679933
22	1	-0.522602	-2.693973	-1.399603
23	1	-0.509394	-1.434851	-2.639630
24	1	0.040998	-3.084422	-3.047270
25	1	2.436334	-3.313809	-3.155822
26	1	4.912064	-0.779887	-0.679249
27	6	5.160074	3.715423	3.409158
28	6	5.161460	-3.715168	-3.408314
29	6	6.474545	4.211731	3.850697
30	6	6.476131	-4.211095	-3.849679
31	8	6.331611	5.229872	4.748487
32	8	7.583525	3.786226	3.478887
33	8	7.584930	-3.784945	-3.478068
34	8	6.333633	-5.229667	-4.747049
35	6	7.556006	-5.832775	-5.282942
36	1	4.289649	4.202899	3.850677
37	1	4.291215	-4.203054	-3.849737
38	6	7.553719	5.833343	5.284575
39	1	6.013957	2.296255	2.120610
40	1	6.014821	-2.295467	-2.120019
41	1	8.142295	5.077318	5.814594
42	1	8.149087	6.258424	4.469884
43	1	7.214318	6.612302	5.967578
44	1	7.216963	-6.612525	-5.965217
45	1	8.143935	-5.076786	-5.813732
46	1	8.151880	-6.256774	-4.468057
47	29	0.000001	-0.000561	0.000004
48	7	-1.535052	0.949091	-0.928706
49	6	-1.422518	1.928951	-1.863742
50	6	-2.560676	2.533531	-2.407970
51	6	-3.842422	2.128178	-1.986566
52	6	-3.931814	1.109761	-1.020460
53	6	-2.763312	0.537501	-0.509083
54	7	-1.535424	-0.949714	0.928370
55	6	-0.033272	2.314577	-2.268758
56	6	-5.079455	2.714044	-2.506862
57	6	-2.763527	-0.537779	0.508615
58	6	-3.932245	-1.109691	1.019891
59	6	-3.843230	-2.128091	1.986049
60	6	-2.561641	-2.533755	2.407637
61	6	-1.423257	-1.929532	1.863496
62	6	-0.034162	-2.315461	2.268730
63	6	-5.080472	-2.713636	2.506213
64	1	0.510204	1.433820	-2.639417
65	1	-0.039815	3.083429	-3.047411
66	1	0.523374	2.693125	-1.399575
67	1	-2.435067	3.313609	-3.156076
68	1	-4.911765	0.780213	-0.679944
69	1	0.522612	-2.693947	1.399604
70	1	0.509379	-1.434853	2.639660
71	1	-0.041000	-3.084440	3.047256
72	1	-2.436336	-3.313814	3.155817
73	1	-4.912064	-0.779885	0.679249
74	6	-5.160071	3.715425	-3.409158
75	6	-5.161464	-3.715148	3.408333
76	6	-6.474541	4.211724	-3.850707
77	6	-6.476136	-4.211073	3.849697
78	8	-6.331608	5.229881	-4.748480
79	8	-7.583521	3.786193	-3.478927
80	8	-7.584935	-3.784930	3.478075
81	8	-6.333640	-5.229642	4.747070
82	6	-7.556016	-5.832749	5.282958
83	1	-4.289645	4.202923	-3.850653
84	1	-4.291219	-4.203021	3.849772
85	6	-7.553716	5.833338	-5.284582
86	1	-6.013954	2.296221	-2.120650
87	1	-6.014822	-2.295474	2.120006
88	1	-8.142269	5.077311	-5.814623
89	1	-8.149107	6.258397	-4.469896
90	1	-7.214316	6.612313	-5.967567

91	1	-7.216977	-6.612519	5.965213
92	1	-8.143933	-5.076766	5.813770
93	1	-8.151902	-6.256723	4.468068

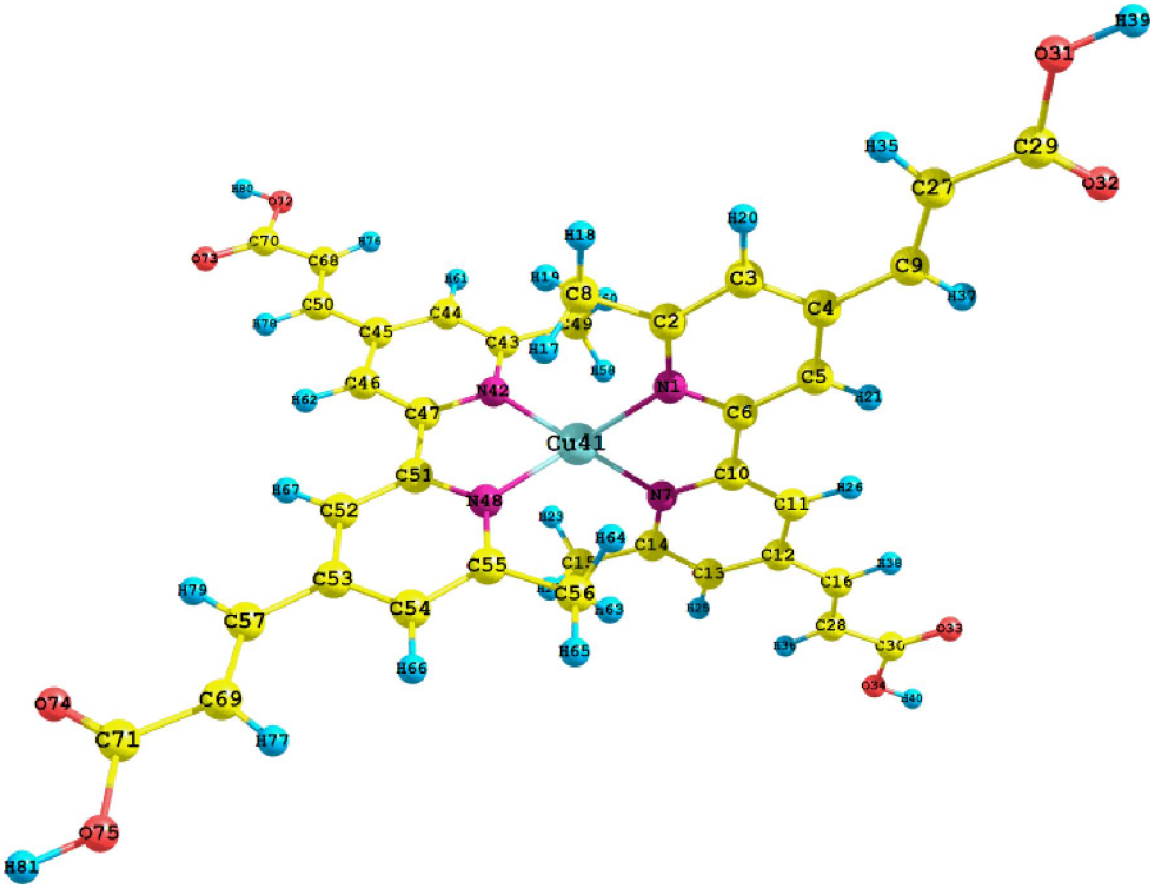
Total Energy: -4007.3727181 Hartree

Infrared (IR) spectrum



5 Molecular system: CuL9

Optimized molecular structure



Geometrical parameters

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	7	1.534828	-0.950002	-0.929030
2	6	1.423311	-1.930475	-1.863652
3	6	2.562217	-2.535550	-2.406443
4	6	3.843051	-2.129908	-1.982973
5	6	3.931398	-1.111205	-1.017216
6	6	2.762498	-0.538053	-0.508203
7	7	1.534707	0.949807	0.929166
8	6	0.034463	-2.316456	-2.269488
9	6	5.082074	-2.714878	-2.498699
10	6	2.762427	0.538048	0.508305
11	6	3.931253	1.111353	1.017327
12	6	3.842771	2.130010	1.983115
13	6	2.561885	2.535446	2.406623
14	6	1.423055	1.930227	1.863830
15	6	0.034166	2.316005	2.269715
16	6	5.081727	2.715113	2.498871
17	1	-0.508858	-1.435892	-2.640830
18	1	0.041581	-3.085599	-3.047824
19	1	-0.522618	-2.694789	-1.400481
20	1	2.437646	-3.316482	-3.153845
21	1	4.911046	-0.782314	-0.675280

22	1	-0.522781	2.694989	1.400907
23	1	-0.509253	1.435233	2.640405
24	1	0.041222	3.084638	3.048561
25	1	2.437214	3.316323	3.154068
26	1	4.910936	0.782610	0.675346
27	6	5.171235	-3.709602	-3.407788
28	6	5.170740	3.709731	3.408094
29	6	6.493086	-4.197883	-3.835224
30	6	6.492497	4.198176	3.835586
31	8	6.384352	-5.204640	-4.748387
32	8	7.593139	-3.771137	-3.436939
33	8	7.592624	3.771650	3.437274
34	8	6.383593	5.204837	4.748849
35	1	4.306681	-4.194354	-3.863216
36	1	4.306083	4.194250	3.863569
37	1	6.014285	-2.301134	-2.102552
38	1	6.013979	2.301551	2.102637
39	1	7.284629	-5.547028	-5.046413
40	1	7.283816	5.547320	5.046928
41	29	-0.000002	-0.000073	-0.000028
42	7	-1.534810	-0.950057	0.928961
43	6	-1.423273	-1.930536	1.863574
44	6	-2.562168	-2.535616	2.406384
45	6	-3.843012	-2.129969	1.982948
46	6	-3.931379	-1.111253	1.017207
47	6	-2.762490	-0.538099	0.508171
48	7	-1.534732	0.949812	-0.929170
49	6	-0.034417	-2.316502	2.269395
50	6	-5.082022	-2.714948	2.498694
51	6	-2.762443	0.538020	-0.508318
52	6	-3.931281	1.111309	-1.017330
53	6	-3.842818	2.129991	-1.983094
54	6	-2.561939	2.535463	-2.406592
55	6	-1.423097	1.930253	-1.863815
56	6	-0.034216	2.316054	-2.269704
57	6	-5.081785	2.715079	-2.498840
58	1	0.508829	-1.435970	2.640922
59	1	-0.041516	-3.085785	3.047594
60	1	0.522727	-2.694637	1.400343
61	1	-2.437579	-3.316556	3.153776
62	1	-4.911035	-0.782352	0.675301
63	1	0.522743	2.695003	-1.400889
64	1	0.509199	1.435298	-2.640440
65	1	-0.041287	3.084718	-3.048520
66	1	-2.437285	3.316357	-3.154021
67	1	-4.910958	0.782532	-0.675363
68	6	-5.171157	-3.709698	3.407757
69	6	-5.170815	3.709748	-3.408006
70	6	-6.492993	-4.197994	3.835222
71	6	-6.492580	4.198175	-3.835495
72	8	-6.384222	-5.204786	4.748343
73	8	-7.593062	-3.771219	3.437011
74	8	-7.592702	3.771553	-3.437275
75	8	-6.383686	5.204929	-4.748659
76	1	-4.306590	-4.194464	3.863143
77	1	-4.306166	4.194325	-3.863433
78	1	-6.014243	-2.301191	2.102585
79	1	-6.014029	2.301463	-2.102643
80	1	-7.284488	-5.547181	5.046397
81	1	-7.283914	5.547392	-5.046744

Total Energy: -3850.3478754 Hartree

Infrared (IR) spectrum