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

Electronic Supporting Information

Synthesis of advanced metal-guided photochromic system for molecular keypad lock: A detailed experimental findings and theoretical understanding

Nandagopal Bar, Pranesh Chowdhury*, Debrupa Biswas, Arindam Ray, Gourab Kanti Das

Polymer & Nano Research Laboratory, Department of Chemistry, Siksha Bhavana, Visva-Bharati University, Santiniketan – 731 235, India

*Corresponding Author: E. mail: pranesh_02@yahoo.co.in.

Telephone: + 91 3463 264983; FAX: +91 3463 261526

Content **Page Number**

1. ^{1}H-NMR Spectra of the ligand (L):

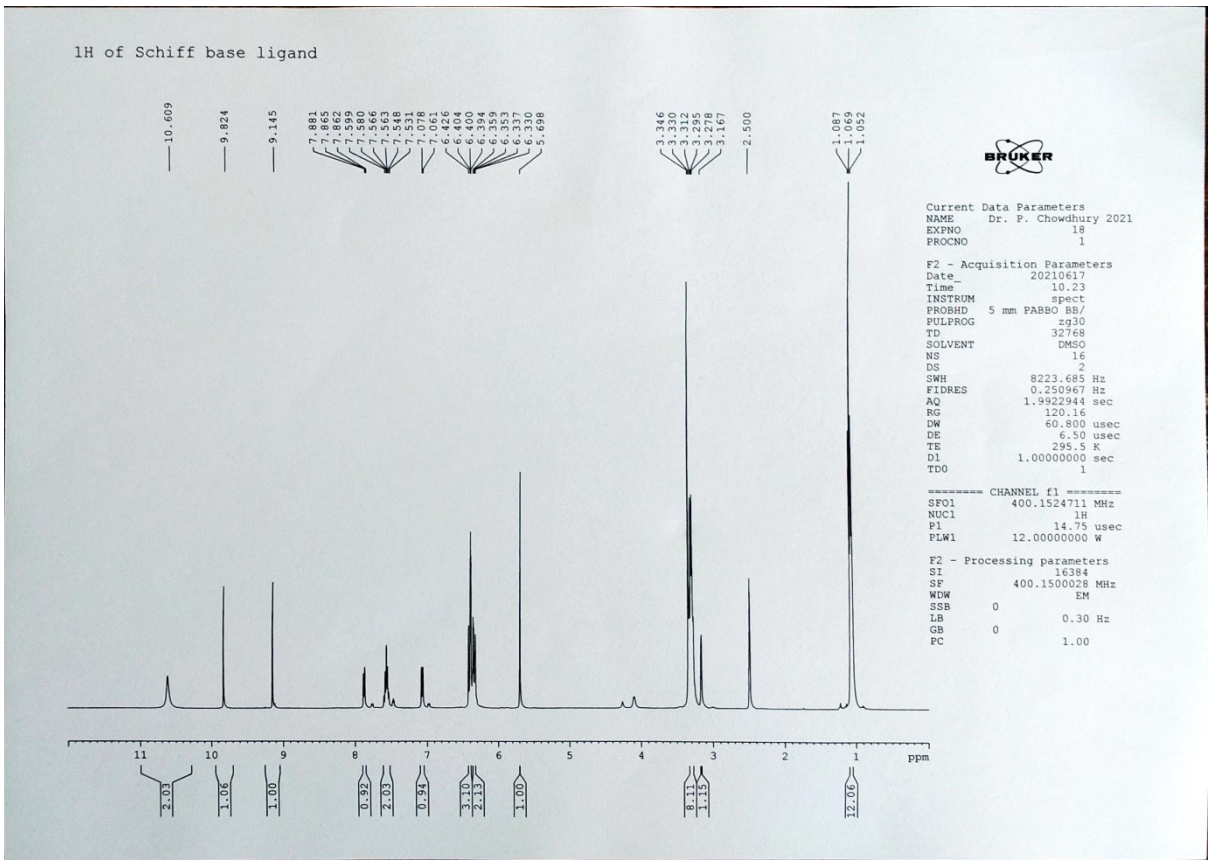


Fig. S1: ^{1}H-NMR spectra of the ligand (L) in d^{6}-DMSO

2. ^{13}C-NMR Spectra of the ligand (L):

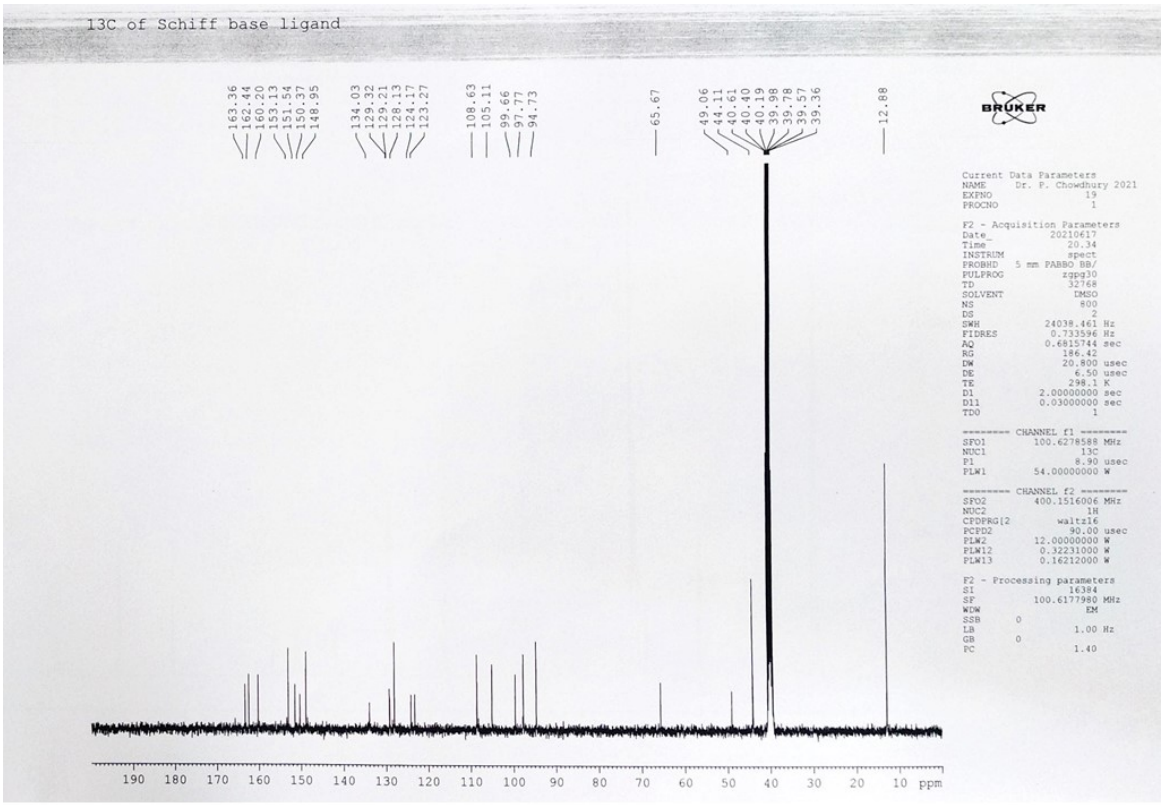


Fig. S2: ^{13}C-NMR spectra of the ligand (L) in d^6-DMSO

3. ^{1}H-NMR Spectra of the 1:

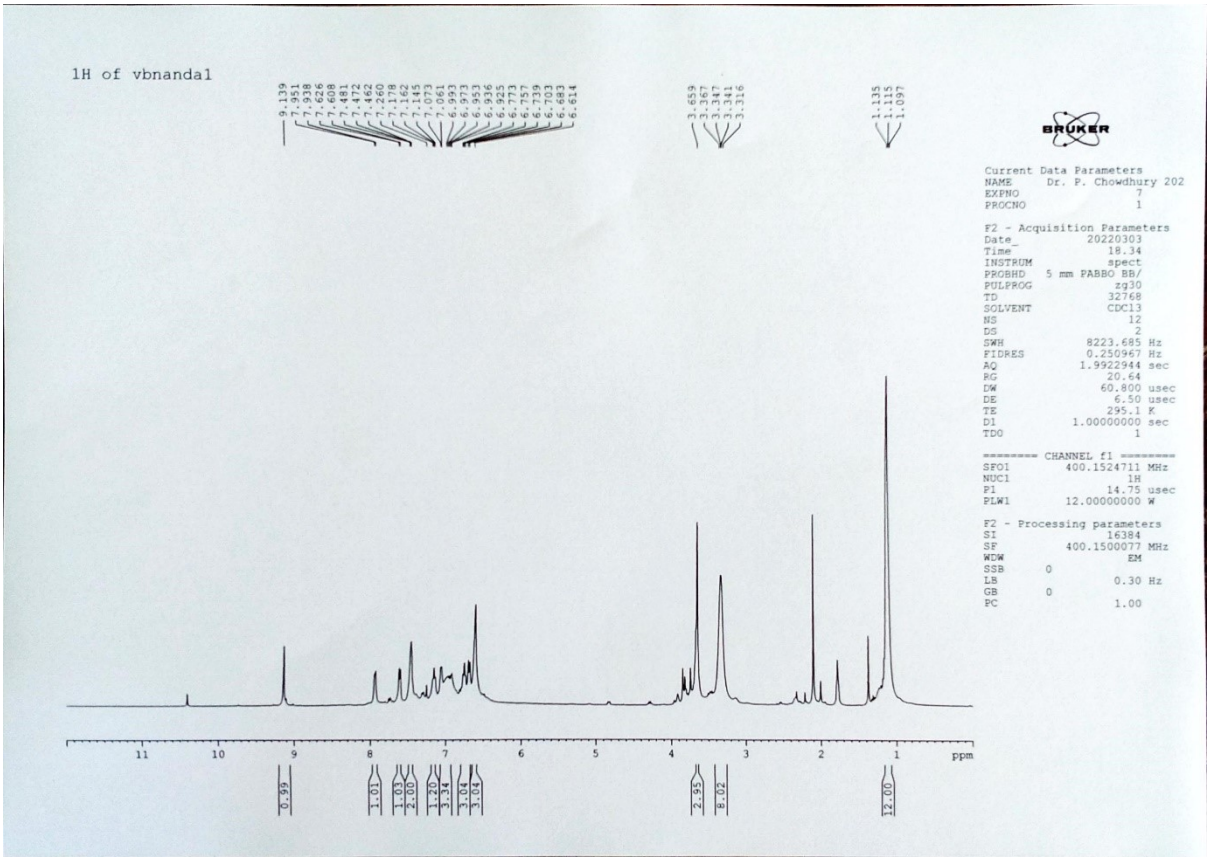


Fig. S3: ^{1}H-NMR spectra of the 1 in $CDCl_3$

4. ^{13}C-NMR Spectra of the 1:

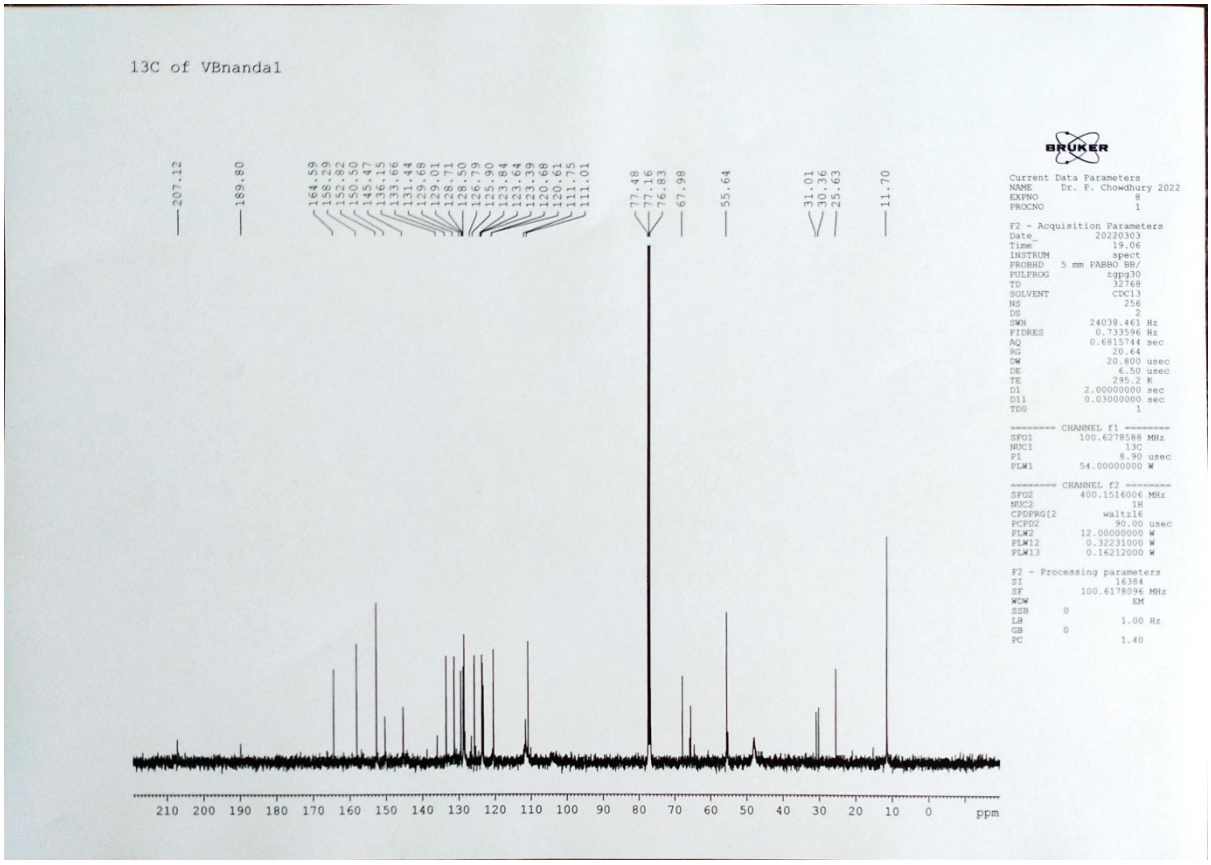


Fig. S4: ^{13}C-NMR spectra of the 1 in $CDCl_3$

5. ESI-Mass spectrometry of Ligand (L):

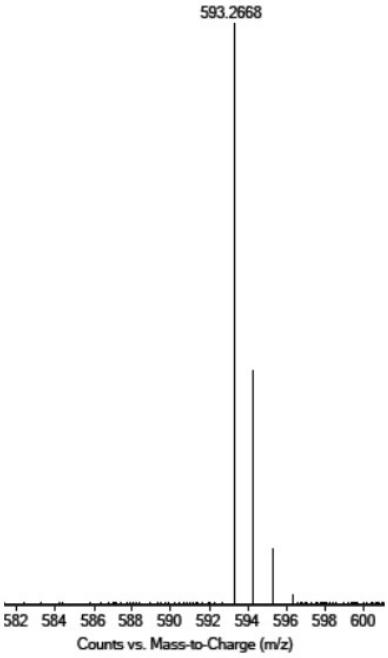


Fig. S5: ESI-Mass spectrometry of the ligand (L), m/z =593

6. FT-IR spectra of the ligand (L):

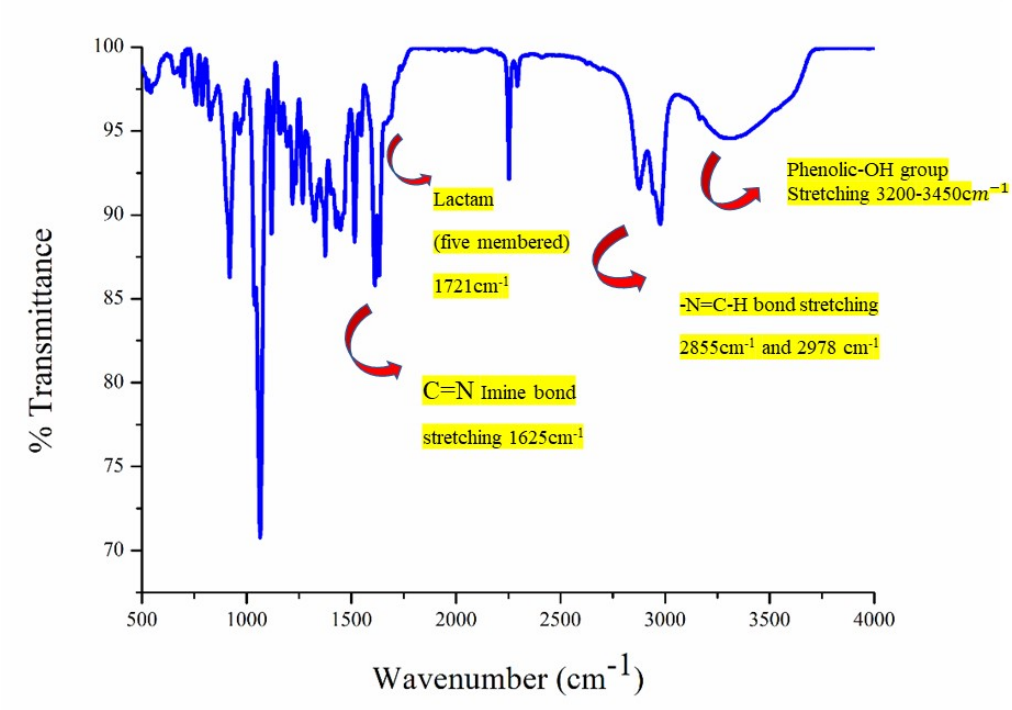


Fig. S6: FT-IR spectra of the ligand (L)

7. The non-photochromic behaviour of the Ligand (L):

UV-Vis spectra:

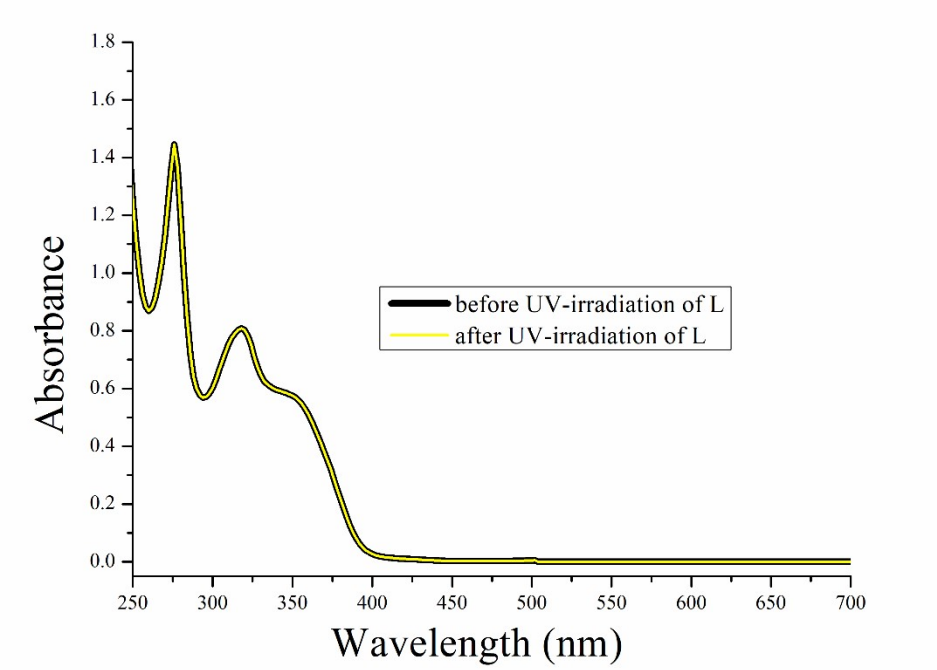


Fig. S7: Absorption spectra of the ligand (L) before and after UV-irradiation

FT-IR spectra:

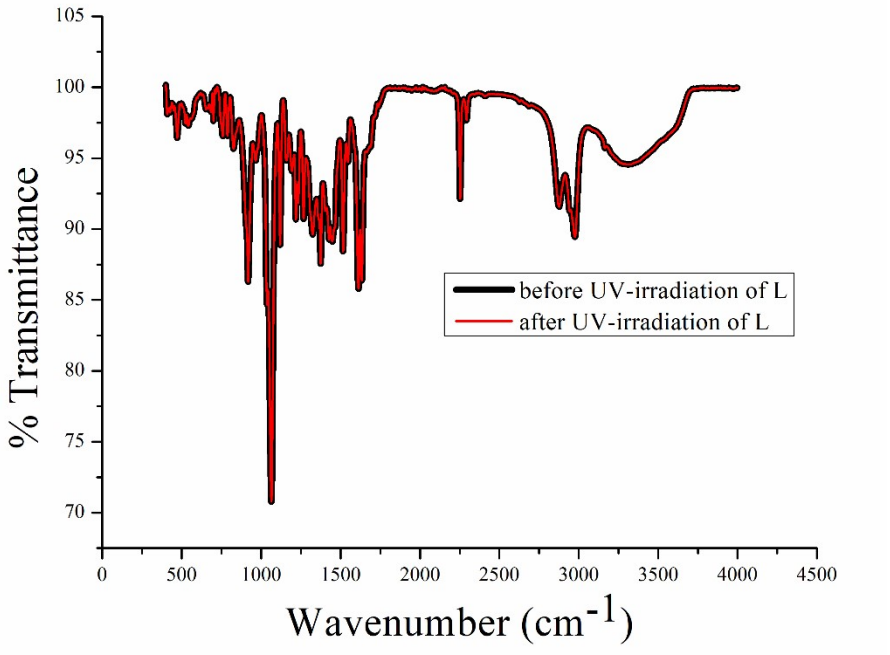


Fig. S8: FT-IR spectra of the ligand (L) before and after UV-irradiation

8. Gaussian 09 Full Reference:

Gaussian 09, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

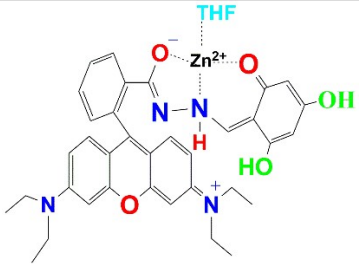
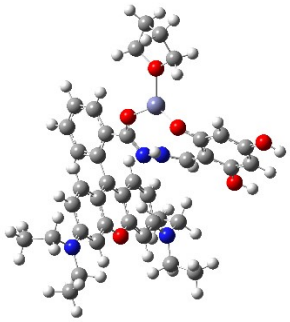
Computational methods:

Computational Method used: Hybrid DFT functional method M06-2X, M06 and M06L.

Basis set used: LANL2DZ for zinc atom and 6-31G (d, p) basis set for other atoms.

Solvent used for calculation by PCM model: Tetrahydrofuran (THF).

9. Coordinate of the stationary points associated to the Potential Energy Surface (PES) using M06-2X hybrid functional:

St.Pt.	General Structure	Ball & Stick model
K		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.50730	-3.11396	-1.53127
C	-1.67460	-2.06817	-1.85753
C	-1.69205	-0.84896	-1.16260
C	-2.60438	-0.73981	-0.11184
C	-3.45673	-1.77395	0.24381
C	-3.44424	-2.99363	-0.46420
C	-0.78324	0.29158	-1.53070
C	-2.06978	1.53416	0.25280
C	-1.14210	1.54706	-0.78752
C	-0.57138	2.78903	-1.10586
H	0.13104	2.84818	-1.93466
C	-0.88836	3.94143	-0.42444
C	-1.82459	3.92226	0.65058
C	-2.41472	2.67977	0.95735
H	-2.46864	-4.01639	-2.12650
H	-4.12450	-1.59755	1.07625
H	-0.43246	4.86898	-0.74125
H	-3.16733	2.56861	1.72453
C	-0.67015	0.49019	-3.03512
C	-1.67246	0.87473	-3.91083
C	0.61441	0.22391	-3.51215
C	-1.34740	0.98351	-5.26285
C	0.95068	0.32595	-4.86128
C	-0.05536	0.71232	-5.73612
H	-2.11413	1.28475	-5.96919
H	0.15526	0.80654	-6.79540
H	1.95660	0.11004	-5.20461
N	-4.29267	-4.00863	-0.14633
C	-5.35128	-3.83410	0.84252
C	-4.24370	-5.29913	-0.82752
C	-4.88159	-4.11866	2.26680

Frequencies

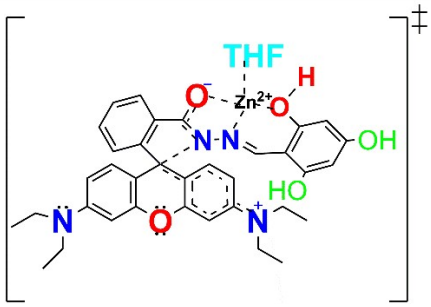
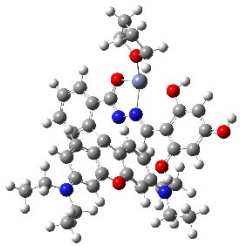
-11.2892	11.7574	16.2658
17.2957	22.3679	26.4150
31.1382	32.4399	39.4681
44.0908	56.4897	59.6142
62.3065	65.0567	71.2232
78.4223	88.3354	97.3790
102.6551	104.1226	114.8681
125.7310	133.2628	138.2143
147.9045	161.0645	163.2915
169.1294	178.4667	185.5215
194.9893	206.0796	210.7513
217.6631	219.4732	223.9428
227.4134	231.1345	236.1403
250.0909	259.0691	266.7758
270.0419	276.3883	291.9930
305.2713	312.6283	328.1308
334.5179	348.7287	357.9098
361.9978	365.3077	386.9221
399.1181	408.9735	419.4378
428.2684	429.9044	434.0423
442.9231	449.9666	462.2120
467.7261	475.4899	479.6125
486.5360	496.1290	498.7286
525.0582	530.2223	534.8861
554.3693	554.7165	565.2363
570.9367	589.5197	601.7652
610.3103	614.6591	617.6145
620.8531	649.3351	651.4076
654.2079	659.7340	682.0345
695.7229	704.3535	709.4429
716.4985	722.0982	727.1625
731.3062	744.5509	759.2346
777.1205	788.9418	791.3153
795.5981	805.1732	807.9126
809.8693	824.3008	826.8353

C	-5.05022	-5.31726	-2.12316	837.6355	846.0595	855.4945
N	-2.13753	5.05212	1.35607	865.7769	867.2997	871.6333
C	-3.24987	4.97637	2.31003	873.0764	893.6953	894.8107
C	-1.71117	6.35958	0.86010	910.4417	912.4312	938.5560
C	-3.50998	6.25250	3.09604	946.4264	949.2158	951.4656
C	-2.55099	6.86138	-0.31223	955.6139	956.5301	969.8441
O	-2.69512	0.38634	0.66369	971.5095	978.5099	979.6253
H	-4.31574	6.05855	3.80692	991.2537	998.8129	1005.4882
H	-2.63033	6.56230	3.66547	1015.8707	1040.2470	1044.1647
H	-3.82820	7.08059	2.45883	1050.9382	1054.6679	1056.7312
H	-4.16832	4.67594	1.78350	1060.2112	1066.8030	1083.7195
H	-3.02026	4.17958	3.02687	1103.7556	1108.9563	1110.1891
H	-1.76021	7.06556	1.68832	1114.1299	1124.8877	1128.5147
H	-0.65294	6.30392	0.59376	1155.3582	1161.1819	1167.4967
H	-5.69996	-3.98261	2.97764	1168.7766	1178.0536	1182.8435
H	-4.52313	-5.14796	2.35217	1185.4785	1192.7324	1206.1080
H	-4.06135	-3.45278	2.54969	1207.1024	1208.0903	1213.5977
H	-5.76603	-2.82526	0.75540	1219.8646	1231.2903	1235.7491
H	-6.16272	-4.51655	0.57320	1245.1753	1253.3770	1257.0832
H	-6.10033	-5.08838	-1.92353	1266.5944	1272.8200	1277.1608
H	-4.67417	-4.57423	-2.83149	1282.5114	1285.0671	1289.0408
H	-5.00006	-6.30189	-2.59397	1292.1442	1311.9524	1313.0062
H	-4.63539	-6.04443	-0.12890	1320.5863	1326.0367	1331.5894
H	-3.20032	-5.57524	-1.00550	1335.0113	1337.1102	1347.6623
C	1.44123	-0.14265	-2.37793	1353.3256	1375.8059	1379.9363
N	0.67732	-0.08428	-1.26617	1384.8386	1391.6826	1396.8982
N	1.27515	-0.41437	-0.08833	1402.3991	1403.1132	1405.6031
O	2.66483	-0.46775	-2.35160	1406.6558	1412.8420	1418.0666
C	0.60673	-0.47678	1.01942	1423.6442	1428.0219	1428.6624
C	2.03685	-1.78818	4.81456	1433.6480	1439.4993	1445.3016
C	2.85416	-2.00145	3.69039	1450.6615	1470.4747	1485.2986
C	2.41750	-1.55955	2.45985	1499.0221	1500.7654	1504.3466
C	1.19024	-0.89821	2.26948	1504.6355	1506.4551	1506.4768
C	0.39991	-0.69771	3.43828	1509.1173	1509.6294	1513.1183
C	0.81337	-1.13198	4.68596	1516.2081	1516.7844	1519.6639
H	3.81361	-2.49994	3.79676	1520.1329	1526.2339	1533.3856
H	0.21050	-0.97431	5.57360	1536.6932	1539.0791	1540.0728
O	3.24246	-1.80677	1.35277	1540.5972	1546.8657	1547.6000
H	-2.67532	1.08287	-3.55197	1583.7880	1601.4623	1604.6208
H	-0.44363	-0.20493	1.05202	1619.0801	1656.0310	1661.5015
H	-2.51181	6.16403	-1.15385	1677.8957	1683.4340	1700.0324
H	-3.59829	6.96976	-0.01574	1701.1755	1710.8657	1722.6667
H	-2.19272	7.83517	-0.65444	1737.8391	3034.3713	3070.5850
H	-0.99583	-2.18479	-2.69985	3072.4703	3082.2473	3084.3620
Zn	3.26150	-0.77428	-0.47885	3086.3000	3088.4679	3099.1856
O	5.17707	-0.30931	-0.53316	3099.9594	3110.7180	3116.1587
H	3.89061	-2.48679	1.58784	3120.0948	3123.9693	3127.5107
C	5.79195	0.16787	-1.78666	3138.5296	3147.0692	3153.9003
C	6.12974	-0.21265	0.57452	3162.1226	3166.8785	3167.1244
C	7.27310	0.23402	-1.46274	3168.0173	3169.0381	3169.5703
C	7.26955	0.62528	0.01834	3171.7538	3176.0163	3179.4541
H	5.36492	1.15012	-2.00433	3182.1521	3184.9649	3187.6660
H	5.52054	-0.53854	-2.57205	3195.7958	3206.5068	3219.2299
H	7.78962	0.96102	-2.09056	3226.2941	3228.3737	3232.7323

H	7.74277	-0.74273	-1.60625	3241.8717	3255.9903	3259.3254
H	8.21315	0.40666	0.51957	3267.0153	3287.8935	3288.4577
H	7.05276	1.69022	0.13711	3827.9071	3878.0097	3879.2294
H	5.61326	0.23796	1.42469			
H	6.45190	-1.22912	0.82084			
O	2.37833	-2.18045	6.04016			
H	3.22757	-2.63891	6.06306			
O	-0.76351	-0.06373	3.24280			
H	-1.27384	0.00297	4.05999			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.785609 Electronic Energy = -2247.15209688
Internal Energy (E)= -2246.31979288 Enthalpy (H)= -2246.31884888
Gibbs Free Energy (G)=-2246.45006088 Gibbs Free Energy of Solvation=-2246.63768364

St.Pt.	General Structure	Ball & Stick model
TS_b		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.92543	-2.81274	-1.70092
C	-2.08529	-1.78733	-2.00796
C	-1.98337	-0.62882	-1.21555
C	-2.79941	-0.58640	-0.08914
C	-3.66207	-1.60716	0.25154
C	-3.76556	-2.75566	-0.54858
C	-1.09958	0.49457	-1.52987
C	-2.14383	1.60846	0.41748
C	-1.30971	1.67541	-0.69109

Frequencies

-345.5989	7.3281	13.0747
17.9675	20.4719	21.9480
24.2768	30.9127	31.9470
41.0025	50.3387	58.4324
61.5140	63.6763	69.5482
75.9286	83.9002	96.6635
99.3426	105.4539	113.4253
122.4830	124.1290	141.9053
154.4500	161.4603	167.5848
178.7531	181.8457	193.5614
198.7254	202.4422	212.0585
223.6017	229.2972	233.1729
235.3426	238.7870	240.0459
255.4586	258.0857	267.5431

C	-0.71944	2.92735	-0.94341	274.9745	288.0189	290.4324
H	-0.07980	3.04119	-1.79998	307.2190	310.8354	323.0443
C	-0.93582	4.01151	-0.15048	336.0796	356.0529	359.0046
C	-1.78548	3.93223	0.99423	369.4182	381.3838	398.5348
C	-2.38831	2.69080	1.24045	401.2160	408.7416	411.9754
H	-2.96984	-3.65130	-2.36350	426.8531	432.3700	441.9104
H	-4.24640	-1.47475	1.13729	446.9144	459.5810	465.5431
H	-0.46501	4.93319	-0.41784	481.7133	485.9766	494.3559
H	-3.07886	2.53726	2.04104	508.5756	523.9454	536.1022
C	-0.79861	0.73151	-2.99435	538.2365	554.2671	564.8216
C	-1.74050	1.20592	-3.88735	576.2720	588.1911	589.5365
C	0.48373	0.44291	-3.43480	616.3475	625.5331	639.0222
C	-1.37097	1.38062	-5.21423	645.6118	651.7849	658.9788
C	0.85901	0.61329	-4.75762	666.5004	687.8788	689.5321
C	-0.08417	1.08735	-5.65097	711.6963	717.9293	723.7671
H	-2.09620	1.74868	-5.91699	734.5661	741.2362	751.2399
H	0.17484	1.22950	-6.68369	756.3435	783.5779	788.8872
H	1.85879	0.37862	-5.07233	794.6272	802.9204	813.2725
N	-4.62149	-3.75883	-0.25049	824.2672	851.4575	852.3909
C	-5.58857	-3.65072	0.83911	857.7032	858.1887	884.6125
C	-4.67822	-4.99787	-1.02468	889.3833	894.0091	901.4063
C	-5.04447	-4.11670	2.18723	909.5860	911.7909	919.7023
C	-5.61088	-4.92685	-2.23111	921.7570	924.6078	935.5244
N	-1.99360	5.00432	1.80577	937.2422	939.4175	941.1042
C	-2.94676	4.86103	2.91314	947.1340	988.3715	991.6577
C	-1.60396	6.34760	1.37442	993.0646	998.4806	1007.9775
C	-2.98070	6.01544	3.90670	1010.9649	1022.5610	1027.1574
C	-2.56829	6.98305	0.37515	1036.7488	1046.2740	1071.5017
O	-2.78254	0.46767	0.75413	1097.7389	1099.0191	1100.8732
H	-3.64923	5.73908	4.71442	1104.2546	1105.9006	1111.4753
H	-2.00366	6.20568	4.33679	1122.0779	1122.6727	1129.3654
H	-3.35943	6.93441	3.47678	1129.9092	1145.7864	1147.7374
H	-3.94953	4.69902	2.52147	1173.8911	1185.4583	1189.5424
H	-2.67311	3.97113	3.46665	1190.5063	1198.7966	1204.7324
H	-1.52808	6.96767	2.25199	1211.5219	1234.8638	1235.3377
H	-0.60244	6.31228	0.96997	1243.0591	1247.9425	1255.8611
H	-5.81235	-4.03261	2.94926	1266.7848	1272.0562	1284.5863
H	-4.73125	-5.15432	2.14122	1292.9355	1295.3302	1299.0967
H	-4.19071	-3.52426	2.49859	1306.8744	1311.0930	1317.1084
H	-5.95421	-2.63409	0.90110	1320.1731	1324.8015	1332.7654
H	-6.44467	-4.25502	0.56765	1336.5116	1345.1450	1364.3294
H	-6.62501	-4.69436	-1.92497	1372.0832	1373.0339	1376.0378
H	-5.29531	-4.16669	-2.93705	1384.2344	1386.6730	1398.4411
H	-5.62808	-5.88202	-2.74559	1401.0705	1406.9346	1416.7496
H	-5.01567	-5.77556	-0.35104	1425.3283	1436.2683	1447.5063
H	-3.67931	-5.28542	-1.32560	1448.7985	1459.2324	1459.3027
C	1.32996	-0.03590	-2.34506	1468.6454	1478.9380	1493.1883
N	0.65424	-0.07049	-1.22688	1499.6230	1507.9461	1516.3936
N	1.36886	-0.51574	-0.14242	1517.6372	1522.0818	1535.6903
O	2.54542	-0.36249	-2.46193	1538.8853	1541.0619	1542.4871
C	0.78538	-0.76201	0.95869	1555.2133	1555.9974	1558.9262
C	2.48643	-2.55944	4.42846	1565.2942	1570.2346	1590.4960
C	3.18025	-2.66080	3.21851	1611.7004	1615.8527	1618.4526
C	2.65502	-2.05724	2.10307	1618.8886	1619.2350	1621.7920

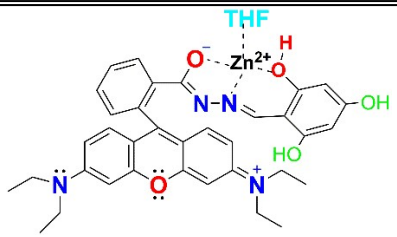
C	1.45477	-1.33803	2.11602	1623.4761	1624.7116	1628.0401
C	0.79137	-1.26088	3.36312	1628.1682	1632.0816	1632.3843
C	1.29537	-1.85311	4.49996	1634.7655	1637.3608	1649.3752
H	4.11047	-3.19903	3.16717	1651.4129	1652.7341	1656.2067
H	0.78571	-1.78405	5.44264	1663.1824	1666.7084	1676.9727
O	3.35372	-2.18579	0.91504	1681.5486	1696.0679	1704.9265
H	-2.73965	1.43436	-3.56529	1705.9986	1731.1866	1758.2136
H	-0.26065	-0.55372	1.07117	1767.7396	1780.2015	1784.3872
H	-2.64811	6.39590	-0.53336	1805.9514	1812.9036	1825.5395
H	-3.56247	7.07740	0.79893	1875.4412	3170.8183	3192.0745
H	-2.22493	7.97658	0.10587	3193.2188	3195.4645	3201.9443
H	-1.48911	-1.86638	-2.89899	3230.2633	3231.8878	3233.5178
Zn	3.32082	-0.77924	-0.71915	3237.6414	3239.5197	3240.3825
O	5.20968	-0.17729	-0.70200	3256.0936	3257.3794	3259.7479
H	3.94002	-2.92952	0.95854	3259.7799	3264.3848	3267.2321
C	5.83755	0.35298	-1.91604	3269.8439	3271.2291	3274.8067
C	6.09801	-0.04306	0.44280	3280.2208	3284.6971	3287.3472
C	7.29376	0.53832	-1.53018	3291.4424	3296.1564	3307.6063
C	7.20711	0.87581	-0.04145	3329.0153	3331.2313	3349.6444
H	5.34563	1.28624	-2.15161	3366.1548	3367.6598	3367.9538
H	5.66815	-0.35884	-2.70959	3378.9284	3385.0105	3386.6992
H	7.76328	1.31858	-2.11423	3395.0837	3421.5824	3426.4188
H	7.84833	-0.38055	-1.68480	3430.6790	3434.1302	3442.5039
H	8.13275	0.69839	0.48972	4124.0368	4166.1469	4175.1084
H	6.92730	1.91359	0.10137			
H	5.52381	0.35238	1.26883			
H	6.46474	-1.03104	0.68969			
O	2.92367	-3.10979	5.54606			
H	3.72706	-3.59646	5.44528			
O	-0.35047	-0.57982	3.37213			
H	-0.77420	-0.59119	4.21709			

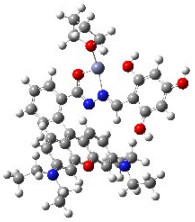
Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.830191 Electronic Energy = -2232.64548814
Internal Energy (E)= -2231.76999414 Enthalpy (H)= -2231.76905014
Gibbs Free Energy (G)=-2231.89980914 Gibbs Free Energy of Solvation=-2232.08530508

St.Pt.	General Structure	Ball & Stick model

I





Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.98072	-2.97935	-1.85715
C	-2.36661	-1.80626	-2.12443
C	-2.49126	-0.67404	-1.27258
C	-3.28684	-0.85655	-0.12138
C	-3.92013	-2.03483	0.17723
C	-3.80485	-3.14268	-0.68819
C	-1.90266	0.57440	-1.50483
C	-2.93839	1.36670	0.53862
C	-2.14154	1.61513	-0.59550
C	-1.65604	2.94376	-0.72867
H	-1.05274	3.19118	-1.58138
C	-1.94135	3.90920	0.17304
C	-2.75315	3.63920	1.33082
C	-3.24368	2.32536	1.47203
H	-2.86879	-3.78543	-2.55068
H	-4.49588	-2.07193	1.07702
H	-1.56055	4.89226	-0.00110
H	-3.88026	2.03467	2.27875
C	-1.18456	0.84433	-2.79470
C	-2.00353	1.25892	-3.83739
C	0.19515	0.71326	-3.01377
C	-1.48375	1.54383	-5.08935
C	0.69776	1.00289	-4.27956
C	-0.12661	1.41388	-5.31104
H	-2.13942	1.86231	-5.87909
H	0.29015	1.62879	-6.27782
H	1.75069	0.89757	-4.44567
N	-4.43544	-4.29798	-0.44322
C	-5.37692	-4.44963	0.66922
C	-4.26410	-5.48950	-1.28098
C	-4.70990	-4.87824	1.97309
C	-5.22166	-5.54078	-2.46790
N	-3.02994	4.59596	2.23469
C	-3.92961	4.26570	3.35431
C	-2.66097	5.99523	1.99365
C	-4.07639	5.33354	4.43014
C	-3.63372	6.73599	1.07960

Frequencies

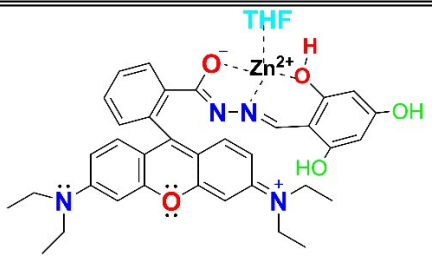
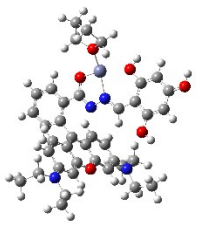
2.8681	10.0930	16.6628
17.5596	19.7651	27.3591
29.0666	33.0586	36.3834
44.6191	54.1157	57.0117
61.0563	67.5497	69.9004
80.5953	92.2265	98.3466
102.6904	107.5761	113.2596
115.9766	129.4336	141.1970
154.2284	160.7922	166.6841
174.2573	177.1115	193.5662
197.6546	206.8877	211.1560
225.3759	230.2920	233.2714
234.2143	239.9723	249.8518
254.1620	265.6988	266.9544
281.1266	294.8121	295.2184
308.5605	320.6070	324.6456
346.0232	355.4601	362.5640
365.6194	376.9073	396.0057
402.0402	406.1382	422.7519
426.2476	430.6232	439.7452
440.4386	455.6927	465.7318
480.9010	489.9806	504.7942
515.2517	525.6560	538.6406
543.8596	556.6655	565.5980
583.9274	594.4479	617.1840
619.5406	631.5227	642.4977
647.0463	649.4227	656.8415
679.6507	689.2307	709.6997
716.4801	726.1900	731.3827
732.0955	736.9033	741.7015
753.3478	782.9691	790.2856
791.0065	801.6899	815.1456
837.8722	850.1120	852.1001
858.1294	859.6532	884.7228
887.1294	890.8264	899.3036
909.3055	912.8081	914.7994
922.8519	926.7875	927.1291
934.5858	936.2687	942.5158
943.4379	988.6333	989.0913
991.6750	998.1220	1007.6873
1009.8374	1019.7703	1021.6099

O	-3.45806	0.14915	0.74593	1024.2416	1046.5528	1069.2207
H	-4.72758	4.93433	5.19950	1099.7641	1102.1841	1103.5529
H	-3.12840	5.57524	4.89681	1108.6092	1109.7425	1110.3602
H	-4.53159	6.24515	4.06360	1125.9672	1128.4778	1132.6584
H	-4.91327	4.02360	2.96012	1144.0901	1145.8770	1153.3265
H	-3.54516	3.37351	3.83316	1175.2548	1185.1302	1186.6759
H	-2.60680	6.49086	2.94775	1188.2182	1191.4764	1200.3599
H	-1.65598	6.03128	1.59893	1210.5091	1223.0607	1232.5084
H	-5.45801	-4.99703	2.74956	1237.2941	1242.7936	1256.6495
H	-4.19781	-5.82703	1.85449	1262.5331	1267.9286	1275.0285
H	-3.98424	-4.14604	2.30979	1279.5922	1291.3643	1300.6209
H	-5.93253	-3.53121	0.79963	1310.7820	1311.6101	1317.3499
H	-6.10195	-5.19450	0.36893	1318.3943	1326.5011	1328.9239
H	-6.25408	-5.52133	-2.13680	1331.7110	1337.1475	1339.0401
H	-5.07198	-4.70324	-3.13992	1373.3402	1376.6828	1386.2165
H	-5.06760	-6.45708	-3.02766	1390.0755	1396.5426	1403.2483
H	-4.42943	-6.34622	-0.64080	1404.1463	1406.8251	1422.1891
H	-3.23559	-5.56031	-1.60680	1429.4881	1448.6992	1455.1795
C	1.18011	0.27617	-1.97945	1458.8087	1466.8541	1467.8917
N	0.74784	-0.03257	-0.80470	1492.1090	1498.8967	1506.0698
N	1.77174	-0.43606	0.03580	1507.8812	1513.4614	1516.9566
O	2.41652	0.23553	-2.34364	1518.1648	1524.0913	1529.1542
C	1.44054	-0.96323	1.13861	1541.1071	1543.5157	1543.7012
C	4.01111	-2.78289	4.01994	1547.0251	1556.1898	1556.9476
C	4.50288	-2.56138	2.73320	1559.9593	1568.0857	1577.3446
C	3.68917	-1.94940	1.80775	1600.4074	1616.2374	1617.1629
C	2.38653	-1.53231	2.09428	1618.5562	1619.5100	1623.1073
C	1.93475	-1.77707	3.41014	1623.8397	1625.4516	1627.8576
C	2.72705	-2.38451	4.35936	1628.7589	1632.8691	1634.2524
H	5.50325	-2.86043	2.47278	1635.0315	1642.4963	1650.7324
H	2.37310	-2.56050	5.35796	1656.1717	1658.0770	1664.4289
O	4.19877	-1.75580	0.53800	1666.1939	1668.1564	1674.9149
H	-3.06060	1.35970	-3.66810	1680.9851	1693.7304	1706.1141
H	0.39619	-1.01239	1.39212	1724.0477	1734.4941	1746.9238
H	-3.69346	6.27597	0.09936	1766.4391	1773.8092	1778.4751
H	-4.63239	6.74911	1.50222	1802.3538	1822.9956	1827.4308
H	-3.31127	7.76394	0.95148	1882.5474	3187.4015	3195.1904
H	-1.77551	-1.71980	-3.01622	3195.9731	3197.6668	3204.7206
Zn	3.56647	-0.20629	-0.86748	3228.6438	3231.8300	3237.1562
O	5.32553	0.71090	-1.06902	3240.8322	3243.2355	3248.8736
H	4.93739	-2.33058	0.39161	3258.7743	3261.6751	3262.2959
C	5.62459	1.45920	-2.28906	3265.2996	3267.9138	3272.2376
C	6.35581	0.91599	-0.06726	3274.0776	3274.5296	3279.2471
C	7.06357	1.90923	-2.10856	3288.6284	3289.1746	3289.7813
C	7.17278	2.08432	-0.59354	3294.2251	3295.9551	3305.4426
H	4.93077	2.28663	-2.33974	3326.2877	3340.2668	3346.6647
H	5.46196	0.79830	-3.12704	3359.0268	3371.7649	3377.1071
H	7.26821	2.81952	-2.65627	3382.5731	3386.4928	3388.9423
H	7.74821	1.14371	-2.45673	3390.2892	3420.9777	3433.0653
H	8.19254	2.05454	-0.23331	3436.7311	3440.3474	3447.5925
H	6.73037	3.02450	-0.28323	4134.6361	4169.8221	4178.8927
H	5.87171	1.10505	0.88055			
H	6.93968	0.00645	-0.00432			
O	4.72928	-3.36338	4.96776			

H	5.58832	-3.63157	4.68139
O	0.69060	-1.38525	3.68616
H	0.43866	-1.59909	4.57150

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.831150 Electronic Energy = -2232.67910934
Internal Energy (E)= -2231.80193634 Enthalpy (H)= -2231.80099234
Gibbs Free Energy (G)=-2231.93526134 Gibbs Free Energy of Solvation=-2232.10830493

St.Pt.	General Structure	Ball & Stick model
I		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-2.40806	-3.90004	-0.03121
C	-1.95575	-2.93747	-0.86350
C	-2.30000	-1.56720	-0.69631
C	-3.12816	-1.27274	0.40841
C	-3.60143	-2.22730	1.27006
C	-3.27294	-3.58544	1.07592
C	-1.88621	-0.52786	-1.53572
C	-3.14254	1.00721	-0.14130
C	-2.32445	0.77794	-1.26361
C	-2.03537	1.91915	-2.05883
H	-1.42989	1.79912	-2.93705
C	-2.51043	3.14800	-1.75607
C	-3.33844	3.36919	-0.59991
C	-3.63838	2.24302	0.19267
H	-2.13355	-4.91510	-0.22496
H	-4.21901	-1.90033	2.07885
H	-2.27061	3.95767	-2.41080

Frequencies

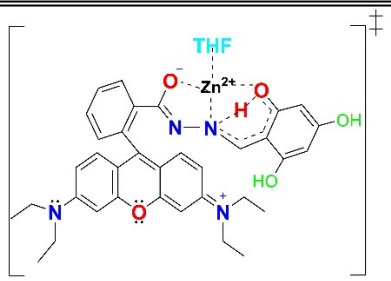
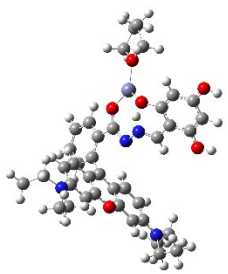
3.0355	10.2401	17.1595
17.6246	26.1462	27.0061
28.4101	32.9867	36.5835
45.7988	54.6422	58.5568
62.8703	65.9135	70.0628
82.1841	93.7076	97.4096
100.4826	111.5509	112.0408
115.9180	129.2572	141.1592
153.2850	159.7985	167.4450
173.5737	176.8850	195.6850
200.9227	208.5202	212.2335
225.3849	230.4379	233.4826
234.2532	240.0642	251.4110
255.4280	262.5822	268.8690
282.2195	294.2915	297.2353
307.9588	320.7466	324.4832
345.6241	354.2946	364.5338
365.3867	378.2023	396.4656
402.6613	419.9709	427.7325
431.4303	436.3917	439.7675
444.6522	455.5836	465.9986
478.2590	489.5833	504.9736

H	-4.27366	2.29761	1.04943	516.2932	528.3182	539.9329
C	-1.14317	-0.82616	-2.80449	543.6870	555.9999	565.4756
C	-1.94613	-1.21035	-3.87128	583.7493	594.5109	617.1833
C	0.24264	-0.71547	-2.99147	619.6829	630.7090	642.5563
C	-1.40392	-1.48265	-5.11640	646.7531	648.5992	657.5205
C	0.76753	-0.98763	-4.25184	679.6098	691.0694	710.3749
C	-0.04054	-1.36908	-5.30725	718.2092	726.2399	731.2068
H	-2.04730	-1.77617	-5.92565	732.9386	736.9496	740.6551
H	0.39344	-1.57385	-6.26865	753.2513	782.8566	790.6658
H	1.82495	-0.89346	-4.39476	791.2389	801.7459	815.2016
N	-3.74411	-4.54683	1.87928	837.4563	850.9904	852.2035
C	-4.72217	-4.26900	2.93429	858.1459	859.8374	884.5117
C	-3.34892	-5.95347	1.75132	891.4340	899.0390	906.3812
C	-4.08378	-3.88084	4.26488	909.6908	911.4474	914.8489
C	-4.21070	-6.73959	0.76764	919.4384	925.1249	926.8699
N	-3.80428	4.59317	-0.29154	927.4523	936.2216	940.5423
C	-4.71122	4.72953	0.86177	942.4750	988.5370	988.8746
C	-3.63463	5.72200	-1.21320	991.0517	998.1339	1007.7292
C	-5.07280	6.15389	1.26151	1009.7230	1019.5057	1021.7237
C	-4.65348	5.74298	-2.34985	1024.2658	1046.6073	1069.2518
O	-3.49316	-0.00910	0.65897	1099.6344	1104.0026	1104.5027
H	-5.70190	6.09612	2.14256	1107.8207	1110.1267	1110.7594
H	-4.19801	6.73879	1.52149	1126.4913	1128.1507	1130.9991
H	-5.63391	6.67903	0.49867	1143.5245	1145.2376	1153.2604
H	-5.62503	4.17515	0.66348	1175.1536	1185.0872	1186.9639
H	-4.23107	4.26553	1.71458	1187.5942	1191.3711	1200.6062
H	-3.70863	6.62988	-0.63939	1210.5936	1222.8329	1232.7415
H	-2.62555	5.71286	-1.59886	1238.0218	1243.0043	1256.5108
H	-4.85445	-3.71180	5.00934	1262.5913	1268.4008	1275.0562
H	-3.43416	-4.66930	4.62933	1279.6199	1291.4075	1308.0967
H	-3.49343	-2.97558	4.17509	1310.1696	1311.5565	1317.7034
H	-5.41124	-3.50743	2.59613	1318.5967	1322.8067	1328.9539
H	-5.31201	-5.16711	3.06143	1331.5167	1337.1776	1339.2101
H	-5.25430	-6.71985	1.06158	1373.4565	1377.5880	1386.3677
H	-4.14030	-6.33751	-0.23679	1389.9793	1393.3661	1403.2060
H	-3.89047	-7.77566	0.74194	1404.1551	1406.5968	1422.3161
H	-3.42987	-6.39021	2.73812	1429.1564	1448.4200	1455.1953
H	-2.30213	-6.01473	1.48792	1458.7898	1466.8030	1469.7817
C	1.21345	-0.33587	-1.92172	1492.0409	1498.9537	1506.6659
N	0.79374	-0.26225	-0.70489	1508.2139	1516.5051	1517.5164
N	1.80174	0.10990	0.16892	1519.2287	1524.4968	1529.0290
O	2.42766	-0.11915	-2.29804	1541.7537	1543.4282	1544.2792
C	1.46077	0.42130	1.34830	1547.1478	1556.2216	1556.9846
C	3.97007	1.99491	4.42344	1559.9699	1568.0023	1577.2893
C	4.42948	2.02133	3.10496	1600.5859	1616.2697	1617.1687
C	3.64112	1.49653	2.11700	1618.5648	1619.3776	1623.1417
C	2.38252	0.92440	2.36219	1623.8104	1625.4797	1627.8531
C	1.95956	0.92311	3.70399	1628.9684	1632.8521	1634.3096
C	2.73644	1.44263	4.72552	1636.4872	1642.3962	1653.7735
H	5.39166	2.45305	2.89944	1656.3143	1657.8593	1666.1078
H	2.38286	1.41639	5.74123	1667.0590	1668.1803	1675.1123
O	4.11710	1.55053	0.82157	1680.9790	1693.5454	1705.4723
H	-3.00878	-1.29046	-3.72810	1723.5419	1734.7995	1747.2606
H	0.42632	0.32373	1.62737	1766.4255	1777.9796	1781.2690

H	-4.58870	4.85152	-2.96396	1802.2466	1820.8643	1825.5049
H	-5.66531	5.80907	-1.96514	1880.7736	3186.8560	3195.1105
H	-4.48055	6.60472	-2.98586	3196.0328	3197.6671	3204.6278
H	-1.32522	-3.21482	-1.68654	3228.2272	3231.4552	3240.5199
Zn	3.58281	0.18866	-0.79020	3241.0367	3242.6546	3249.0616
O	5.40875	-0.53308	-1.14660	3251.3885	3261.7283	3262.3839
C	6.36072	-1.04538	-0.17557	3265.3880	3268.1251	3272.1110
C	5.81988	-0.86740	-2.50863	3274.1214	3274.3087	3279.4293
C	7.55802	-1.47974	-1.00552	3288.6878	3289.4631	3290.5045
C	6.91330	-1.90452	-2.32538	3295.5294	3296.1624	3309.6873
H	5.89394	-1.87672	0.33746	3327.7755	3339.8434	3353.2792
H	6.57422	-0.25682	0.53133	3359.3495	3371.8729	3374.3218
H	8.10910	-2.27681	-0.52433	3376.1635	3386.5636	3389.3621
H	8.23393	-0.64608	-1.16071	3391.6351	3420.4203	3433.3136
H	7.60739	-1.90409	-3.15531	3436.8716	3440.5849	3447.0995
H	6.48481	-2.89728	-2.24158	4128.9829	4170.4498	4175.1754
H	4.94625	-1.21710	-3.03711			
H	6.18600	0.04228	-2.96585			
H	4.82481	2.17814	0.76365			
O	4.77672	2.51311	5.33490			
O	0.76244	0.38909	3.94734			
H	4.42467	2.47521	6.21108			
H	0.52346	0.44194	4.85969			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.831327 Electronic Energy = -2232.68111972
Internal Energy (E)= -2231.80384672 Enthalpy (H)= -2231.80290272
Gibbs Free Energy (G)=-2231.93665172 Gibbs Free Energy of Solvation=-2232.10914876

St.Pt.	General Structure	Ball & Stick model
TS_a		

Cartesian co-ordinate

Frequencies

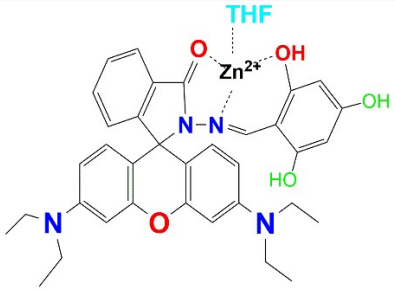
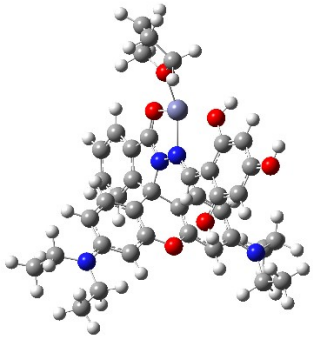
Atoms	X	Y	Z
C	3.49303	-3.05152	1.44758
C	2.74704	-1.99219	1.82825
C	2.78800	-0.74819	1.13841
C	3.63686	-0.70050	0.01074
C	4.40369	-1.75873	-0.40029
C	4.37653	-2.97559	0.31278
C	2.05688	0.39087	1.49028
C	3.06053	1.53522	-0.39736
C	2.20723	1.55706	0.72327
C	1.58836	2.80627	0.99985
H	0.95099	2.89077	1.85955
C	1.79046	3.89805	0.22917
C	2.64724	3.85357	-0.92728
C	3.28296	2.62587	-1.19989
H	3.43595	-3.95107	2.02279
H	5.00731	-1.62196	-1.27165
H	1.31080	4.81071	0.50992
H	3.96812	2.50245	-2.00971
C	1.25224	0.41692	2.75627
C	1.98389	0.59713	3.92366
C	-0.14547	0.32810	2.82942
C	1.35738	0.69182	5.15524
C	-0.75793	0.43411	4.07418
C	-0.01993	0.61001	5.23038
H	1.94555	0.83323	6.04345
H	-0.51793	0.68336	6.17969
H	-1.82651	0.37386	4.12885
N	5.13608	-4.01820	-0.04255
C	6.12763	-3.92770	-1.11818
C	5.06222	-5.32044	0.62812
C	5.55748	-4.25134	-2.49613
C	5.97255	-5.42764	1.84798
N	2.83391	4.93287	-1.70701
C	3.78069	4.83188	-2.83241
C	2.31135	6.24750	-1.31934
C	3.81913	6.02292	-3.78060
C	3.18497	6.97717	-0.30206
O	3.72291	0.41702	-0.72042
H	4.51947	5.78608	-4.57348
H	2.85532	6.20901	-4.24030
H	4.16525	6.93248	-3.30564
H	4.78002	4.65838	-2.44146
H	3.50597	3.96176	-3.41559
H	2.21699	6.84117	-2.21238
H	1.30291	6.13058	-0.94974
H	6.34130	-4.19150	-3.24356
H	5.14768	-5.25531	-2.52151
H	4.76928	-3.56085	-2.77501
H	6.58435	-2.94774	-1.10585

-1093.0775	6.1063	10.0489
15.8373	17.2023	20.3275
26.7752	28.5149	32.3007
37.2271	46.0850	56.2069
56.6555	62.3208	65.5822
72.5860	81.2328	85.3975
99.2442	104.9152	109.4599
112.6192	121.1274	125.2963
129.7496	148.7194	161.9375
163.1608	171.7245	183.8985
198.2150	201.0965	208.8800
222.7144	225.1072	233.9624
234.6006	238.4736	249.5766
251.3743	256.4927	265.4651
279.3664	283.5900	299.6701
302.6857	320.5618	322.6821
339.4512	348.9039	359.0826
365.1630	374.5313	381.4999
396.9821	402.2507	424.9650
431.3038	436.1946	439.7794
446.6980	457.9208	488.7116
489.7039	503.5908	505.4092
516.3673	530.1781	539.2662
554.2704	565.2608	567.7140
594.3309	606.7271	615.6763
629.2065	642.6438	647.1850
654.9689	669.7884	679.8314
689.2077	710.1903	715.6820
726.0633	728.2409	729.8417
736.6977	744.0987	751.6716
759.7117	788.2208	790.6866
792.2670	805.7371	826.0260
836.8456	851.2557	852.1028
858.0325	859.8830	884.8364
889.6697	899.5393	904.1704
909.2434	913.3439	914.6259
923.0802	925.1390	927.5837
931.9178	934.5636	937.3179
942.6265	987.3066	987.7214
989.9179	997.5680	1004.0227
1007.7623	1017.9074	1019.8202
1024.3635	1047.3676	1069.3292
1096.7534	1099.0440	1102.8120
1105.0864	1110.0757	1110.6728
1114.4102	1129.9094	1143.4499
1144.2463	1149.5898	1156.5282
1175.1474	1185.0735	1186.7654
1191.1352	1193.4243	1210.3786
1217.8227	1227.7734	1232.5360
1242.2125	1243.8437	1256.2077
1262.1495	1266.3526	1275.9114
1285.7206	1291.9039	1310.3072
1310.6711	1316.4216	1316.6243
1319.4095	1327.3937	1329.6555

H	6.91789	-4.62629	-0.87698	1331.3407	1337.3705	1339.3168
H	7.00877	-5.25848	1.57690	1371.9269	1386.2424	1388.9170
H	5.70607	-4.70523	2.61133	1389.9757	1403.1022	1404.8607
H	5.89764	-6.42030	2.27887	1407.3884	1410.6001	1422.7053
H	5.34475	-6.06428	-0.10525	1429.7860	1448.8792	1455.6513
H	4.03557	-5.53875	0.88756	1460.0216	1467.6832	1483.7137
C	-1.02177	0.10078	1.64259	1493.8187	1499.2231	1507.4797
N	-0.49913	-0.42496	0.59989	1509.5387	1517.2265	1517.6495
N	-1.39487	-0.53101	-0.43536	1518.2662	1524.0851	1529.7965
O	-2.27101	0.43388	1.79368	1542.1700	1543.6276	1547.6949
C	-1.35968	-1.50558	-1.25164	1556.3300	1556.9284	1559.9780
C	-4.54280	-1.74586	-4.04636	1568.1530	1577.7903	1602.7825
C	-4.55077	-0.73737	-3.07797	1616.2467	1617.1450	1618.5136
C	-3.49942	-0.67409	-2.20630	1618.8626	1622.4582	1623.7679
C	-2.41893	-1.58336	-2.24644	1623.8934	1625.6910	1627.6004
C	-2.44878	-2.57725	-3.23178	1627.8452	1632.8105	1634.3670
C	-3.50134	-2.66283	-4.12731	1643.0196	1649.5933	1656.2707
H	-5.34587	-0.01853	-3.05716	1658.0678	1662.7635	1663.9646
H	-3.51118	-3.43131	-4.88035	1667.7232	1668.2416	1674.9453
O	-3.45348	0.30581	-1.25356	1680.9078	1688.9505	1693.9011
H	3.05467	0.67524	3.86689	1724.0849	1736.0147	1763.5136
H	-0.60081	-2.26768	-1.19172	1766.4541	1772.4739	1788.6880
H	3.28094	6.41605	0.62104	1809.1662	1812.4719	1823.6513
H	4.18202	7.14504	-0.69423	1840.4014	2063.4484	3187.6762
H	2.75109	7.94337	-0.06690	3195.7367	3195.7588	3197.5764
H	2.10936	-2.08699	2.68621	3204.7471	3231.6654	3234.7565
Zn	-3.79583	0.23537	0.73175	3241.2847	3245.6582	3249.2817
O	-5.66137	0.15587	1.31488	3250.8435	3253.3261	3262.0693
C	-6.81923	0.19665	0.41976	3262.3596	3265.3491	3267.3514
C	-6.08265	0.09518	2.71563	3273.0651	3274.0079	3275.0236
C	-7.99693	0.44949	1.34485	3278.9173	3288.3687	3289.5930
C	-7.56314	-0.23292	2.64289	3292.8619	3296.3746	3298.1159
H	-6.87496	-0.76293	-0.07576	3317.9865	3321.8930	3340.5265
H	-6.64635	0.97805	-0.30558	3350.7535	3361.1481	3369.1641
H	-8.91372	0.04288	0.93924	3372.2280	3386.8406	3387.4558
H	-8.13618	1.51364	1.49836	3392.3074	3406.5426	3412.1592
H	-8.09390	0.13407	3.51120	3432.9580	3437.6564	3439.8214
H	-7.71087	-1.30531	2.58205	3448.1004	4172.5132	4174.2154
H	-5.48133	-0.65609	3.20661			
H	-5.89156	1.06601	3.15218			
H	-2.41796	0.23282	-0.90153			
O	-5.57907	-1.77157	-4.87217			
O	-1.42375	-3.42881	-3.25140			
H	-5.51296	-2.44738	-5.52910			
H	-1.50191	-4.07355	-3.93752			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.826927 Electronic Energy = -2232.63711276
Internal Energy (E)= -2231.76476976 Enthalpy (H)= -2231.76382576
Gibbs Free Energy (G)=-2231.89649676 Gibbs Free Energy of Solvation=-2232.07670509

St.Pt.	General Structure	Ball & Stick model
E		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-3.75286	-2.87661	-1.49099
C	-2.90266	-1.87350	-1.84313
C	-2.85574	-0.64248	-1.12731
C	-3.71975	-0.53592	-0.00283
C	-4.58938	-1.53401	0.37406
C	-4.65300	-2.73619	-0.37338
C	-2.02721	0.43769	-1.45951
C	-2.93661	1.64503	0.45105
C	-2.07269	1.60296	-0.67286
C	-1.33126	2.78737	-0.93907
H	-0.68678	2.81158	-1.81220
C	-1.43286	3.89245	-0.14819
C	-2.29757	3.91349	1.00505
C	-3.05618	2.74788	1.26957
H	-3.76635	-3.78114	-2.08366
H	-5.20141	-1.36373	1.24887
H	-0.86839	4.77386	-0.41796
H	-3.75899	2.68467	2.08703
C	-1.22569	0.40959	-2.71614
C	-1.94619	0.53749	-3.90694
C	0.17875	0.33386	-2.77220
C	-1.29631	0.60519	-5.13547
C	0.81982	0.41501	-4.01151
C	0.09263	0.54914	-5.18748
H	-1.87589	0.70906	-6.04645
H	0.60708	0.60741	-6.14033
H	1.90201	0.36614	-4.03648
N	-5.52078	-3.71327	-0.05930

Frequencies

7.7831	10.9635	17.3106
17.6634	27.1296	28.4688
30.8846	31.8724	39.0195
45.3943	49.6342	54.4004
59.3731	61.2586	70.3219
73.5824	85.3809	86.7069
93.9008	102.1705	109.6210
112.2749	124.5352	132.5481
139.5270	151.4143	158.8918
160.7500	171.6222	174.1327
180.8306	195.5146	196.4785
206.6707	215.3764	223.4364
224.2867	229.0500	235.1982
243.3894	265.9217	269.7840
273.3674	278.3633	287.4626
296.8044	303.7706	308.0688
325.7982	337.4777	345.4280
361.4660	368.8821	381.8037
390.8798	405.8172	409.3468
421.6060	424.8791	430.8588
436.9502	448.2964	450.4155
460.6554	473.5655	480.3195
484.1175	492.4476	514.2777
516.6636	534.6047	545.9841
562.2212	565.1469	571.7273
591.2562	599.8989	607.0082
616.0198	636.6447	645.6774
649.7060	659.5649	661.0143
669.7138	679.7813	684.9354
692.8268	704.5997	708.4404
720.2732	728.4575	732.6650
751.6361	755.0043	759.3409

C	-6.52799	-3.53998	0.99054	779.7616	793.5563	808.6657
C	-5.55108	-4.99897	-0.76387	809.2967	810.0553	811.8927
C	-6.00253	-3.92384	2.37025	825.0784	837.1763	843.9018
C	-6.41693	-4.95459	-2.01886	846.7364	848.3766	850.5033
N	-2.38880	5.00382	1.79609	852.4621	867.2431	868.7387
C	-3.38772	5.00033	2.88084	877.5637	879.3284	896.6263
C	-1.71969	6.25571	1.42874	916.5666	920.8007	933.7044
C	-3.39439	6.23912	3.76251	935.8338	943.3096	947.1856
C	-2.48982	7.04506	0.37391	947.4476	956.5697	957.7322
O	-3.71766	0.58232	0.75880	975.7520	983.7118	997.2295
H	-4.16549	6.10441	4.52348	998.6947	1005.8039	1012.3004
H	-2.44213	6.37936	4.27878	1034.0605	1035.6234	1047.4770
H	-3.63700	7.14769	3.20701	1049.6683	1049.8399	1067.7193
H	-4.38283	4.86082	2.43788	1070.0205	1084.5925	1096.0987
H	-3.18844	4.12716	3.51174	1105.3739	1108.2173	1112.3774
H	-1.60122	6.84811	2.33415	1117.4629	1126.6667	1130.4217
H	-0.70544	6.02531	1.09636	1150.5244	1157.7026	1163.0068
H	-6.78323	-3.79341	3.12259	1170.9066	1179.3886	1189.0304
H	-5.68767	-4.97054	2.38470	1193.5752	1194.6064	1199.2505
H	-5.14383	-3.30805	2.65068	1206.9357	1213.9621	1214.2143
H	-6.89053	-2.50924	0.97094	1230.1276	1233.2725	1235.2948
H	-7.38057	-4.16841	0.71932	1249.7983	1254.8852	1257.8662
H	-7.44445	-4.67776	-1.76941	1261.3994	1273.7648	1285.2022
H	-6.03518	-4.22322	-2.73601	1293.9736	1296.9049	1300.2729
H	-6.43693	-5.93473	-2.50030	1311.9327	1316.4862	1319.0312
H	-5.94332	-5.73415	-0.05602	1321.3203	1333.9928	1339.6732
H	-4.52942	-5.31251	-0.98996	1339.9824	1349.6838	1371.2898
C	1.02804	0.12712	-1.56937	1377.0377	1378.4504	1383.9901
N	0.45776	-0.37836	-0.50756	1395.1797	1397.4014	1408.5551
N	1.34953	-0.46158	0.54487	1408.9714	1412.2695	1418.0294
O	2.28900	0.44092	-1.68164	1418.4461	1422.6040	1429.4157
C	1.41383	-1.48519	1.36635	1432.3329	1433.8321	1435.4221
C	4.47119	-2.16061	4.16327	1437.6142	1447.6604	1453.3582
C	4.69263	-1.21745	3.15801	1467.8849	1475.4837	1493.2025
C	3.69877	-0.93967	2.22927	1497.5520	1501.5713	1504.0799
C	2.43613	-1.63650	2.32223	1504.5816	1506.4986	1509.7595
C	2.26890	-2.62306	3.33973	1510.5054	1510.8063	1515.7981
C	3.26211	-2.87806	4.25848	1517.5574	1524.4744	1527.2452
H	5.64163	-0.69904	3.11179	1530.2393	1533.9667	1542.5824
H	3.11668	-3.61220	5.04518	1546.5298	1552.1601	1553.4335
O	3.92268	-0.06324	1.26649	1560.7937	1567.7936	1574.0800
H	-3.02914	0.60285	-3.86084	1576.8072	1583.1798	1601.7243
H	0.64194	-2.24144	1.24209	1627.0145	1632.8460	1640.2804
H	-2.61137	6.46583	-0.54563	1647.5684	1673.9927	1685.6665
H	-3.48648	7.30592	0.73994	1694.3370	1712.9373	1722.7746
H	-1.96296	7.97084	0.13210	1738.5615	3059.3104	3075.2290
H	-2.24581	-2.00095	-2.69723	3084.0200	3087.2778	3091.8126
Zn	3.79891	-0.08187	-0.63012	3106.2042	3106.6101	3107.2976
O	5.54718	-0.11981	-1.53751	3111.5202	3114.1110	3117.4886
C	6.79774	-0.30309	-0.79066	3120.4086	3124.5906	3147.4587
C	5.82242	0.25723	-2.92697	3152.8899	3153.0942	3167.6122
C	7.85015	0.33570	-1.67891	3170.9469	3171.7321	3174.8430
C	7.31851	0.03330	-3.08383	3175.5852	3177.5219	3180.2655
H	6.95101	-1.37900	-0.67053	3180.9802	3182.0016	3188.4113

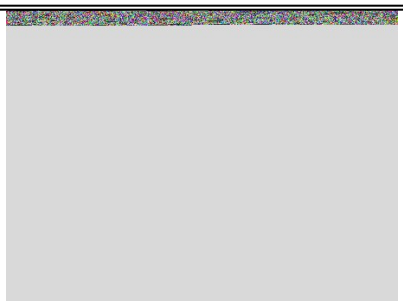
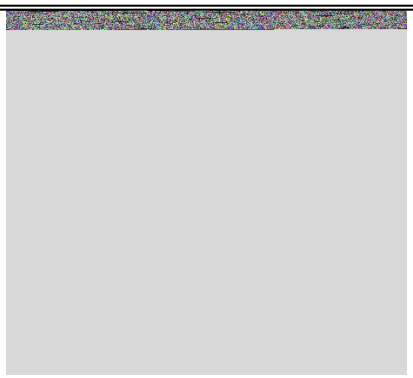
H	6.66701	0.16751	0.18553	3192.7937	3193.1287	3217.0631
H	8.83979	-0.08660	-1.50091	3221.9181	3223.2729	3226.1391
H	7.89578	1.41419	-1.50484	3234.6027	3235.4201	3241.8320
H	7.74473	0.68375	-3.84844	3246.6459	3252.8604	3261.2667
H	7.52330	-1.00495	-3.35808	3275.9018	3277.2806	3287.2215
H	5.20230	-0.37047	-3.56876	3521.9652	3868.8980	3871.0530
H	5.54311	1.30774	-3.04546			
H	1.91820	0.35202	0.77747			
O	5.47072	-2.35450	5.02403			
O	1.08211	-3.25654	3.34378			
H	5.24384	-3.00977	5.69596			
H	1.05623	-3.93211	4.03295			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.786829 Electronic Energy = -2247.15318190
Internal Energy (E)= -2246.3184529 Enthalpy (H)= -2246.3175079
Gibbs Free Energy (G)=-2246.4541319 Gibbs Free Energy of Solvation=-2246.62195113

10. Coordinate of the stationary points associated to the TD-DFT analysis:

TD-DFT method with B3LYP functional and 6-31G (d, p) basis set.

St.Pt.	General Structure	Ball & Stick model
E		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-4.26320	-2.69485	-1.29267
C	-3.25579	-1.83897	-1.70941
C	-3.00591	-0.58836	-1.09420
C	-3.83310	-0.28192	0.00148
C	-4.86125	-1.12369	0.45090
C	-5.11439	-2.36075	-0.20558
C	-2.01312	0.34405	-1.50391
C	-2.76616	1.78345	0.32146
C	-1.91456	1.56257	-0.77262
C	-1.03223	2.62782	-1.07207
H	-0.37690	2.51760	-1.93040
C	-0.99585	3.80547	-0.34062
C	-1.85120	4.01523	0.77511
C	-2.75620	2.96067	1.08468
H	-4.41510	-3.62150	-1.82950
H	-5.43561	-0.79979	1.30987
H	-0.31389	4.58365	-0.65360
H	-3.47501	3.03324	1.88946
C	-1.22570	0.12271	-2.73941
C	-1.91859	0.18725	-3.95563
C	0.16833	-0.09914	-2.77191
C	-1.26289	0.04109	-5.17303
C	0.81960	-0.22584	-4.00388
C	0.11432	-0.16365	-5.19754
H	-1.82520	0.09895	-6.09899
H	0.63548	-0.27286	-6.14227
H	1.89207	-0.38108	-4.00901
N	-6.12711	-3.17163	0.20095
C	-7.08754	-2.76505	1.22745
C	-6.33867	-4.49291	-0.38658

Frequencies

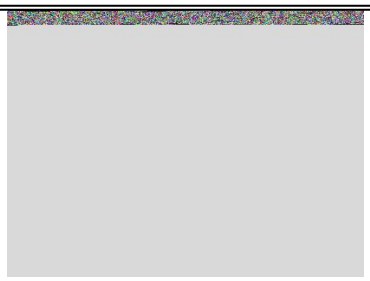
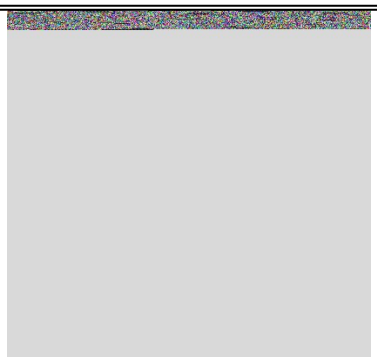
-38.1790	5.1771	7.1485
14.8700	17.3130	21.9359
27.2355	27.5631	30.6512
43.0837	45.4126	46.0276
52.1575	56.0013	57.8908
66.6662	70.4384	85.2118
91.3644	95.5548	102.8223
107.9489	113.1139	117.3633
135.6621	142.4515	151.2253
155.4875	162.0309	172.7782
189.9503	194.2561	204.4057
212.6912	219.1774	223.7287
228.5966	231.1469	232.6541
236.8082	258.0241	262.2828
267.4515	269.7280	284.0531
286.4520	304.8390	315.6152
327.6637	332.4943	341.3424
352.2102	365.7882	378.9849
385.8901	402.1311	404.1830
412.3955	423.8221	425.5829
429.8241	441.4801	445.3605
447.9147	456.0763	462.9623
476.2440	485.9434	506.9601
512.9451	531.9809	546.1355
556.5108	563.1839	572.6493
572.8112	582.8778	587.0461
602.3216	623.2298	627.1899
632.8656	639.4161	644.1930
653.0268	667.9674	680.4707
694.5470	696.4858	697.1329
708.0900	716.2412	728.7082
732.2968	749.6420	752.1411
778.2980	799.4724	802.0012
805.0210	806.7912	807.8790

C	-6.60751	-3.09994	2.63906	811.3923	815.2466	816.7646
C	-7.19639	-4.43595	-1.65022	844.7100	850.4596	854.1314
N	-1.83033	5.16447	1.51395	857.8497	858.6092	866.7868
C	-2.83171	5.35395	2.57679	872.8076	875.8874	886.6880
C	-1.01891	6.29909	1.08170	910.4024	921.2678	930.6157
C	-2.65414	6.60377	3.42332	936.1256	938.3813	942.4046
C	-1.69072	7.10360	-0.03184	945.2399	953.6830	954.1689
O	-3.68593	0.86549	0.69929	966.1701	969.9708	979.5404
H	-3.43535	6.60267	4.18612	981.6864	998.7871	1010.6268
H	-1.69052	6.61482	3.93764	1026.1433	1035.7770	1043.1062
H	-2.76448	7.52303	2.84395	1045.7049	1046.0063	1067.8023
H	-3.83228	5.35874	2.12062	1069.5774	1080.7036	1091.3260
H	-2.78633	4.48008	3.23559	1092.6710	1098.9048	1102.3832
H	-0.83103	6.93180	1.94790	1115.9779	1122.3948	1123.2696
H	-0.04063	5.92833	0.76672	1148.2218	1148.6794	1153.7794
H	-7.36024	-2.80068	3.37202	1158.7099	1169.0522	1175.7395
H	-6.43748	-4.17429	2.74435	1183.6725	1187.0835	1191.7332
H	-5.67225	-2.58208	2.86902	1206.2386	1209.2532	1210.3345
H	-7.29820	-1.69781	1.12041	1222.8124	1225.5562	1227.4584
H	-8.02309	-3.28856	1.01205	1236.6017	1249.5024	1252.4939
H	-8.17543	-4.00153	-1.43332	1260.0837	1271.6612	1272.3371
H	-6.71826	-3.82871	-2.42292	1282.2827	1291.6039	1292.4496
H	-7.34989	-5.44316	-2.04394	1298.4813	1304.5069	1311.3799
H	-6.82737	-5.10415	0.37735	1313.4608	1316.2191	1328.2468
H	-5.36885	-4.95781	-0.58307	1331.5479	1332.1340	1338.5121
C	1.00569	-0.21999	-1.54877	1370.6785	1371.2766	1372.5070
N	0.41918	-0.56470	-0.42978	1376.9290	1383.0451	1388.9378
N	1.31869	-0.58884	0.61558	1390.6617	1393.1791	1398.3740
O	2.28466	-0.01074	-1.70209	1403.1475	1404.7574	1410.4689
C	1.37535	-1.54567	1.51225	1412.3181	1414.6721	1419.4072
C	4.48333	-2.07792	4.29281	1421.7032	1425.2550	1431.9427
C	4.70431	-1.22725	3.20808	1443.5457	1447.3864	1462.6438
C	3.69434	-0.99701	2.28339	1466.8284	1484.6800	1495.8759
C	2.41792	-1.64646	2.46032	1498.0502	1500.6237	1503.3084
C	2.24745	-2.53579	3.56083	1503.5104	1504.4184	1506.7496
C	3.25658	-2.74476	4.47558	1506.8979	1510.3815	1512.1862
H	5.66646	-0.74410	3.09568	1516.5388	1518.9396	1523.2553
H	3.10948	-3.40658	5.32400	1527.6721	1529.7808	1542.3291
O	3.91614	-0.20580	1.24691	1542.6810	1545.2420	1549.7503
H	-2.98925	0.36769	-3.93494	1550.6604	1557.9326	1569.6707
H	0.58381	-2.29009	1.46456	1572.6447	1604.6267	1617.6421
H	-1.87626	6.48005	-0.91046	1620.2328	1634.7978	1645.8936
H	-2.64876	7.50556	0.30813	1658.5865	1683.1958	1705.4938
H	-1.05429	7.94093	-0.32714	1716.1851	3040.2228	3084.1115
H	-2.63433	-2.12093	-2.55258	3084.7768	3087.2254	3093.2659
Zn	3.83564	-0.31545	-0.64060	3097.7659	3099.6212	3105.3612
O	5.56036	-0.33596	-1.58797	3106.3591	3108.2472	3113.8758
C	6.85101	-0.40048	-0.89331	3120.0814	3122.1089	3143.4451
C	5.75151	-0.19440	-3.03354	3146.7805	3163.7191	3170.9772
C	7.85331	0.05828	-1.93875	3171.4879	3172.8685	3173.8451
C	7.23435	-0.46155	-3.24084	3175.0777	3176.2114	3176.5051
H	7.00915	-1.43871	-0.58925	3178.6216	3179.5451	3182.8283
H	6.78186	0.24060	-0.01269	3189.4211	3192.6627	3218.7700
H	8.84627	-0.35172	-1.75050	3221.5102	3230.8458	3231.9677

H	7.92476	1.14915	-1.95003	3234.7553	3240.4905	3245.2302
H	7.61492	0.05230	-4.12434	3255.9524	3266.8767	3269.3340
H	7.41885	-1.53278	-3.35671	3274.5394	3280.4472	3281.3616
H	5.09179	-0.91103	-3.52601	3524.2244	3878.1500	3879.9725
H	5.46712	0.82549	-3.30591			
H	1.94386	0.20428	0.74812			
O	5.50147	-2.23252	5.14238			
O	1.04331	-3.13244	3.64514			
H	5.27395	-2.82737	5.86789			
H	1.01408	-3.73773	4.39639			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.781632 Electronic Energy = -2247.14714564
Internal Energy (E)= -2246.31779664 Enthalpy (H)= -2246.31685164
Gibbs Free Energy (G)=-2246.45438164 Gibbs Free Energy of Solvation=-2246.62305393

St.Pt.	General Structure	Ball & Stick model
K		

Cartesian co-ordinate

Atoms	X	Y	Z
C	-3.64895	-2.30838	-1.14926
C	-2.53733	-1.63677	-1.58150
C	-2.11641	-0.43034	-0.99127
C	-2.87880	0.09496	0.07672
C	-4.01377	-0.54844	0.52826
C	-4.43793	-1.76541	-0.07339
C	-0.87142	0.27222	-1.49074
C	-1.49139	1.99587	0.25900
C	-0.69261	1.59851	-0.80425

Frequencies

9.5295	13.1064	14.0525
19.4001	20.8483	24.0889
30.9738	33.6021	39.2884
47.5010	53.9256	60.0355
62.7934	66.1188	73.4882
75.6264	88.0157	97.0816
107.7924	109.8827	116.3097
125.3811	136.0926	143.7683
151.4475	156.4212	157.8554
166.4939	175.6940	180.6981
190.9703	192.9480	207.0381
216.7779	220.1879	224.3078
227.6471	228.8877	231.0641
238.2279	252.5437	260.4022

C	0.30310	2.50099	-1.20403	265.4721	266.9549	268.8483
H	0.93118	2.24357	-2.05368	285.6979	301.0240	312.5720
C	0.49779	3.70807	-0.57296	326.4941	330.6750	338.3128
C	-0.31155	4.09805	0.53315	348.7421	350.8981	354.0497
C	-1.33326	3.20274	0.91843	359.6893	373.5139	395.3592
H	-3.94668	-3.22167	-1.64522	400.5301	411.5200	424.5108
H	-4.53953	-0.10358	1.36163	435.8243	437.0818	444.6109
H	1.26839	4.36618	-0.94901	449.7334	469.1975	475.2148
H	-2.02674	3.42288	1.71692	489.0034	490.7257	508.6169
C	-0.88892	0.37537	-3.01479	523.7221	529.4564	534.4193
C	-1.79689	1.03635	-3.82153	554.0360	563.6675	570.4766
C	0.19222	-0.31074	-3.56503	573.0860	577.1967	590.2467
C	-1.58979	0.99502	-5.20409	595.0438	600.2777	608.1400
C	0.41040	-0.35548	-4.93656	613.3287	620.4998	646.8975
C	-0.50396	0.30811	-5.75329	652.5099	655.3169	669.3940
H	-2.28001	1.51175	-5.86190	681.7530	686.2985	697.5094
H	-0.36914	0.29745	-6.82913	706.2340	713.6084	716.9341
H	1.26251	-0.88553	-5.34754	728.5607	737.8826	746.6118
N	-5.55264	-2.39100	0.34044	755.3870	776.2338	794.7502
C	-6.45109	-1.80711	1.34499	795.3377	798.4042	808.2091
C	-5.97295	-3.69680	-0.18652	810.6150	814.9068	823.1882
C	-6.02855	-2.18597	2.76428	830.1275	841.2468	851.4149
C	-6.83893	-3.54678	-1.43715	862.2870	867.2060	868.8626
N	-0.11669	5.27812	1.19253	870.8511	879.9368	893.7152
C	-1.10309	5.67234	2.20539	909.5961	913.2240	923.0780
C	0.78576	6.28340	0.63355	937.3770	944.6479	946.7380
C	-0.78710	6.96476	2.94259	950.0458	956.0799	956.1333
C	0.17683	7.04863	-0.53919	974.6576	979.2772	981.2520
O	-2.53358	1.21466	0.73301	991.5558	999.3234	1004.0847
H	-1.56006	7.12499	3.69682	1012.3157	1035.2180	1036.4537
H	0.17480	6.91132	3.45767	1037.9469	1051.7874	1056.5171
H	-0.78800	7.83484	2.28236	1065.8756	1068.7093	1078.2726
H	-2.09641	5.75096	1.73864	1090.5184	1094.3307	1104.7930
H	-1.16101	4.86567	2.94493	1114.9726	1119.2702	1121.5770
H	1.05996	6.97149	1.43184	1153.9801	1161.0877	1169.8344
H	1.71807	5.79216	0.34498	1170.3425	1178.6281	1181.0447
H	-6.73582	-1.75862	3.47677	1185.2900	1189.1932	1196.0230
H	-6.02577	-3.27035	2.89513	1207.2049	1210.8520	1211.6271
H	-5.02912	-1.80822	2.99095	1215.5865	1222.2593	1224.2695
H	-6.48672	-0.72652	1.20419	1232.2818	1233.9907	1252.4584
H	-7.44994	-2.19201	1.12712	1254.4287	1271.5404	1274.2669
H	-7.72871	-2.94863	-1.22848	1275.2452	1277.7142	1283.5963
H	-6.28318	-3.06617	-2.24557	1284.1123	1303.4129	1306.0997
H	-7.16295	-4.53315	-1.77267	1314.5711	1323.9522	1329.1838
H	-6.53611	-4.18296	0.61339	1330.5201	1330.9382	1335.2766
H	-5.09075	-4.30947	-0.37157	1342.4705	1344.0253	1367.7705
C	0.96571	-0.87781	-2.46406	1370.6149	1377.9495	1381.6832
N	0.33055	-0.61019	-1.30940	1385.4826	1389.9725	1392.5019
N	1.01237	-0.86533	-0.14627	1393.4229	1398.9798	1415.4071
O	2.09401	-1.46186	-2.50179	1418.2281	1422.6351	1426.2232
C	0.38117	-0.90064	1.05041	1427.3317	1427.7299	1439.0381
C	2.21048	-2.04552	4.74316	1447.3276	1454.0376	1464.7265
C	2.80671	-2.45137	3.55090	1498.1580	1498.6963	1503.1124
C	2.21347	-2.10513	2.34559	1503.4152	1504.5266	1506.1310

C	1.03856	-1.32719	2.23301	1507.0477	1507.7821	1510.1280
C	0.46936	-0.94808	3.49295	1512.1279	1515.5652	1518.4120
C	1.02840	-1.29384	4.70255	1519.7593	1522.2441	1529.0089
H	3.72145	-3.03808	3.55968	1529.2874	1530.2387	1533.7573
H	0.57903	-0.98653	5.64095	1542.3489	1548.2679	1551.6079
O	2.81969	-2.62095	1.17145	1560.7083	1562.3361	1569.6225
H	-2.63159	1.58659	-3.39819	1588.6387	1605.8424	1642.5562
H	-0.59873	-0.46252	1.16600	1647.8909	1670.4830	1671.9705
H	-0.10154	6.37089	-1.35095	1685.4095	1691.0096	1699.5652
H	-0.72439	7.58148	-0.22318	1716.9012	3029.1875	3082.7209
H	0.88581	7.78227	-0.92972	3087.6961	3092.5686	3094.6066
H	-1.95996	-2.03678	-2.40850	3094.9720	3095.7559	3109.1618
Zn	2.81052	-1.58599	-0.63091	3113.8963	3120.3063	3120.3852
O	4.77631	-1.39143	-0.85917	3122.1548	3126.5756	3158.6285
H	3.19159	-3.49090	1.36394	3163.1124	3169.9273	3171.6495
C	5.37519	-1.02946	-2.14672	3172.3721	3175.4820	3176.7612
C	5.79362	-1.45642	0.18547	3179.7967	3184.6763	3187.3637
C	6.86648	-1.21255	-1.92247	3189.2296	3189.6322	3191.1119
C	7.02412	-0.82631	-0.44825	3191.5561	3192.8788	3205.5883
H	5.11025	0.01110	-2.35324	3210.4586	3228.0315	3238.5577
H	4.93911	-1.67929	-2.90626	3239.2717	3240.5100	3246.8990
H	7.45705	-0.58606	-2.59164	3254.9551	3280.2295	3283.0447
H	7.15290	-2.25558	-2.08193	3286.5831	3290.4356	3310.1517
H	7.94644	-1.20208	-0.00418	3874.1331	3891.5015	3898.3308
H	6.99984	0.26025	-0.32969			
H	5.41277	-0.92604	1.06052			
H	5.95285	-2.51131	0.42842			
O	2.70397	-2.33303	5.96350			
H	3.50866	-2.85994	5.90104			
O	-0.67236	-0.22000	3.41126			
H	-0.96289	0.02262	4.29812			

Statistical Thermodynamic Analysis

Temperature=298.15 K Pressure=1 atm
Zero-point correction= 0.783235 Electronic Energy = -2247.13759144
Internal Energy (E)= -2246.30609444 Enthalpy (H)= -2246.30515044
Gibbs Free Energy (G)=-2246.44135844 Gibbs Free Energy of Solvation=-2246.62840216