Electronic Supplementary Material (ESI) for Dalton Transactions.

Benzothiazole integrated into a cryptand for ESIPT based selective chemosensor for the Zn2+ ion

Mayank Gupta, Sunanda Sahana, Vivekanand Sharma and Parimal K. Bharadwaj*

Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India

Table S1. The crystal and refinement data of **L**.

Parameters	**L**
Empirical formula	C114H125N22O7S6
Formula wt.	2107.71
Temperature (K)	100(2)
Radiation Source	Mo Kα
Wavelength (Å)	0.71073
Crystal system	Monoclinc
Space group	*C* 2/c
a, Å	35.135(11)
b, Å	14.185(4)
c, Å	24.132(6)
α (°)	90
β (°)	112.963(11)
γ (°)	90
U, Å^3	11074(5)
Z	4
ρcalc (g/cm3)	1.264
μ, mm-1	0.189
F(000)	4460.0
Refl. Collected	64632
*R*int	0.1438
Independent refl.	9751
Refinement method	Full-matrix least-squares on F2
GOOF	1.021
Final R indices [I>2σ(I)]	R1 = 0.0831 wR2 = 0.2108
R indices (all data)	R1 = 0.1492 wR2 = 0.2607

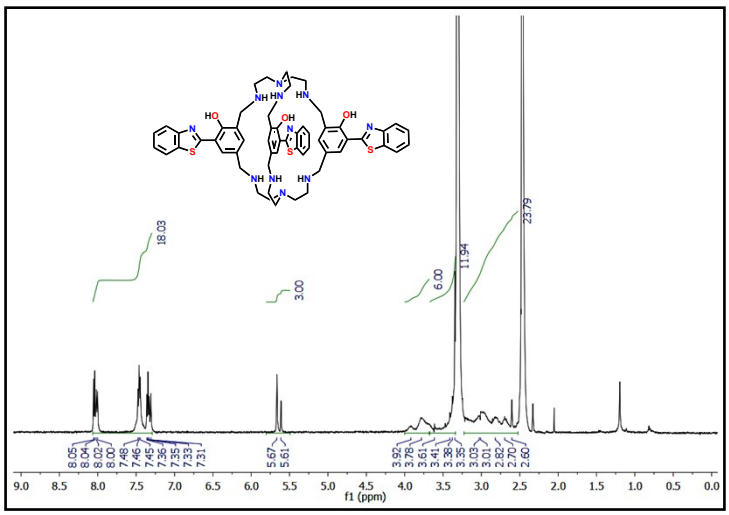

Figure S1. 1H NMR spectrum of **L**.

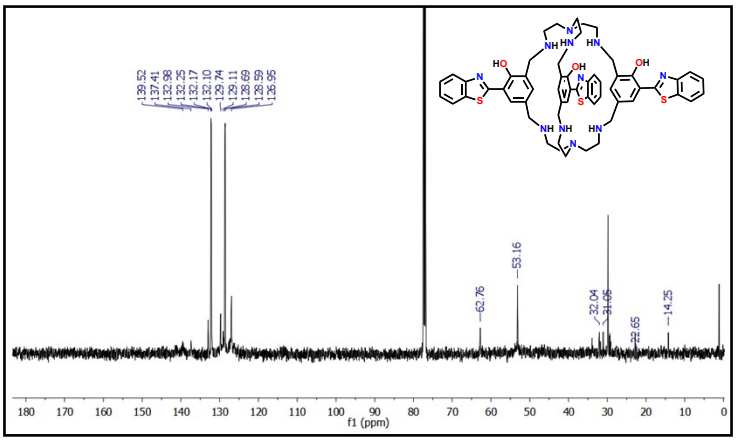

Figure S2. 13C NMR spectrum of **L**.

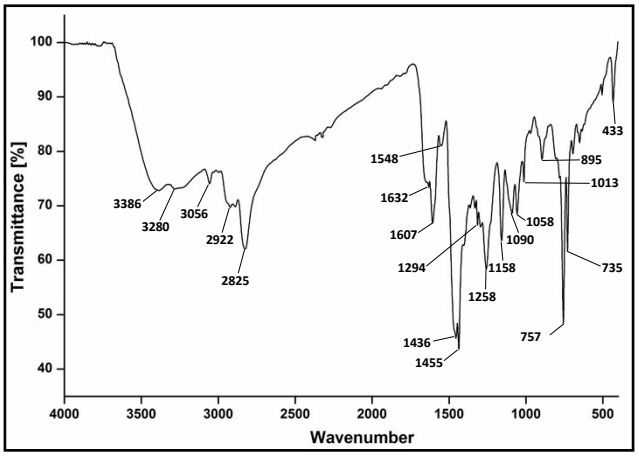

Figure S3. IR spectrum of **L.**

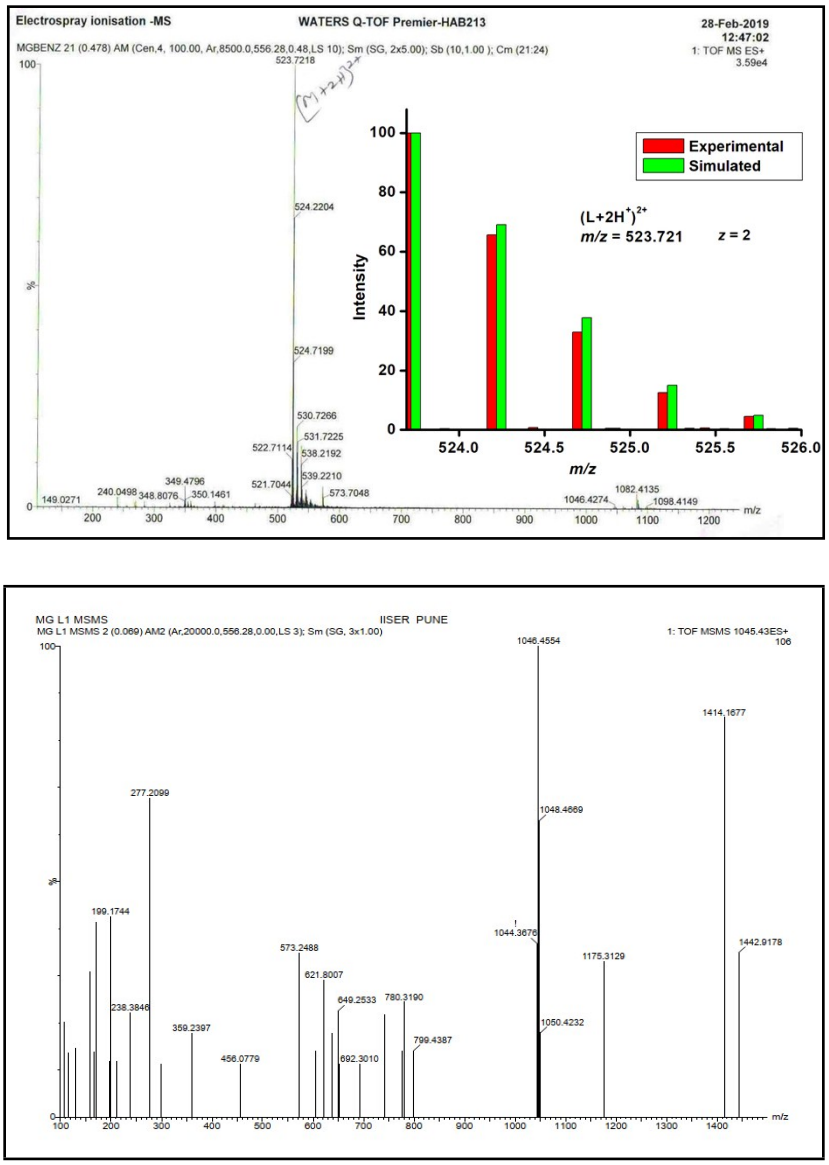

Figure S4. ESI-MS, (above) and MS/MS (below) spectra of **L** (positive mode).

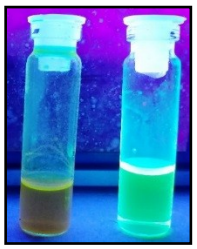

Figure S5. Color of the solution changes from yellow to fluoresecent green upon addition of Zn2+.

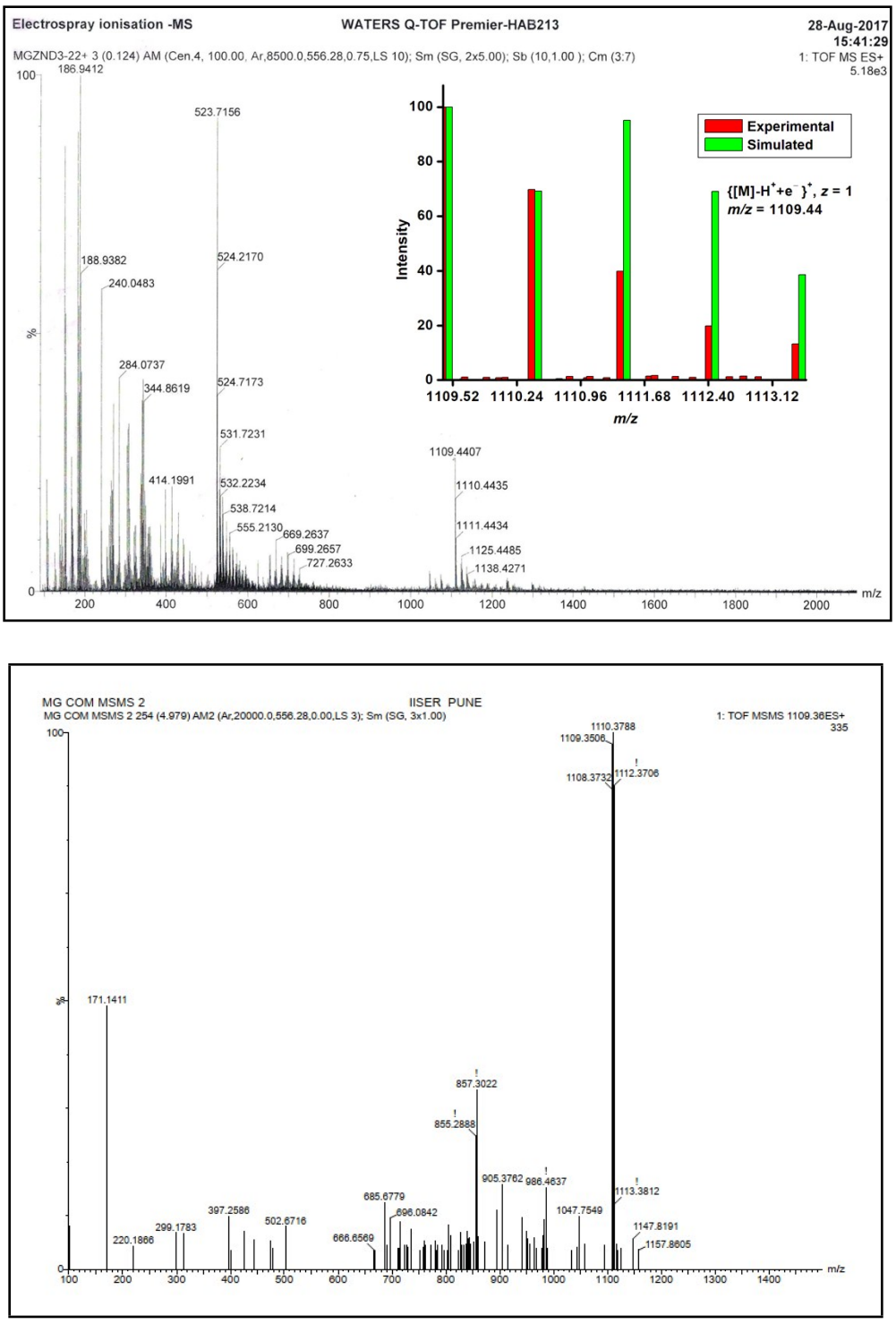

Figure S6. ESI-MS (above) and MS/MS spectra after addition of Zn2+ in crptand **L** (positive mode).

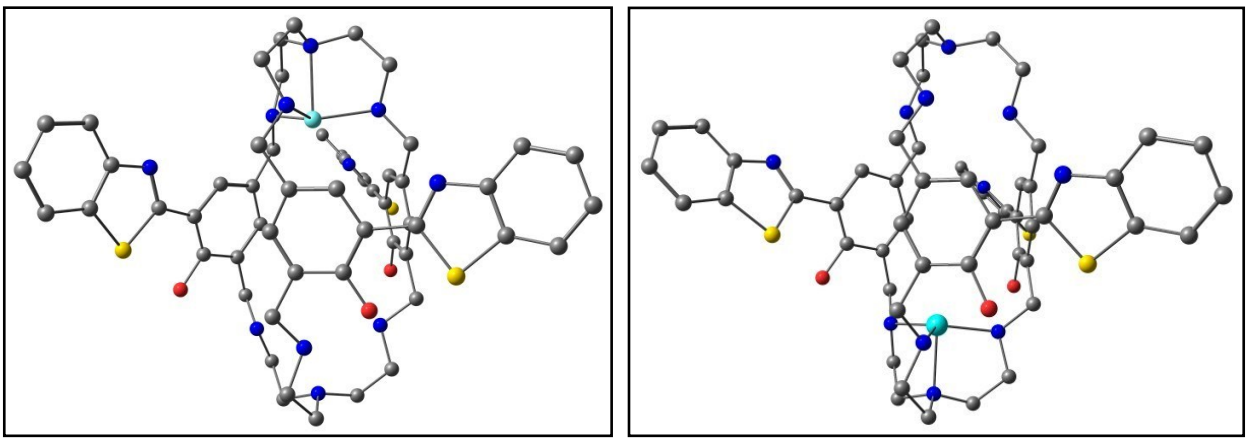

Figure S7. Optimized structures of Cryptand having metal at side cavity 1 (left) and cavity 2 (right).

Coordinates

Metal free Cryptand

		Coordinates (Angstroms)		
Serial No.	Atomic No.	X	Y	Z
1	16	2.720478	-5.10529	-0.55721
2	16	-5.86239	0.410725	1.122797
3	16	3.938153	4.379329	-1.77513
4	8	-3.69165	1.838048	2.061326
5	1	-3.06443	2.130312	2.789559
6	8	0.619417	-3.84533	-1.85055
7	1	0.170881	-3.38902	-2.64394
8	7	2.500174	-4.15947	1.873062
9	7	0.341582	-1.05879	-5.50739
10	7	-1.05331	1.114277	-3.82257
11	7	2.691294	-0.52911	-3.55893
12	7	-5.05702	-0.30969	-1.26092
13	7	-0.28395	1.131403	5.485993
14	7	-0.93595	-2.35526	-3.30765
15	7	-1.10932	-1.17938	3.761476
16	1	-0.44753	-1.89831	4.048634
17	6	-3.46538	1.213134	-0.23397
18	6	-1.50221	1.948079	-1.49738
19	7	-1.4767	2.594875	3.289692
20	6	-2.98607	1.890841	0.905194
21	6	-1.27379	-2.2996	1.535509
22	6	-0.07354	-2.99107	1.6419

23	1	0.407134	-3.15365	2.600617
24	6	0.591497	-3.51333	0.514524
25	6	-1.24043	-2.68232	-0.87828
26	6	-1.05197	2.623182	-0.3493
27	1	-0.11676	3.17727	-0.37935
28	6	-2.70289	1.259286	-1.42328
29	1	-3.08979	0.712094	-2.27387
30	6	1.880539	-4.17991	0.721175
31	6	3.975844	-5.49128	0.599243
32	6	-0.64433	2.016523	-2.74534
33	1	-0.59974	3.071436	-3.08127
34	1	0.381925	1.743048	-2.47365
35	6	-1.84085	-2.15544	0.259032
36	1	-2.78211	-1.62474	0.148564
37	6	-0.23591	1.304524	-5.02505
38	1	-0.47618	2.244651	-5.55511
39	1	0.808088	1.378435	-4.70368
40	6	-4.70406	0.429422	-0.24124
41	7	1.814291	0.550346	3.552564
42	1	0.868863	0.223455	3.335377
43	6	-1.76816	2.606935	0.839995
44	6	-0.35781	0.125065	-5.99616
45	1	-1.41845	-0.11839	-6.12862
46	1	0.008686	0.436674	-6.99142
47	6	-0.00342	-3.35702	-0.75576
48	6	3.673781	-4.88415	1.842276
49	6	-2.00523	-1.7535	2.745448
50	1	-2.69111	-0.96153	2.424637
51	1	-2.6421	-2.54908	3.178936
52	6	-1.47281	-2.52031	-4.66062
53	1	-2.30123	-1.81811	-4.8494
54	1	-1.88445	-3.53195	-4.76295
55	6	-1.91894	-2.59411	-2.23163
56	1	-2.40076	-3.55818	-2.45098
57	1	-2.71714	-1.83951	-2.20904
58	6	1.774068	-1.10009	-5.79441
59	1	2.101073	-0.09547	-6.08805
60	1	1.995504	-1.75323	-6.65797
61	6	5.995499	-6.40149	1.511497
62	1	6.901285	-6.9899	1.398256
63	6	3.166598	-1.02853	-2.26667

64	1	4.215763	-1.38257	-2.30915
65	1	2.567899	-1.91182	-2.01994
66	6	2.621559	-1.55775	-4.59717
67	1	2.164228	-2.45012	-4.15601
68	1	3.617332	-1.87049	-4.96474
69	6	5.137443	-6.24955	0.425412
70	1	5.366208	-6.71178	-0.52998
71	6	2.038745	0.366772	4.988803
72	1	3.081279	0.620624	5.215521
73	1	1.904748	-0.6846	5.295235
74	6	-0.35449	-2.32529	-5.69158
75	1	0.372094	-3.13311	-5.55518
76	1	-0.77202	-2.44388	-6.70961
77	6	1.131181	1.291787	5.810333
78	1	1.338976	1.135769	6.886149
79	1	1.412685	2.324721	5.582122
80	6	-0.89725	-0.10187	5.979548
81	1	-1.44704	0.061828	6.9223
82	1	-0.10423	-0.82007	6.218261
83	6	-1.03389	3.287011	4.502535
84	1	-1.6901	4.146035	4.68931
85	1	-0.01268	3.68612	4.383732
86	6	-1.83873	-0.73849	4.952543
87	1	-2.39612	-1.55995	5.440574
88	1	-2.58763	-0.00351	4.63344
89	6	-1.09649	2.331753	5.698521
90	1	-0.81084	2.872198	6.618119
91	1	-2.13793	2.019717	5.826432
92	6	4.553116	-5.04728	2.925597
93	1	4.316183	-4.5815	3.876883
94	6	5.704631	-5.80418	2.751545
95	1	6.390721	-5.93838	3.582733
96	6	2.778299	3.705732	-0.57613
97	6	-1.26464	3.369513	2.048308
98	1	-0.20969	3.641592	1.903431
99	1	-1.83008	4.30647	2.159331
100	6	3.224889	5.956309	-1.5249
101	6	2.193362	5.850797	-0.55817
102	6	1.473057	6.997027	-0.18907
103	1	0.68312	6.910574	0.549775
104	6	1.790233	8.214283	-0.7795

105	1	1.239387	9.10731	-0.49952
106	6	2.816204	8.306159	-1.73615
107	1	3.048354	9.267749	-2.18434
108	6	3.54173	7.180507	-2.11925
109	1	4.332624	7.25604	-2.85879
110	6	2.791825	-0.14625	2.687697
111	1	2.65543	-1.23731	2.686357
112	1	3.784868	0.047066	3.118458
113	6	-6.26912	-0.93469	-1.05407
114	6	-6.88235	-0.66539	0.193444
115	6	-8.11126	-1.23685	0.536256
116	1	-8.57752	-1.02838	1.494338
117	6	-8.7269	-2.08066	-0.38473
118	1	-9.6834	-2.53258	-0.1389
119	6	-8.12734	-2.35433	-1.62756
120	1	-8.62874	-3.01596	-2.32792
121	6	-6.90516	-1.78975	-1.96935
122	1	-6.43154	-1.99189	-2.92474
123	6	2.681389	1.77645	1.032356
124	6	2.814435	2.265196	-0.28701
125	6	2.993583	1.350897	-1.34306
126	6	3.024323	-0.0246	-1.13525
127	6	2.923538	-0.48383	0.186039
128	1	2.961498	-1.55228	0.383351
129	6	2.771562	0.38251	1.264891
130	7	1.974119	4.580577	-0.05528
131	8	2.500476	2.632771	2.058602
132	1	2.190866	2.065992	2.825051
133	1	-2.02467	1.304652	-4.06279
134	1	3.310414	0.210478	-3.88302
135	1	-0.94977	1.721421	3.239419
136	1	-0.57284	-1.39926	-3.2477
137	1	3.05318	1.747561	-2.35141

Cryptand with metal (Outside)

		Coordinates (Angstroms)		
Serial No.	Atomic No.	X	Y	Z
1	16	-3.85649	4.9666	-0.26736
2	16	-2.88601	-5.02544	-2.3821
3	16	3.549752	-0.02906	4.320948

4	8	-0.298	-4.08991	-2.17613
5	1	0.531924	-3.69081	-2.58458
6	8	-4.3578	2.382015	0.562741
7	1	-2.6146	3.670647	4.406462
8	7	-2.16246	4.597055	-2.22821
9	7	-3.68769	0.439727	4.65625
10	7	-1.9093	-1.8483	3.67359
11	7	-1.3047	2.190356	3.574669
12	7	-3.96995	-4.16353	-0.16183
13	7	2.814795	-0.4276	-4.11196
14	7	-4.35498	0.138832	1.903309
15	7	-0.12062	0.047978	-3.64892
16	1	-0.05245	1.055173	-3.50598
17	6	-1.5926	-3.66449	-0.21276
18	6	-0.54326	-2.55342	1.701693
19	7	1.950686	-2.66656	-2.41487
20	6	-0.36936	-3.61673	-0.90908
21	6	-2.27529	0.383614	-2.44982
22	6	-2.31588	1.774021	-2.40868
23	1	-1.82053	2.372884	-3.16758
24	6	-2.99094	2.473349	-1.39127
25	6	-3.68438	0.316041	-0.45602
26	6	0.670576	-2.54675	0.994471
27	1	1.556596	-2.11464	1.457771
28	6	-1.65058	-3.12414	1.091693
29	1	-2.60959	-3.14771	1.59368
30	6	-2.91973	3.938982	-1.39067
31	6	-3.1549	6.37468	-1.0331
32	6	-0.57643	-1.92539	3.081699
33	1	0.145667	-2.45895	3.732536
34	1	-0.20649	-0.89537	3.002941
35	6	-2.9638	-0.32964	-1.45673
36	1	-2.94914	-1.41581	-1.47233
37	6	-1.89262	-1.2352	5.004266
38	1	-1.49828	-1.91647	5.781423
39	1	-1.21866	-0.37331	4.960397
40	6	-2.82349	-4.21808	-0.78764
41	7	3.221224	1.492964	-1.8223
42	1	2.441331	0.841531	-1.95115
43	6	0.777256	-3.07176	-0.28584
44	6	-3.28349	-0.73815	5.415062

45	1	-4.01293	-1.53778	5.237212
46	1	-3.2938	-0.54886	6.504769
47	6	-3.68933	1.730089	-0.41515
48	6	-2.2702	5.961643	-2.05872
49	6	-1.5443	-0.33214	-3.56601
50	1	-1.59987	-1.41686	-3.41411
51	1	-2.05974	-0.1223	-4.52353
52	6	-5.27897	-0.35491	2.925885
53	1	-5.13347	-1.4311	3.115354
54	1	-6.30917	-0.22432	2.571268
55	6	-4.50259	-0.45926	0.560836
56	1	-5.56804	-0.38503	0.297532
57	1	-4.24323	-1.5263	0.537029
58	6	-3.17833	1.716384	5.155148
59	1	-2.37523	1.515803	5.874741
60	1	-3.95687	2.267791	5.713125
61	6	-2.66544	8.671458	-1.508
62	1	-2.80985	9.729234	-1.30605
63	6	-0.97257	2.735385	2.256029
64	1	-1.12322	3.831921	2.210088
65	1	-1.68521	2.314107	1.537292
66	6	-2.62636	2.625788	4.045192
67	1	-4.50022	1.689632	1.297527
68	1	-3.31189	2.604695	3.192198
69	6	-3.35625	7.729161	-0.75039
70	1	-4.03514	8.041628	0.037819
71	6	3.848266	1.662201	-3.15929
72	1	4.825612	2.139032	-3.02567
73	1	3.242478	2.352097	-3.76447
74	6	-5.07756	0.455981	4.214256
75	1	-5.35624	1.494295	4.003714
76	1	-5.77425	0.091216	4.991933
77	6	4.048899	0.337727	-3.90339
78	1	4.562819	0.562058	-4.85784
79	1	4.724867	-0.29351	-3.32227
80	6	1.905486	0.180914	-5.08924
81	1	2.240407	-0.00303	-6.12757
82	1	1.928858	1.268228	-4.9531
83	6	3.216408	-2.69591	-3.16163
84	1	3.440644	-3.73167	-3.44801
85	1	4.054145	-2.34714	-2.53963

86	6	0.451679	-0.28098	-4.95227
87	1	-0.11896	0.16216	-5.79184
88	1	0.378315	-1.36785	-5.08319
89	6	3.103299	-1.84039	-4.42241
90	1	4.024495	-1.93929	-5.02102
91	1	2.288023	-2.23666	-5.03431
92	6	-1.58109	6.927528	-2.81123
93	1	-0.90539	6.606073	-3.59799
94	6	-1.78468	8.272526	-2.53043
95	1	-1.25828	9.028243	-3.10694
96	6	3.571952	0.528771	2.647178
97	6	2.101678	-3.09882	-1.01341
98	1	2.845662	-2.49576	-0.4688
99	1	2.493832	-4.12618	-1.03878
100	6	4.677833	-1.30458	3.90184
101	6	5.002533	-1.21153	2.52869
102	6	5.88135	-2.14842	1.962226
103	1	6.10812	-2.10474	0.902475
104	6	6.422447	-3.13625	2.777402
105	1	7.103436	-3.86504	2.347642
106	6	6.101975	-3.21044	4.143218
107	1	6.540348	-3.99052	4.758693
108	6	5.222135	-2.29686	4.718707
109	1	4.966778	-2.35646	5.772258
110	6	2.641289	2.812147	-1.34914
111	1	1.835168	3.118336	-2.02889
112	1	3.451146	3.543751	-1.42116
113	6	-4.98281	-4.7609	-0.88265
114	6	-4.59526	-5.30337	-2.13166
115	6	-5.52135	-5.93593	-2.96667
116	1	-5.22038	-6.35008	-3.92457
117	6	-6.84341	-6.02433	-2.53821
118	1	-7.57837	-6.51388	-3.17118
119	6	-7.23953	-5.48924	-1.29845
120	1	-8.27757	-5.57189	-0.98831
121	6	-6.32171	-4.8587	-0.46827
122	1	-6.61329	-4.44206	0.491022
123	6	3.149623	2.26776	0.98652
124	6	2.703427	1.584264	2.151375
125	6	1.367563	1.745232	2.579231
126	6	0.444041	2.437513	1.799947

127	6	0.834912	2.810434	0.492349
128	1	0.079192	3.1787	-0.20088
129	6	2.151713	2.690145	0.069393
130	7	4.368486	-0.17237	1.854677
131	8	4.419775	2.369752	0.671178
132	1	-2.29511	-2.7889	3.751859
133	1	-0.6088	2.519642	4.24381
134	1	1.583672	-1.71072	-2.44398
135	1	-3.40875	-0.02012	2.260269
136	1	1.03666	1.260338	3.49345
137	30	4.745839	0.694615	-0.25028
138	7	6.664857	-0.47259	-1.44342
139	8	7.566261	-1.06148	-1.99597
140	8	5.547274	-1.06552	-1.12684
141	8	6.715222	0.767122	-1.12513

Cryptand with Metal (Cavity 1)

		Coordinates (Angstroms)		
Serial No.	Atomic No.	X	Y	Z
1	16	1.666889	5.515089	0.205807
2	16	5.270196	-3.6292	0.53258
3	8	0.306062	3.775536	1.937736
4	1	0.083957	3.319974	2.849682
5	7	1.160864	4.382903	-2.09502
6	7	0.899169	1.094986	5.816393
7	7	-0.54547	-1.26339	4.58094
8	7	2.67619	1.077129	3.413631
9	7	-0.82311	-0.97949	-4.89424
10	7	-0.65192	2.243833	3.754134
11	7	-2.15282	0.887432	-3.17771
12	1	-1.71909	1.738018	-3.54397
13	6	-3.19165	-1.93679	1.082465
14	6	-1.2194	-2.41826	2.481732
15	7	-0.91492	-2.47384	-2.40013
16	6	-2.36944	-2.27136	0.016239
17	6	-2.04533	1.909792	-0.94405
18	6	-1.05937	2.833887	-1.2995
19	1	-0.91097	3.153464	-2.3281
20	6	-0.23317	3.448402	-0.34718
21	6	-1.4762	2.25941	1.405304

22	6	-0.4789	-2.69678	1.335544
23	1	0.564249	-2.98871	1.436527
24	6	-2.5844	-2.07118	2.358012
25	6	0.814064	4.357619	-0.83006
26	6	2.523817	6.091341	-1.20726
27	6	-0.58784	-2.53842	3.856423
28	1	-1.10918	-3.33248	4.421148
29	1	0.445109	-2.87969	3.726548
30	6	-2.23129	1.631787	0.422123
31	1	-3.0139	0.940991	0.724726
32	6	0.302859	-1.34014	5.775903
33	1	-0.00556	-2.14662	6.466948
34	1	1.320885	-1.58815	5.447952
35	6	-4.55836	-1.49012	0.793957
36	7	1.416794	0.100795	-3.40073
37	6	-1.05684	-2.66312	0.046224
38	6	0.318962	-0.0228	6.560824
39	1	-0.71394	0.233846	6.826092
40	1	0.840473	-0.19403	7.519054
41	6	-0.45261	3.170329	1.025512
42	6	2.1162	5.351046	-2.34287
43	6	-2.96266	1.316716	-1.9896
44	1	-3.49112	0.439323	-1.60408
45	1	-3.71932	2.038097	-2.32914
46	6	-1.02008	2.486616	5.157351
47	1	-1.78504	1.76488	5.487767
48	1	-1.45976	3.486608	5.250303
49	6	-1.81569	2.060484	2.872468
50	1	-2.55689	2.821264	3.155323
51	1	-2.29604	1.082575	3.025542
52	6	2.358261	1.160355	5.880092
53	1	2.735769	0.134486	5.973131
54	1	2.712803	1.69693	6.779164
55	6	4.035756	7.365347	-2.55298
56	1	4.780543	8.148985	-2.6531
57	8	4.15409	-1.19201	2.219808
58	1	4.353902	-2.14392	2.156642
59	6	3.525612	1.502107	2.295006
60	1	4.601273	1.469964	2.552424
61	1	3.286332	2.546539	2.065978
62	6	3.010863	1.79562	4.64676

63	1	2.692539	2.840035	4.532485
64	1	4.100896	1.826759	4.834128
65	6	3.487599	7.100511	-1.30202
66	1	3.79655	7.667232	-0.42929
67	6	1.258727	0.411615	-4.84903
68	1	2.23746	0.53808	-5.32795
69	1	0.734604	1.370415	-4.93326
70	6	0.228114	2.374764	6.036937
71	1	0.915893	3.180739	5.764168
72	1	-0.04835	2.538171	7.092662
73	6	0.489868	-0.71926	-5.54674
74	1	0.366843	-0.48889	-6.61268
75	1	1.084716	-1.63751	-5.49031
76	6	-1.91867	-0.11447	-5.41228
77	1	-2.44908	-0.59701	-6.24322
78	1	-1.46666	0.798878	-5.81488
79	6	-0.55138	-3.14713	-3.67871
80	1	-0.88146	-4.19324	-3.67084
81	1	0.541849	-3.15602	-3.75085
82	6	-2.9055	0.268184	-4.30017
83	1	-3.66305	0.9548	-4.69739
84	1	-3.43463	-0.60705	-3.90744
85	6	-1.1901	-2.4207	-4.8677
86	1	-0.91479	-2.92152	-5.80519
87	1	-2.27989	-2.49026	-4.78147
88	6	2.683949	5.633382	-3.59739
89	1	2.362782	5.074677	-4.47154
90	6	3.636781	6.63788	-3.69121
91	1	4.079164	6.872781	-4.65462
92	6	3.812538	-2.93168	-0.216
93	6	-0.33596	-3.14232	-1.19085
94	1	0.741989	-2.96079	-1.14943
95	1	-0.46975	-4.22825	-1.30257
96	6	4.80806	-5.19346	-0.10894
97	6	3.620274	-5.05073	-0.86657
98	6	3.070755	-6.17634	-1.50079
99	1	2.160965	-6.07426	-2.08434
100	6	3.708934	-7.40239	-1.36723
101	1	3.294865	-8.2803	-1.85342
102	6	4.888284	-7.52603	-0.60988
103	1	5.368451	-8.49545	-0.52059

104	6	5.452582	-6.42475	0.028253
105	1	6.363584	-6.52434	0.609186
106	6	2.216877	1.108802	-2.62729
107	1	1.632212	2.023946	-2.49423
108	1	3.102364	1.372789	-3.22294
109	6	-6.8874	-0.64966	0.789125
110	6	-6.35289	-1.06671	-0.45465
111	6	-7.15805	-1.00388	-1.6044
112	1	-6.75979	-1.33964	-2.55688
113	6	-8.45777	-0.53015	-1.48899
114	1	-9.09361	-0.48406	-2.36775
115	6	-8.97045	-0.115	-0.24546
116	1	-9.99166	0.247484	-0.18132
117	6	-8.19301	-0.16871	0.908185
118	1	-8.59475	0.147125	1.86539
119	6	2.973969	-0.83241	-1.20636
120	6	3.496079	-1.49856	-0.11246
121	6	3.66662	-0.70273	1.050225
122	6	3.311942	0.667162	1.04686
123	6	2.808205	1.238026	-0.12037
124	1	2.557008	2.295692	-0.11855
125	6	2.63554	0.495172	-1.31121
126	7	3.08774	-3.76999	-0.90166
127	1	-1.49619	-1.03893	4.871094
128	1	2.83809	0.084524	3.573896
129	1	-0.04346	1.415635	3.741569
130	8	-3.24775	-1.83249	3.52742
131	1	-4.19567	-2.04426	3.454852
132	16	-5.65879	-0.82475	2.025019
133	7	-5.04699	-1.52328	-0.41673
134	30	-0.53445	-0.40008	-2.72738
135	1	1.955077	-0.77048	-3.33038
136	1	-1.93281	-2.54548	-2.2855

Cryptand with metal (Cavity 2)

		Coordinates (Angstroms)		
Serial No.	Atomic No.	X	Y	Z
1	16	-5.22915	-2.31499	0.322507
2	16	-1.04039	6.336437	0.325894
3	8	-2.8677	-3.06726	2.007163

4	1	-3.74887	-3.39684	1.744481
5	7	-4.32094	-3.13468	-1.98738
6	7	-0.56931	-0.03171	5.542332
7	7	1.60972	0.700768	3.777833
8	7	-1.95364	1.291281	3.344981
9	7	0.869915	0.081981	-5.45491
10	7	-0.746	-2.14158	3.563568
11	7	0.354759	-2.28315	-3.58153
12	1	-0.35115	-2.94748	-3.89804
13	6	3.560013	-0.71654	0.078254
14	6	2.472122	1.026163	1.453933
15	7	2.530953	1.337342	-3.29734
16	6	3.14656	-0.09516	-1.12245
17	6	-0.16192	-2.75369	-1.19125
18	6	-1.52996	-2.74121	-1.44272
19	1	-1.9064	-2.6559	-2.45434
20	6	-2.49112	-2.82556	-0.41247
21	6	-0.65453	-2.93943	1.194867
22	6	2.047475	1.656555	0.28763
23	1	1.481807	2.585591	0.346944
24	6	3.258815	-0.14723	1.335028
25	6	-3.9123	-2.81984	-0.7993
26	6	-6.39025	-2.62183	-0.95649
27	6	2.25493	1.653872	2.803975
28	1	3.207317	1.976902	3.246117
29	1	1.609769	2.53353	2.716111
30	6	0.258482	-2.83757	0.144597
31	1	1.322665	-2.85781	0.366023
32	6	1.527579	1.264127	5.155428
33	1	2.531182	1.448709	5.55725
34	1	1.027045	2.236667	5.087712
35	6	4.369937	-1.95487	-0.02717
36	7	-1.24006	0.934555	-3.71137
37	1	-0.49513	0.310691	-3.39755
38	6	2.411675	1.108156	-0.95471
39	6	0.768294	0.317744	6.091921
40	1	1.339479	-0.60931	6.206777
41	1	0.684026	0.764452	7.091501
42	6	-2.03311	-2.9469	0.909789
43	6	-5.69412	-3.0386	-2.11775
44	6	0.882706	-2.71686	-2.29082

45	1	1.674675	-2.01055	-2.00682
46	1	1.364696	-3.71324	-2.33543
47	6	-0.42338	-2.45783	4.985173
48	1	0.667413	-2.50745	5.077432
49	1	-0.81419	-3.44592	5.257328
50	6	-0.17733	-3.15672	2.608423
51	1	-0.4773	-4.15126	2.965318
52	1	0.913548	-3.09879	2.656607
53	6	-1.59773	1.010436	5.800264
54	1	-1.08856	1.976033	5.884272
55	1	-2.11003	0.838158	6.756055
56	6	-8.47267	-2.78883	-2.10921
57	1	-9.5547	-2.70079	-2.12205
58	8	-1.52465	3.719856	2.063721
59	1	-1.14305	4.608402	1.920516
60	6	-2.95136	1.335743	2.21703
61	1	-3.76919	1.999639	2.530155
62	1	-3.36883	0.332707	2.091951
63	6	-2.62325	1.080818	4.663094
64	1	-3.20645	0.155342	4.596555
65	1	-3.33335	1.892278	4.864255
66	6	-7.77969	-2.49198	-0.9375
67	1	-8.30844	-2.17559	-0.04429
68	6	-1.54183	0.555178	-5.09105
69	1	-2.36217	1.180891	-5.46484
70	1	-1.87767	-0.49397	-5.17806
71	6	-1.01364	-1.39902	5.922746
72	1	-2.10628	-1.43262	5.858407
73	1	-0.75035	-1.62848	6.963566
74	6	-0.30779	0.790967	-5.9667
75	1	-0.53229	0.52088	-7.01335
76	1	-0.09335	1.864579	-5.95517
77	6	0.924486	-1.3433	-5.8005
78	1	1.578767	-1.5254	-6.6696
79	1	-0.07716	-1.66901	-6.10287
80	6	2.383067	1.890634	-4.64083
81	1	3.308006	2.419977	-4.90414
82	1	1.567981	2.619334	-4.62021
83	6	1.389785	-2.20686	-4.62271
84	1	1.687052	-3.20322	-4.99301
85	1	2.286726	-1.76472	-4.17381

86	6	2.125863	0.786083	-5.67601
87	1	2.193397	1.244025	-6.67906
88	1	2.949863	0.065659	-5.61508
89	6	-6.41382	-3.33209	-3.28673
90	1	-5.88038	-3.65666	-4.17398
91	6	-7.79658	-3.20408	-3.27098
92	1	-8.36694	-3.43059	-4.16637
93	6	-0.48906	4.837421	-0.47825
94	6	2.090479	1.819237	-2.17634
95	1	-1.09728	3.19735	-2.48011
96	1	1.53103	2.754723	-2.17662
97	6	0.366105	7.159981	-0.32565
98	6	1.103388	6.252529	-1.12471
99	6	2.262089	6.694709	-1.78122
100	1	2.828601	6.002174	-2.39526
101	6	2.654188	8.0185	-1.62958
102	1	3.546819	8.375203	-2.13389
103	6	1.909591	8.907921	-0.83367
104	1	2.236013	9.938406	-0.7333
105	6	0.756538	8.49169	-0.17251
106	1	0.182961	9.183844	0.435223
107	6	-2.37706	0.843427	-2.80289
108	1	-2.69098	-0.19154	-2.58002
109	1	-3.23701	1.318337	-3.29596
110	6	5.415399	-4.21234	0.277958
111	6	5.820909	-3.43978	-0.83806
112	6	6.786851	-3.95393	-1.7162
113	1	7.099966	-3.35917	-2.56793
114	6	7.320649	-5.21259	-1.46712
115	1	8.070331	-5.62033	-2.13821
116	6	6.906534	-5.96675	-0.35529
117	1	7.339968	-6.94676	-0.18022
118	6	5.949135	-5.47665	0.531181
119	1	5.63527	-6.06308	1.388758
120	6	-1.45341	2.815711	-1.5299
121	6	-1.24079	3.573217	-0.36888
122	6	-1.7079	3.069099	0.85908
123	6	-2.35845	1.824954	0.918021
124	6	-2.5456	1.100479	-0.26647
125	1	-3.07024	0.149051	-0.22191
126	6	-2.10753	1.583944	-1.50322

127	7	0.597523	4.961217	-1.17847
128	1	3.053118	0.447006	-3.10619
129	8	3.692687	-0.65432	2.542889
130	1	4.327887	-1.38543	2.399294
131	16	4.199792	-3.31813	1.173039
132	7	5.21908	-2.19972	-0.96584
133	30	-0.31311	-0.06929	3.335011
134	1	2.258135	-0.09573	3.796929
135	1	-1.54883	2.234936	3.351157
136	1	-1.76125	-2.24017	3.447958

Thermal Corrections

Parameters (Energy given in HF)	Metal Free Cryptand	Metal in Cavity 1	Metal in Cavity 2	Metal Outside to Cryptand
Zero-point correction	1.138768	1.120793	1.122310	1.147796
Thermal correction to energy	1.203321	1.186138	1.187426	1.217912
Thermal correction to enthalpy	1.204265	1.187082	1.188371	1.218856
Thermal correction to Gibbs free energy	1.035348	1.018499	1.020781	1.036068
Sum of electronic and zero-point energies	-4231.434994	-4295.173033	-4295.257201	-4576.682393
Sum of electronic and thermal energies	-4231.370441	-4295.107687	-4295.192084	-4576.612278
Sum of electronic and thermal enthalpies	-4231.369497	-4295.106743	-4295.191140	-4576.611333
Sum of electronic and thermal free energies	-4231.538414	-4295.275326	-4295.358730	-4576.794122