Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Ferrocenyl pyrazaboles: Design, Synthesis, Structure, and Properties

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I. Crystallographic Data

Single crystal X-ray structural studies of **11a, 11b,** and **4d** were performed on a CCD Agilent Technologies (Oxford Diffraction) SUPER NOVA diffractometer. Data were collected at 150(2) K using graphite-monochromated Mo Kα radiation (λ_α = 0.71073 Å). The strategy for the Data collection was evaluated by using the CrysAlisPro CCD software. The data were collected by the standard 'phi-omega scan techniques, and were scaled and reduced using CrysAlisPro RED software. The structures were solved by direct methods using SHELXS-97, and refined by full matrix least-squares with SHELXL-97, refining on F^2. The positions of all the atoms were obtained by direct methods. All non-hydrogen atoms were refined anisotropically. The remaining hydrogen atoms were placed in geometrically constrained positions, and refined with isotropic temperature factors, generally 1.2U_{eq} of their parent atoms. The crystal, and refinement data are summarized in Table 1. The CCDC numbers **950018, 891091,** and **891092** contain the supplementary crystallographic data for **11a, 11b,** and **11d** respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk (or from the Cambridge Crystallographic Data Centre, 12 union Road, Cambridge CB21 EZ, UK; Fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

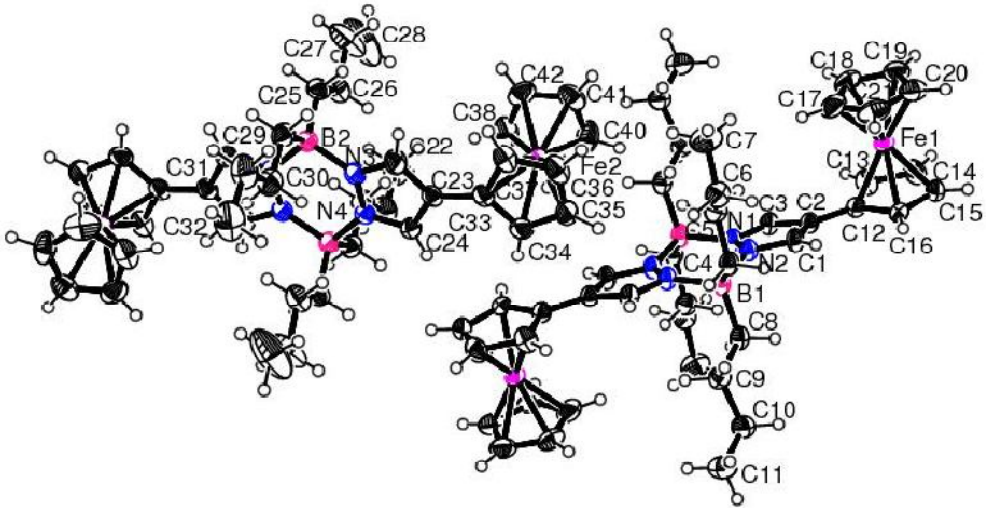


Figure S1. Crystal structure of **11a** (50% probability for thermal ellipsoids).

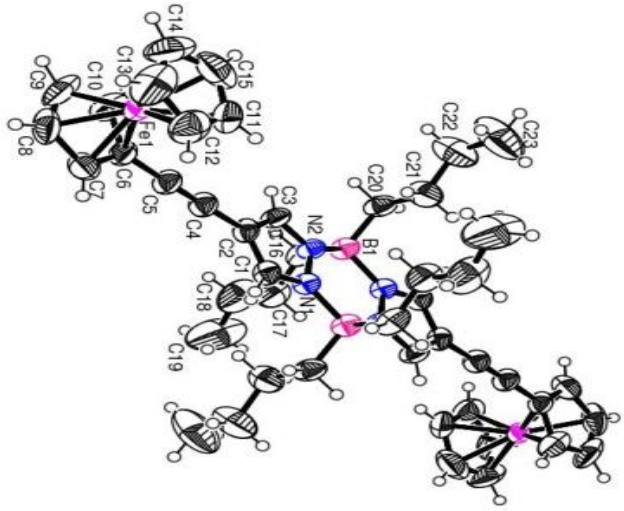


Figure S2. Crystal structure of **11b** (50% probability for thermal ellipsoids): Top view.

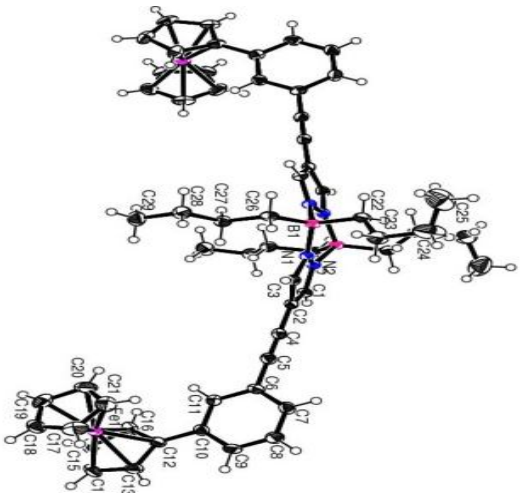


Figure S3. Crystal structure of **11d** (50% probability for thermal ellipsoids): Side view.

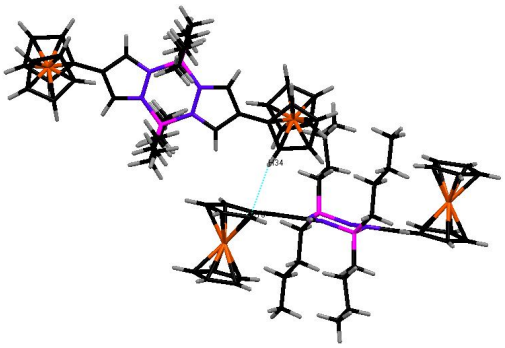


Figure S4. The two symmetry independent molecules in the crystal structures of **11a.**

Table 1. Selected bond lengths and angles of compound 11a.

Compound 11a			
Bond lengths (Å)		**Bond angles °**	
B(1)-N(1)#1	1.586(3)	N(2)#1-B(1)-N(1)	103.9(2)
B(1)-N(2)	1.588(3)	N(2)#1-B(1)-C(26)	109.3(2)
B(1)-C(4)	1.608(3)	N(1)-B(1)-C(26)	107.6(2)
B(1)-C(8)	1.625(3)	N(2)#1-B(1)-C(22)	106.9(2)
N(1)-C(3)	1.342(3)	N(1)-B(1)-C(22)	112.0(2)
N(1)-N(2)	1.359(2)	C(26)-B(1)-C(22)	116.4(2)
N(2)-C(1)	1.343(3)	C(3)-N(1)-N(2)	108.1(2)
C(1)-C(2)	1.387(3)	C(3)-N(1)-B(1)	126.5(2)
C(2)-C(3)	1.386(3)	N(2)-N(1)-B(1)	125.3(2)
B(1)-B(1)	3.267	C(1)-N(2)-B(1)#1	126.6(2)

Table 2. Selected bond lengths, and bond angles of compound 11b.

Compound 11b			
Bond lengths (Å)		**Bond angles °**	
B(1)-N(1)	1.571(8)	N(1)1-B(1)-N(2)	105.3(4)
B(1)-N(2)	1.591(7)	N(1)1-B(1)-C(20)	111.0(5)
B(1)-C(20)	1.598(10)	N(2)-B(1)-C(20)	111.0(5)
B(1)-C(16)	1.619(10)	N(1)1-B(1)-C(16)	109.1(5)
N(1)-C(1)	1.350(7)	N(2)-B(1)-C(16)	109.0(5)
N(1)-N(2)	1.350(6)	C(20)-B(1)-C(16)	111.3(5)

N(2)-C(3)	1.332(7)	C(1)-N(1)-N(2)	107.4(4)
C(1)-C(2)	1.377(8)	N (2)-C (3)-C (2)	177.6 (7)
C(2)-C(3)	1.380(9)	C(1)-N(1)-B(1)1	124.9(5)
B(1)-B(1)	3.251	N(2)-N(1)-B(1)1	126.8(4)

Table 3. Selected bond lengths and bond angles of compound 11d.

Compound 11d			
Bond lengths (Å)		**Bond angles °**	
B(1)-N(1)	1.597(4)	N(2)1-B(1)-N(1)	103.9(2)
B(1)-N(2)1	1.596(4)	N(2)1-B(1)-C(26)	109.3(2)
B(1)-C(26)	1.613(4)	N(1)-B(1)-C(26)	107.6(2)
B(1)-C(22)	1.614(4)	N(2)1-B(1)-C(22)	106.9(2)
N(1)-C(3)	1.334(4)	N(1)-B(1)-C(22)	112.0(2)
N(1)-N(2)	1.354(3)	C(26)-B(1)-C(22)	116.4(2)
N(2)-C(1)	1.337(4)	C(3)-N(1)-N(2)	108.1(2)
C(1)-C(2)	1.395(4)	C(3)-N(1)-B(1)	126.5(2)
C(2)-C(3)	1.389(4)	N(2)-N(1)-B(1)	125.3(2)
B(1)-B(1)	3.179	C(1)-N(2)-B(1)1	126.6(2)

DFT Calculations.

Calculation method: B3LYP/6-31+G** for C, H, N, B, and Lanl2DZ for Fe with Gaussian 09

DFT Data for ferrocenyl pyrazaboles.

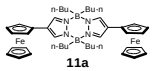
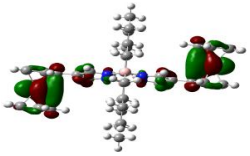
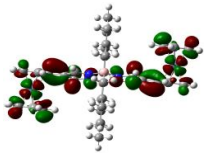
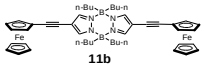
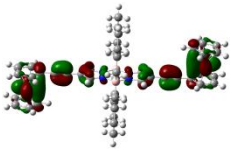
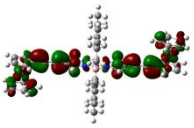
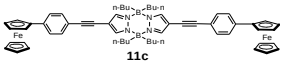
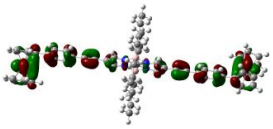
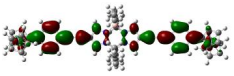
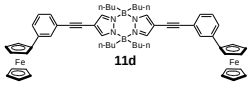
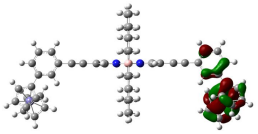
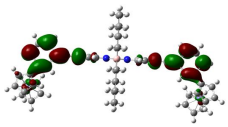
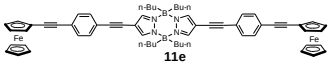
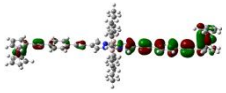
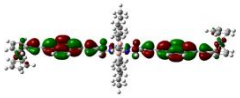
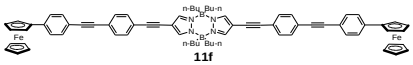
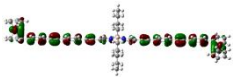
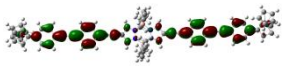
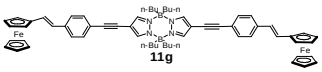
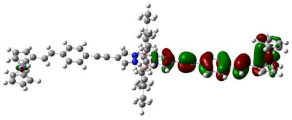
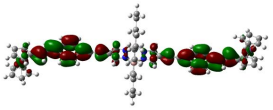
Ferrocenyl pyrazaboles	HOMO-1	LUMO+1
 11a		
 11b		
 11c		
 11d		
 11e		
 11f		
 11g		

Figure S5- HOMO-1, and LUMO+1 frontier orbitals of BODIPYs at the B3LYP/6-31+G** for C, N, B, H, and Lanl2DZ for Fe level

Ferrocenyl pyrazabole 11a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.151997	0.381451	0.766869
2	7	0	-1.254706	0.380486	-0.584705
3	6	0	-2.501471	0.765777	-0.912929
4	1	0	-2.794272	0.823266	-1.949813
5	6	0	-3.240228	1.028444	0.245281
6	6	0	-2.334136	0.771457	1.278326
7	1	0	-2.459386	0.856309	2.346553
8	6	0	0.608061	1.326220	2.495481
9	1	0	-0.172274	1.540254	3.243068
10	1	0	1.481723	1.028403	3.097027
11	6	0	-0.188043	-1.226238	2.629448
12	1	0	0.714813	-1.414800	3.232030
13	1	0	-0.935174	-0.889150	3.365570
14	6	0	0.943740	2.627149	1.753795
15	1	0	0.073173	2.958485	1.170543
16	1	0	1.739368	2.442353	1.017956
17	5	0	0.130909	0.025596	1.633279
18	6	0	-0.661167	-2.555518	2.025907
19	1	0	0.081004	-2.923231	1.303756
20	1	0	-1.582297	-2.394681	1.448236
21	7	0	1.151847	-0.381444	-0.766775
22	7	0	1.254653	-0.380165	0.584792
23	6	0	2.501430	-0.765430	0.913013
24	1	0	2.794303	-0.822698	1.949888
25	6	0	3.240099	-1.028370	-0.245189
26	6	0	2.333935	-0.771606	-1.278226
27	1	0	2.459129	-0.856657	-2.346443
28	6	0	-0.608353	-1.325990	-2.495380
29	1	0	0.171983	-1.540168	-3.242928
30	1	0	-1.481925	-1.028021	-3.096978
31	6	0	0.188132	1.226362	-2.629352
32	1	0	-0.714740	1.415184	-3.231829
33	1	0	0.935116	0.889147	-3.365562
34	6	0	-0.944306	-2.626845	-1.753699
35	1	0	-0.073823	-2.958355	-1.170420
36	1	0	-1.739914	-2.441884	-1.017875
37	5	0	-0.131009	-0.025433	-1.633187
38	6	0	0.661640	2.555487	-2.025756
39	1	0	-0.080363	2.923329	-1.303500
40	1	0	1.582790	2.394368	-1.448195
41	6	0	1.380801	3.771094	2.680273
42	1	0	0.586835	3.959528	3.416428

43	1	0	2.256973	3.449997	3.261142
44	6	0	0.920071	3.650641	-3.070901
45	1	0	1.661844	3.287656	-3.796287
46	1	0	-0.000456	3.823876	-3.645749
47	6	0	1.401369	4.973604	-2.466417
48	1	0	2.338659	4.839102	-1.913869
49	1	0	1.577254	5.730194	-3.238793
50	1	0	0.664262	5.380363	-1.764498
51	6	0	1.707956	5.071422	1.939013
52	1	0	2.522796	4.925175	1.220438
53	1	0	0.839757	5.437372	1.378774
54	1	0	2.014401	5.863448	2.630832
55	6	0	-0.919417	-3.650651	3.071121
56	1	0	-1.661361	-3.287801	3.796397
57	1	0	0.001098	-3.823587	3.646079
58	6	0	-1.381581	-3.770708	-2.680177
59	1	0	-0.587646	-3.959300	-3.416323
60	1	0	-2.257687	-3.449445	-3.261055
61	6	0	-1.709004	-5.070965	-1.938907
62	1	0	-2.015599	-5.862939	-2.630719
63	1	0	-0.840886	-5.437079	-1.378652
64	1	0	-2.523827	-4.924543	-1.220348
65	6	0	-1.400291	-4.973797	2.466700
66	1	0	-1.576092	-5.730358	3.239124
67	1	0	-2.337534	-4.839589	1.914003
68	1	0	-0.662978	-5.380438	1.764928
69	6	0	-4.622108	1.492513	0.360858
70	26	0	-6.377741	0.401191	0.032414
71	6	0	-5.430860	1.463455	1.545594
72	6	0	-5.411358	2.099168	-0.672898
73	6	0	-6.692505	2.057195	1.246539
74	6	0	-6.681289	2.448038	-0.125780
75	6	0	-5.868177	-1.526449	-0.557096
76	6	0	-6.677888	-0.905767	-1.555853
77	6	0	-7.929988	-0.564229	-0.959929
78	6	0	-7.893260	-0.972703	0.407570
79	6	0	-6.618859	-1.567318	0.656501
80	1	0	-5.141689	1.035993	2.495909
81	1	0	-5.096226	2.259949	-1.694896
82	1	0	-7.523336	2.157861	1.930933
83	1	0	-7.500679	2.902119	-0.665671
84	1	0	-4.849906	-1.867184	-0.686014
85	1	0	-6.385187	-0.705359	-2.577413
86	1	0	-8.749248	-0.055655	-1.449504
87	1	0	-8.679035	-0.826036	1.135908
88	1	0	-6.271675	-1.952974	1.605223
89	6	0	4.621964	-1.492485	-0.360802
90	26	0	6.377740	-0.401316	-0.032484
91	6	0	5.411230	-2.099240	0.672875
92	6	0	5.430627	-1.463480	-1.545604
93	6	0	6.681090	-2.448204	0.125652
94	6	0	6.692241	-2.057334	-1.246659

95	6	0	5.868703	1.526544	0.556725
96	6	0	6.619435	1.567009	-0.656857
97	6	0	7.893650	0.972045	-0.407800
98	6	0	7.930220	0.563761	0.959760
99	6	0	6.678202	0.905760	1.555598
100	1	0	5.096138	-2.260038	1.694884
101	1	0	5.141406	-1.035947	-2.495871
102	1	0	7.500490	-2.902350	0.665476
103	1	0	7.523005	-2.158064	-1.931126
104	1	0	4.850539	1.867623	0.685572
105	1	0	6.272383	1.952610	-1.605650
106	1	0	8.679391	0.825044	-1.136109
107	1	0	8.749305	0.054994	1.449428
108	1	0	6.385404	0.705595	2.577178

Total Energy (HF) = -2151.1883873 Hartree

Ferrocenyl pyrazabole 11b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.236335	-0.249353	-0.686089
2	7	0	1.245329	-0.248422	0.672089
3	6	0	2.496981	-0.498523	1.088596
4	1	0	2.729729	-0.541741	2.140788
5	6	0	3.338667	-0.669320	-0.020462
6	6	0	2.482086	-0.500768	-1.118469
7	1	0	2.700863	-0.548326	-2.173449
8	6	0	0.244409	1.289367	-2.590689
9	1	0	1.078054	1.049798	-3.269797
10	1	0	-0.624157	1.393168	-3.260154
11	6	0	-0.285124	-1.335528	-2.552276
12	1	0	-1.127788	-1.112859	-3.225983
13	1	0	0.574492	-1.459589	-3.229808
14	6	0	0.521829	2.648423	-1.933629
15	1	0	1.402730	2.574617	-1.280513
16	1	0	-0.314625	2.921979	-1.275432
17	5	0	-0.012800	-0.010874	-1.641446
18	6	0	-0.556310	-2.674616	-1.853107
19	1	0	-1.427872	-2.579085	-1.190171
20	1	0	0.288476	-2.931690	-1.198865
21	7	0	-1.236532	0.252666	0.686544
22	7	0	-1.245794	0.250418	-0.671628
23	6	0	-2.497602	0.499782	-1.088126

24	1	0	-2.730530	0.542074	-2.140315
25	6	0	-3.339125	0.671340	0.020934
26	6	0	-2.482274	0.504087	1.118932
27	1	0	-2.700911	0.552357	2.173907
28	6	0	-0.245406	-1.286422	2.591221
29	1	0	-1.078181	-1.045964	3.271078
30	1	0	0.623612	-1.391331	3.259925
31	6	0	0.285533	1.338189	2.552677
32	1	0	1.127337	1.114669	3.227177
33	1	0	-0.574547	1.463383	3.229413
34	6	0	-0.524967	-2.645075	1.934228
35	1	0	-1.406574	-2.570251	1.282162
36	1	0	0.310419	-2.919353	1.274998
37	5	0	0.012494	0.013646	1.641906
38	6	0	0.558886	2.676845	1.853518
39	1	0	1.431174	2.580301	1.191667
40	1	0	-0.284832	2.934612	1.198194
41	6	0	0.748824	3.784990	-2.941358
42	1	0	1.590115	3.520914	-3.597342
43	1	0	-0.129334	3.864659	-3.597255
44	6	0	0.803231	3.841580	2.824261
45	1	0	-0.067468	3.946548	3.486551
46	1	0	1.649820	3.592110	3.479140
47	6	0	1.075051	5.176133	2.122616
48	1	0	0.230842	5.469131	1.487882
49	1	0	1.244636	5.983436	2.843257
50	1	0	1.960804	5.113131	1.479843
51	6	0	1.019751	5.141534	-2.282904
52	1	0	0.178581	5.450661	-1.651763
53	1	0	1.909957	5.101669	-1.644466
54	1	0	1.181161	5.927045	-3.029072
55	6	0	-0.800638	-3.839369	-2.823831
56	1	0	0.069191	-3.943041	-3.487467
57	1	0	-1.648523	-3.590755	-3.477359
58	6	0	-0.751988	-3.781617	2.941978
59	1	0	-1.591987	-3.516645	3.599254
60	1	0	0.127015	-3.862619	3.596578
61	6	0	-1.025647	-5.137619	2.283533
62	1	0	-1.186709	-5.923191	3.029712
63	1	0	-1.916926	-5.096479	1.646665
64	1	0	-0.185954	-5.447525	1.650815
65	6	0	-1.069714	-5.174475	-2.122183
66	1	0	-1.239683	-5.981712	-2.842809
67	1	0	-0.224018	-5.466758	-1.489095
68	1	0	-1.954356	-5.112700	-1.477771
69	6	0	-4.727211	0.943907	0.033751
70	6	0	-5.918188	1.185229	0.053142
71	6	0	-7.305580	1.477869	0.086580
72	26	0	-8.887396	0.123161	-0.000546
73	6	0	-8.125477	1.580703	1.266775
74	6	0	-8.151209	1.760762	-1.044948
75	6	0	-9.443826	1.933619	0.862550

76	6	0	-9.459811	2.043842	-0.561371
77	6	0	-8.106773	-1.794317	-0.177215
78	6	0	-8.951760	-1.504861	-1.290695
79	6	0	-10.260092	-1.224925	-0.790620
80	6	0	-10.222781	-1.340643	0.631744
81	6	0	-8.891320	-1.691946	1.010975
82	1	0	-7.785207	1.402956	2.276943
83	1	0	-7.834892	1.742385	-2.078147
84	1	0	-10.293534	2.060691	1.518828
85	1	0	-10.323864	2.269463	-1.170966
86	1	0	-7.046512	-2.002552	-0.221550
87	1	0	-8.647302	-1.472382	-2.327702
88	1	0	-11.120078	-0.942953	-1.382613
89	1	0	-11.048788	-1.160038	1.305874
90	1	0	-8.532499	-1.826344	2.022095
91	6	0	4.726600	-0.942663	-0.033139
92	6	0	5.917376	-1.184998	-0.052218
93	6	0	7.304475	-1.479068	-0.085083
94	26	0	8.887962	-0.126190	-0.000160
95	6	0	8.149625	-1.761049	1.047020
96	6	0	8.124381	-1.584973	-1.265011
97	6	0	9.457913	-2.046636	0.564091
98	6	0	9.442240	-1.938856	-0.860015
99	6	0	8.109130	1.792808	0.167944
100	6	0	8.898779	1.686249	-1.016488
101	6	0	10.228086	1.334204	-0.630461
102	6	0	10.258960	1.222193	0.792348
103	6	0	8.948798	1.505129	1.285909
104	1	0	7.833221	-1.740554	2.080155
105	1	0	7.784472	-1.408569	-2.275534
106	1	0	10.321588	-2.272288	1.174208
107	1	0	10.291900	-2.068129	-1.515926
108	1	0	7.048974	2.002625	0.207058
109	1	0	8.544644	1.818472	-2.029546
110	1	0	11.056888	1.150787	-1.300383
111	1	0	11.115926	0.940661	1.388916
112	1	0	8.639752	1.475750	2.321650

Total Energy (HF) = - 2303.4941111 Hartree

Ferrocenyl pyrazabole 11c

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.250365	-0.062542	-0.456152
2	7	0	1.254259	-0.074304	0.902626

3	6	0	2.520754	-0.219353	1.322237
4	1	0	2.753111	-0.252140	2.374889
5	6	0	3.378108	-0.306734	0.215048
6	6	0	2.514284	-0.200628	-0.885466
7	1	0	2.740159	-0.220088	-1.939869
8	6	0	0.126742	1.382614	-2.360768
9	1	0	0.989775	1.226264	-3.027173
10	1	0	-0.737582	1.400757	-3.043499
11	6	0	-0.161546	-1.280430	-2.326911
12	1	0	-1.030313	-1.141309	-2.989651
13	1	0	0.697791	-1.316180	-3.015186
14	6	0	0.260790	2.762449	-1.701893
15	1	0	1.133347	2.773868	-1.034051
16	1	0	-0.609024	2.955060	-1.058271
17	5	0	-0.013293	0.062796	-1.414475
18	6	0	-0.289662	-2.642411	-1.630901
19	1	0	-1.160018	-2.638193	-0.960007
20	1	0	0.582994	-2.815419	-0.985453
21	7	0	-1.262840	0.205876	0.911773
22	7	0	-1.267547	0.207894	-0.447033
23	6	0	-2.535300	0.339577	-0.866984
24	1	0	-2.768446	0.363396	-1.919711
25	6	0	-3.392930	0.427201	0.239974
26	6	0	-2.527717	0.336744	1.340815
27	1	0	-2.753425	0.359349	2.395195
28	6	0	-0.144819	-1.239767	2.817941
29	1	0	-1.002886	-1.075689	3.488857
30	1	0	0.722800	-1.265068	3.496235
31	6	0	0.154812	1.421783	2.781255
32	1	0	1.018577	1.275736	3.449055
33	1	0	-0.708140	1.465661	3.464548
34	6	0	-0.294428	-2.618766	2.160518
35	1	0	-1.169454	-2.622197	1.495695
36	1	0	0.571152	-2.820667	1.514111
37	5	0	0.000819	0.078564	1.870089
38	6	0	0.298985	2.782010	2.085026
39	1	0	1.171847	2.768648	1.417421
40	1	0	-0.569388	2.963775	1.436307
41	6	0	0.393945	3.914632	-2.708604
42	1	0	1.266739	3.731693	-3.350902
43	1	0	-0.477426	3.909247	-3.378266
44	6	0	0.441116	3.960394	3.059726
45	1	0	-0.431554	3.981684	3.727327
46	1	0	1.310989	3.787289	3.708687
47	6	0	0.585283	5.317138	2.362878
48	1	0	-0.285853	5.534431	1.734044
49	1	0	0.684314	6.133475	3.086472
50	1	0	1.469484	5.338041	1.715301
51	6	0	0.523837	5.291589	-2.049618
52	1	0	-0.350523	5.517716	-1.428381
53	1	0	1.406640	5.339459	-1.401637
54	1	0	0.615952	6.088363	-2.795596

55	6	0	-0.423159	-3.821919	-2.605421
56	1	0	0.446375	-3.832993	-3.277350
57	1	0	-1.298172	-3.658617	-3.250006
58	6	0	-0.435752	-3.768768	3.168648
59	1	0	-1.303751	-3.575875	3.814510
60	1	0	0.438489	-3.772392	3.834559
61	6	0	-0.583477	-5.144603	2.511078
62	1	0	-0.680759	-5.939962	3.257906
63	1	0	-1.469834	-5.183194	1.867299
64	1	0	0.285402	-5.380471	1.885820
65	6	0	-0.548270	-5.180512	-1.908474
66	1	0	-0.642356	-5.997538	-2.631949
67	1	0	0.328953	-5.388402	-1.284912
68	1	0	-1.428336	-5.211615	-1.255738
69	6	0	-4.799770	0.564460	0.244170
70	6	0	-6.010707	0.675388	0.246703
71	6	0	4.782725	-0.465188	0.207913
72	6	0	5.990940	-0.602380	0.199049
73	6	0	-7.428930	0.796528	0.247212
74	6	0	-8.149877	0.865737	1.455343
75	6	0	-8.150874	0.846225	-0.963465
76	6	0	-9.535078	0.977883	1.448825
77	1	0	-7.610587	0.838491	2.396793
78	6	0	-9.534780	0.951807	-0.959096
79	1	0	-7.611556	0.792939	-1.903850
80	6	0	-10.260514	1.016155	0.245161
81	1	0	-10.063806	1.053834	2.393856
82	1	0	-10.067513	0.966705	-1.904967
83	6	0	7.404950	-0.764801	0.183532
84	6	0	8.121987	-0.736524	-1.030682
85	6	0	8.125827	-0.961520	1.377602
86	6	0	9.500773	-0.894605	-1.042848
87	1	0	7.583044	-0.583621	-1.960282
88	6	0	9.505647	-1.125537	1.353936
89	1	0	7.590073	-0.994734	2.320883
90	6	0	10.226255	-1.091376	0.147094
91	1	0	10.029929	-0.849645	-1.989648
92	1	0	10.032731	-1.301680	2.286438
93	6	0	11.686715	-1.284404	0.132677
94	26	0	13.150021	0.132259	-0.350781
95	6	0	12.589059	-1.089000	1.233567
96	6	0	12.481284	-1.727660	-0.980534
97	6	0	13.907698	-1.420522	0.806484
98	6	0	13.840578	-1.816555	-0.562717
99	6	0	12.210466	1.931741	-0.798441
100	6	0	12.966183	1.479734	-1.922298
101	6	0	14.333707	1.377938	-1.522868
102	6	0	14.422361	1.765956	-0.151889
103	6	0	13.110065	2.108208	0.295719
104	1	0	12.320569	-0.714046	2.211365
105	1	0	12.109902	-1.958857	-1.969110
106	1	0	14.805311	-1.346791	1.404699

107	1	0	14.676956	-2.105458	-1.184187
108	1	0	11.138459	2.070832	-0.768124
109	1	0	12.568927	1.231478	-2.896988
110	1	0	15.152314	1.035166	-2.140804
111	1	0	15.320187	1.768201	0.450885
112	1	0	12.840260	2.417007	1.296331
113	6	0	-11.728298	1.142581	0.251236
114	26	0	-13.121959	-0.286044	-0.377816
115	6	0	-12.614493	0.789759	1.325673
116	6	0	-12.548871	1.659736	-0.809948
117	6	0	-13.950128	1.097034	0.934495
118	6	0	-13.909054	1.636902	-0.385860
119	6	0	-12.097073	-1.975679	-1.023594
120	6	0	-12.894922	-1.449870	-2.084677
121	6	0	-14.258779	-1.464644	-1.660461
122	6	0	-14.302801	-1.997556	-0.336651
123	6	0	-12.966723	-2.313454	0.056675
124	1	0	-12.322820	0.328001	2.258615
125	1	0	-12.193925	2.013952	-1.767564
126	1	0	-14.840403	0.914648	1.520331
127	1	0	-14.761596	1.945505	-0.975020
128	1	0	-11.018818	-2.058152	-1.020006
129	1	0	-12.528605	-1.079463	-3.032276
130	1	0	-15.105283	-1.104802	-2.229050
131	1	0	-15.188442	-2.111380	0.273217
132	1	0	-12.662723	-2.709280	1.015943

Total Energy (HF) = - 2765.6134873 Hartree

Ferrocenyl pyrazabole 11d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.250312	1.447718	-0.555525
2	7	0	-1.236101	1.669170	0.785027
3	6	0	-2.504856	1.739545	1.216623
4	1	0	-2.725192	1.915650	2.257627
5	6	0	-3.381381	1.559473	0.137110
6	6	0	-2.528023	1.378315	-0.960571
7	1	0	-2.769871	1.203197	-1.996981
8	6	0	0.004078	-0.236760	-2.156978
9	1	0	-0.872326	-0.314975	-2.819705
10	1	0	0.865132	-0.309567	-2.840100
11	6	0	-0.008210	2.388320	-2.690083

12	1	0	0.854813	2.198091	-3.347616
13	1	0	-0.880578	2.190777	-3.332952
14	6	0	0.018678	-1.450838	-1.218173
15	1	0	-0.849765	-1.413169	-0.545612
16	1	0	0.901971	-1.407663	-0.565510
17	5	0	0.006636	1.260829	-1.512722
18	6	0	-0.011145	3.873645	-2.302525
19	1	0	0.868012	4.100107	-1.683364
20	1	0	-0.883481	4.093636	-1.671419
21	7	0	1.297095	1.669896	0.759689
22	7	0	1.282666	1.454801	-0.581908
23	6	0	2.551248	1.393235	-1.015167
24	1	0	2.771313	1.223258	-2.057251
25	6	0	3.428011	1.573003	0.064258
26	6	0	2.574880	1.743939	1.163791
27	1	0	2.816910	1.917578	2.200404
28	6	0	0.046109	3.355308	2.361991
29	1	0	0.921097	3.430298	3.026943
30	1	0	-0.816347	3.430807	3.043060
31	6	0	0.051660	0.729853	2.893301
32	1	0	-0.808932	0.924438	3.552736
33	1	0	0.926550	0.922488	3.534258
34	6	0	0.037892	4.569730	1.423495
35	1	0	0.908176	4.529596	0.753427
36	1	0	-0.843641	4.529543	0.768333
37	5	0	0.040049	1.858110	1.716709
38	6	0	0.045806	-0.755300	2.505259
39	1	0	-0.836452	-0.977030	1.888744
40	1	0	0.914980	-0.979569	1.871348
41	6	0	0.014615	-2.798659	-1.954261
42	1	0	-0.868836	-2.849622	-2.605939
43	1	0	0.884288	-2.844803	-2.624528
44	6	0	0.056485	-1.705185	3.712125
45	1	0	0.940088	-1.491319	4.329542
46	1	0	-0.813110	-1.487819	4.347907
47	6	0	0.049477	-3.187544	3.325246
48	1	0	0.925047	-3.442831	2.717144
49	1	0	0.058727	-3.834983	4.208758
50	1	0	-0.840992	-3.439880	2.737910
51	6	0	0.027798	-4.009383	-1.015593
52	1	0	0.917716	-4.005273	-0.375551
53	1	0	-0.848455	-4.009992	-0.356968
54	1	0	0.024522	-4.951993	-1.573483
55	6	0	-0.023171	4.823083	-3.509722
56	1	0	-0.903052	4.603517	-4.130442
57	1	0	0.850249	4.611013	-4.142051
58	6	0	0.044148	5.917334	2.159954
59	1	0	0.925923	5.965367	2.814116
60	1	0	-0.827319	5.965989	2.827742
61	6	0	0.037348	7.128236	1.221448
62	1	0	0.041605	8.070742	1.779522
63	1	0	0.915730	7.126492	0.565685

64	1	0	-0.850533	7.126734	0.578611
65	6	0	-0.027068	6.305538	-3.123188
66	1	0	-0.036381	6.952637	-4.006938
67	1	0	-0.907084	6.555457	-2.519290
68	1	0	0.859108	6.563588	-2.531891
69	6	0	4.844633	1.583802	0.043309
70	6	0	6.059388	1.594249	0.016495
71	6	0	-4.798182	1.564328	0.154381
72	6	0	-6.013024	1.572175	0.176449
73	6	0	7.488258	1.613965	-0.026227
74	6	0	8.171705	2.757964	-0.484171
75	6	0	8.225645	0.486229	0.372025
76	6	0	9.562208	2.756787	-0.530775
77	1	0	7.604842	3.629318	-0.794568
78	6	0	9.627031	0.477449	0.324902
79	1	0	7.691257	-0.398313	0.701780
80	6	0	10.284914	1.633464	-0.127474
81	1	0	10.090642	3.640647	-0.876270
82	6	0	-7.442331	1.591866	0.207644
83	6	0	-8.160542	0.423797	0.513686
84	6	0	-8.145344	2.780806	-0.070113
85	6	0	-9.562281	0.419178	0.557793
86	1	0	-7.610169	-0.491275	0.704456
87	6	0	-9.536097	2.783250	-0.028966
88	1	0	-7.593471	3.683658	-0.309256
89	6	0	-10.239125	1.620368	0.286882
90	1	0	-10.079782	3.700837	-0.234548
91	1	0	-11.322874	1.647367	0.341581
92	1	0	11.370090	1.656924	-0.146419
93	6	0	-10.310071	-0.804916	0.906274
94	26	0	-10.450096	-2.572762	-0.202988
95	6	0	-9.818698	-1.922654	1.663730
96	6	0	-11.678879	-1.093052	0.580982
97	6	0	-10.872067	-2.871578	1.809114
98	6	0	-12.022647	-2.359188	1.138422
99	6	0	-9.331447	-2.357028	-1.941607
100	6	0	-10.698901	-2.606491	-2.266623
101	6	0	-11.061656	-3.870206	-1.708562
102	6	0	-9.918039	-4.401700	-1.039183
103	6	0	-8.848905	-3.465670	-1.182309
104	1	0	-8.818368	-2.025051	2.060671
105	1	0	-12.328236	-0.474196	-0.022515
106	1	0	-10.800187	-3.825351	2.313285
107	1	0	-12.975700	-2.859605	1.036581
108	1	0	-8.772424	-1.464288	-2.186551
109	1	0	-11.353634	-1.940654	-2.811880
110	1	0	-12.039570	-4.329358	-1.757075
111	1	0	-9.878571	-5.333115	-0.491295
112	1	0	-7.856100	-3.567113	-0.765947
113	6	0	10.398373	-0.704438	0.757729
114	26	0	10.377454	-2.617145	-0.088749
115	6	0	11.712370	-1.074519	0.313161

116	6	0	9.993259	-1.686689	1.724846
117	6	0	12.109866	-2.256997	1.002953
118	6	0	11.047084	-2.634365	1.877413
119	6	0	9.038650	-2.621828	-1.676722
120	6	0	8.656884	-3.602103	-0.711290
121	6	0	9.731702	-4.533169	-0.578344
122	6	0	10.777678	-4.127755	-1.461464
123	6	0	10.349078	-2.946711	-2.140767
124	1	0	12.285300	-0.566549	-0.450214
125	1	0	9.048706	-1.700519	2.250833
126	1	0	13.037264	-2.793943	0.859033
127	1	0	11.030095	-3.502032	2.522453
128	1	0	8.457377	-1.758029	-1.968654
129	1	0	7.728315	-3.620971	-0.157435
130	1	0	9.761807	-5.376609	0.097773
131	1	0	11.738386	-4.611623	-1.572496
132	1	0	10.928015	-2.379943	-2.856895

Total Energy (HF) = - 2765.610203 Hartree

Ferrocenyl pyrazabole 11e

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.266918	0.185597	-0.544409
2	7	0	-1.270371	0.189644	0.814631
3	6	0	-2.539918	0.296831	1.235713
4	1	0	-2.772529	0.319188	2.288625
5	6	0	-3.399865	0.366563	0.129105
6	6	0	-2.534106	0.290737	-0.972566
7	1	0	-2.761407	0.307034	-2.026743
8	6	0	-0.120102	-1.250342	-2.441204
9	1	0	-0.982240	-1.111025	-3.112455
10	1	0	0.747184	-1.261950	-3.120315
11	6	0	0.120230	1.417836	-2.425703
12	1	0	0.986570	1.286608	-3.093176
13	1	0	-0.743795	1.436550	-3.108791
14	6	0	-0.238156	-2.626803	-1.772139
15	1	0	-1.115231	-2.645923	-1.110252
16	1	0	0.629702	-2.801198	-1.120824
17	5	0	-0.002439	0.078471	-1.504423
18	6	0	0.233306	2.786531	-1.740254
19	1	0	1.108571	2.800047	-1.075795
20	1	0	-0.636907	2.951334	-1.089527
21	7	0	1.254638	-0.016437	0.820939

22	7	0	1.255920	-0.039399	-0.537935
23	6	0	2.524040	-0.159203	-0.959372
24	1	0	2.755093	-0.195384	-2.012218
25	6	0	3.385509	-0.218227	0.146644
26	6	0	2.522136	-0.121992	1.248593
27	1	0	2.750688	-0.128164	2.302625
28	6	0	0.095826	1.413452	2.716606
29	1	0	0.966444	1.288557	3.379697
30	1	0	-0.765214	1.411177	3.403707
31	6	0	-0.122004	-1.257120	2.702797
32	1	0	-0.996558	-1.139644	3.362031
33	1	0	0.735758	-1.261639	3.393944
34	6	0	0.184539	2.791134	2.045658
35	1	0	1.057369	2.826047	1.378993
36	1	0	-0.690137	2.947628	1.398779
37	5	0	-0.010654	0.083024	1.781155
38	6	0	-0.206060	-2.627525	2.016565
39	1	0	-1.077097	-2.657199	1.347237
40	1	0	0.670821	-2.775191	1.370526
41	6	0	-0.347350	-3.789083	-2.769991
42	1	0	-1.215938	-3.622676	-3.422413
43	1	0	0.530436	-3.778829	-3.431166
44	6	0	-0.298028	-3.804254	2.999004
45	1	0	0.572561	-3.781688	3.669302
46	1	0	-1.176884	-3.666524	3.644333
47	6	0	-0.378384	-5.170986	2.311443
48	1	0	0.503901	-5.353148	1.686965
49	1	0	-0.442480	-5.985624	3.040837
50	1	0	-1.258562	-5.236969	1.661514
51	6	0	-0.467029	-5.161744	-2.100222
52	1	0	0.402730	-5.371201	-1.466853
53	1	0	-1.356828	-5.215395	-1.462302
54	1	0	-0.540247	-5.966031	-2.840168
55	6	0	0.342510	3.960732	-2.724077
56	1	0	-0.533529	3.956180	-3.387600
57	1	0	1.213216	3.804021	-3.376073
58	6	0	0.276360	3.956728	3.041260
59	1	0	1.153055	3.809826	3.687516
60	1	0	-0.596139	3.928837	3.708903
61	6	0	0.361782	5.330796	2.369114
62	1	0	0.424489	6.137242	3.107678
63	1	0	1.244566	5.402401	1.723335
64	1	0	-0.517763	5.521375	1.743286
65	6	0	0.457247	5.325701	-2.037923
66	1	0	0.531525	6.138697	-2.768181
67	1	0	-0.415095	5.526189	-1.405203
68	1	0	1.344727	5.373502	-1.396310
69	6	0	4.792716	-0.348063	0.148451
70	6	0	6.003449	-0.462760	0.147296
71	6	0	-4.808206	0.482855	0.122715
72	6	0	-6.020376	0.580804	0.112683
73	6	0	7.419309	-0.600557	0.143865

74	6	0	8.155127	-0.522954	1.345051
75	6	0	8.119070	-0.820279	-1.061315
76	6	0	9.535368	-0.659965	1.340958
77	1	0	7.628144	-0.354535	2.278582
78	6	0	9.499259	-0.957537	-1.064902
79	1	0	7.563873	-0.882636	-1.991609
80	6	0	10.236504	-0.880339	0.136082
81	1	0	10.090567	-0.599660	2.271354
82	1	0	10.026261	-1.127610	-1.998113
83	6	0	-7.438424	0.691853	0.094376
84	6	0	-8.136749	0.787298	-1.127822
85	6	0	-8.178455	0.706399	1.295371
86	6	0	-9.519601	0.890698	-1.147935
87	1	0	-7.578399	0.778490	-2.058270
88	6	0	-9.561598	0.809692	1.274787
89	1	0	-7.652590	0.634651	2.241890
90	6	0	-10.261440	0.902511	0.052775
91	1	0	-10.045701	0.963491	-2.094219
92	1	0	-10.119926	0.819605	2.205223
93	6	0	11.651657	-1.021486	0.132636
94	6	0	12.861695	-1.151261	0.132673
95	6	0	14.269085	-1.316900	0.138510
96	26	0	15.705405	0.147760	-0.231933
97	6	0	15.143116	-1.165945	1.274562
98	6	0	15.093058	-1.687260	-0.984564
99	6	0	16.471781	-1.454794	0.854803
100	6	0	16.440845	-1.776288	-0.536650
101	6	0	14.730751	1.937967	-0.633672
102	6	0	15.543361	1.561887	-1.745326
103	6	0	16.896505	1.480017	-1.295195
104	6	0	16.919223	1.804876	0.094753
105	6	0	15.580043	2.087104	0.503938
106	1	0	14.828386	-0.870709	2.265348
107	1	0	14.734650	-1.853581	-1.990445
108	1	0	17.355996	-1.404528	1.475048
109	1	0	17.297351	-2.013499	-1.152482
110	1	0	13.653834	2.036452	-0.638844
111	1	0	15.191544	1.345155	-2.744564
112	1	0	17.748896	1.189948	-1.894165
113	1	0	17.792278	1.804388	0.732923
114	1	0	15.260908	2.339732	1.505695
115	6	0	-11.679884	1.002034	0.028736
116	6	0	-12.893393	1.089769	0.001139
117	6	0	-14.305538	1.203278	-0.036408
118	26	0	-15.676073	-0.357586	-0.207534
119	6	0	-15.198757	1.187839	1.094611
120	6	0	-15.117073	1.368612	-1.216129
121	6	0	-16.527449	1.356100	0.613607
122	6	0	-16.477217	1.467675	-0.809605
123	6	0	-14.626734	-2.148737	-0.282386
124	6	0	-15.393387	-1.979763	-1.474717
125	6	0	-16.769513	-1.882589	-1.104339

126	6	0	-16.852438	-1.990787	0.316675
127	6	0	-15.527652	-2.154622	0.824845
128	1	0	-14.896731	1.055937	2.123840
129	1	0	-14.741433	1.397219	-2.228997
130	1	0	-17.423107	1.363190	1.219351
131	1	0	-17.328117	1.573147	-1.468226
132	1	0	-13.548331	-2.204512	-0.223923
133	1	0	-14.998150	-1.906110	-2.478443
134	1	0	-17.599412	-1.721337	-1.778621
135	1	0	-17.756402	-1.927351	0.906913
136	1	0	-15.252401	-2.237053	1.867285

Total Energy (HF) = - 2917.9212204 Hartree

Ferrocenyl pyrazabole 11f

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.265390	0.070140	0.960540
2	7	0	-1.264777	0.069945	-0.398606
3	6	0	-2.535263	0.140395	-0.823894
4	1	0	-2.765319	0.153350	-1.877552
5	6	0	-3.400327	0.189583	0.279900
6	6	0	-2.536408	0.140723	1.384615
7	1	0	-2.767374	0.154297	2.438072
8	6	0	0.071149	1.340297	2.852141
9	1	0	-0.792201	1.321630	3.536080
10	1	0	0.942247	1.240711	3.518852
11	6	0	-0.072696	-1.335579	2.852961
12	1	0	0.790180	-1.316450	3.537484
13	1	0	-0.944298	-1.235603	3.518952
14	6	0	0.128697	2.715352	2.172441
15	1	0	-0.745491	2.844675	1.519004
16	1	0	1.004637	2.768232	1.510900
17	5	0	-0.000458	0.002080	1.924401
18	6	0	-0.129669	-2.711056	2.174072
19	1	0	0.745125	-2.840799	1.521524
20	1	0	-1.005007	-2.764379	1.511773
21	7	0	1.265117	-0.069008	-0.397758
22	7	0	1.265049	-0.066639	0.961386
23	6	0	2.535860	-0.136501	1.386245
24	1	0	2.766266	-0.148105	2.439849
25	6	0	3.400316	-0.187553	0.282055
26	6	0	2.535793	-0.140498	-0.822261
27	1	0	2.766408	-0.155430	-1.875769
28	6	0	-0.072389	-1.337910	-2.289441

29	1	0	0.791566	-1.320604	-2.972653
30	1	0	-0.942759	-1.236878	-2.956882
31	6	0	0.073947	1.337788	-2.290158
32	1	0	-0.789473	1.319998	-2.974037
33	1	0	0.944878	1.236435	-2.956820
34	6	0	-0.132778	-2.712916	-1.609891
35	1	0	0.740706	-2.843846	-0.955848
36	1	0	-1.009285	-2.764343	-0.948975
37	5	0	0.000462	0.000191	-1.361560
38	6	0	0.133623	2.713205	-1.611386
39	1	0	-0.740551	2.844507	-0.958333
40	1	0	1.009445	2.765096	-0.949602
41	6	0	0.184413	3.889887	3.160015
42	1	0	-0.692326	3.845706	3.821221
43	1	0	1.059358	3.769270	3.814057
44	6	0	0.191701	3.886919	-2.599812
45	1	0	1.066511	3.764142	-3.253631
46	1	0	-0.685025	3.843903	-3.261112
47	6	0	0.251481	5.258213	-1.919291
48	1	0	1.137770	5.345724	-1.280291
49	1	0	0.290020	6.070469	-2.653118
50	1	0	-0.626899	5.425022	-1.285146
51	6	0	0.241665	5.260789	2.478483
52	1	0	1.127668	5.349394	1.839242
53	1	0	-0.637137	5.425595	1.844394
54	1	0	0.278896	6.073645	3.211713
55	6	0	-0.186284	-3.884964	3.162343
56	1	0	-1.061877	-3.763959	3.815447
57	1	0	0.689803	-3.840322	3.824380
58	6	0	-0.189885	-3.887248	-2.597639
59	1	0	0.687567	-3.844719	-3.258008
60	1	0	-1.063970	-3.764829	-3.252495
61	6	0	-0.250514	-5.258100	-1.916300
62	1	0	-0.288463	-6.070821	-2.649643
63	1	0	0.627221	-5.424635	-1.281193
64	1	0	-1.137439	-5.345062	-1.278107
65	6	0	-0.242809	-5.256309	2.481644
66	1	0	-0.280575	-6.068697	3.215365
67	1	0	-1.128249	-5.345435	1.841697
68	1	0	0.636561	-5.421420	1.848420
69	6	0	4.810966	-0.269597	0.280276
70	6	0	6.024991	-0.341917	0.275326
71	6	0	-4.810988	0.271424	0.277485
72	6	0	-6.025023	0.343555	0.272288
73	6	0	7.444694	-0.427340	0.265267
74	6	0	8.153429	-0.489682	-0.953264
75	6	0	8.175417	-0.451558	1.472019
76	6	0	9.537616	-0.572679	-0.964271
77	1	0	7.601881	-0.472039	-1.887599
78	6	0	9.559783	-0.534328	1.460487
79	1	0	7.641032	-0.404292	2.415259
80	6	0	10.269926	-0.596231	0.242230

81	1	0	10.072353	-0.620019	-1.907241
82	1	0	10.111539	-0.551957	2.394638
83	6	0	-7.444746	0.428653	0.262365
84	6	0	-8.175259	0.453342	1.469237
85	6	0	-8.153713	0.490202	-0.956069
86	6	0	-9.559639	0.535787	1.457917
87	1	0	-7.640688	0.406658	2.412401
88	6	0	-9.537927	0.572877	-0.966864
89	1	0	-7.602340	0.472178	-1.890499
90	6	0	-10.270022	0.596895	0.239758
91	1	0	-10.111235	0.553763	2.392157
92	1	0	-10.072841	0.619574	-1.909766
93	6	0	-11.688827	0.678982	0.226977
94	6	0	-12.904470	0.746612	0.213070
95	6	0	-14.324417	0.820885	0.192553
96	6	0	-15.069283	0.815018	1.388785
97	6	0	-15.027226	0.901464	-1.028276
98	6	0	-16.456677	0.884096	1.361052
99	1	0	-14.545595	0.763522	2.337999
100	6	0	-16.413305	0.964508	-1.045690
101	1	0	-14.469619	0.907507	-1.959439
102	6	0	-17.162136	0.952674	0.146394
103	1	0	-17.003726	0.901641	2.298490
104	1	0	-16.928377	1.008260	-2.000258
105	6	0	-18.632901	1.033221	0.130220
106	26	0	-19.972034	-0.425253	-0.546951
107	6	0	-19.524991	0.633886	1.183443
108	6	0	-19.452405	1.544281	-0.934916
109	6	0	-20.862920	0.907931	0.776305
110	6	0	-20.817656	1.472636	-0.533450
111	6	0	-18.886373	-2.074162	-1.199702
112	6	0	-19.675936	-1.551910	-2.268658
113	6	0	-21.047451	-1.611976	-1.874659
114	6	0	-21.104708	-2.169611	-0.561730
115	6	0	-19.769057	-2.455284	-0.144712
116	1	0	-19.234575	0.165123	2.113222
117	1	0	-19.094305	1.926847	-1.880293
118	1	0	-21.756170	0.688057	1.344629
119	1	0	-21.669881	1.765909	-1.130885
120	1	0	-17.806549	-2.127080	-1.174498
121	1	0	-19.300138	-1.155377	-3.201868
122	1	0	-21.891395	-1.265833	-2.455492
123	1	0	-21.999992	-2.320599	0.025677
124	1	0	-19.474750	-2.860108	0.813801
125	6	0	11.688709	-0.678666	0.229184
126	6	0	12.904334	-0.746539	0.214915
127	6	0	14.324252	-0.821236	0.193841
128	6	0	15.069541	-0.816123	1.389815
129	6	0	15.026593	-0.901503	-1.027278
130	6	0	16.456905	-0.885724	1.361572
131	1	0	14.546196	-0.764826	2.339228
132	6	0	16.412638	-0.965041	-1.045200

133	1	0	14.468655	-0.906919	-1.958246
134	6	0	17.161886	-0.954066	0.146632
135	1	0	17.004285	-0.903874	2.298806
136	1	0	16.927430	-1.008483	-1.999937
137	6	0	18.632600	-1.035299	0.129853
138	26	0	19.972191	0.422477	-0.547885
139	6	0	19.525320	-0.636408	1.182711
140	6	0	19.451405	-1.546785	-0.935616
141	6	0	20.862939	-0.911147	0.775026
142	6	0	20.816856	-1.475837	-0.534705
143	6	0	18.886957	2.070335	-1.204027
144	6	0	19.679918	1.548513	-2.270673
145	6	0	21.050290	1.609803	-1.872871
146	6	0	21.103426	2.167760	-0.559902
147	6	0	19.766380	2.452399	-0.146657
148	1	0	19.235502	-0.167471	2.112591
149	1	0	19.092669	-1.929185	-1.880819
150	1	0	21.756546	-0.691719	1.342961
151	1	0	21.668677	-1.769568	-1.132489
152	1	0	17.807021	2.122384	-1.181841
153	1	0	19.307018	1.151470	-3.204835
154	1	0	21.896143	1.264275	-2.451284
155	1	0	21.996937	2.319629	0.029972
156	1	0	19.469048	2.857206	0.810930

Total Energy (HF) = - 3380.0407566 Hartree

Ferrocenyl pyrazabole 11g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.241462	0.374494	-0.682900
2	7	0	-1.311723	0.201143	0.663164
3	6	0	-2.601847	0.244324	1.030167
4	1	0	-2.885928	0.132679	2.064655
5	6	0	-3.407574	0.450931	-0.099897
6	6	0	-2.487724	0.524984	-1.156958
7	1	0	-2.663850	0.671954	-2.210816
8	6	0	0.005920	-0.900221	-2.628036
9	1	0	-0.824047	-0.714644	-3.328106
10	1	0	0.906357	-0.858837	-3.261247
11	6	0	0.215173	1.760760	-2.397987
12	1	0	1.113457	1.691056	-3.031747
13	1	0	-0.614760	1.820519	-3.119856
14	6	0	-0.135164	-2.321487	-2.066223
15	1	0	-1.037366	-2.386824	-1.442007

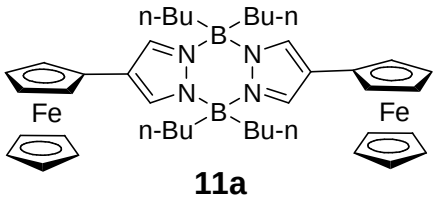
16	1	0	0.706855	-2.542895	-1.395588
17	5	0	0.067183	0.354356	-1.587963
18	6	0	0.272446	3.076163	-1.608905
19	1	0	1.120007	3.056247	-0.909774
20	1	0	-0.626037	3.175041	-0.983824
21	7	0	1.210988	-0.002972	0.769168
22	7	0	1.281408	0.166776	-0.577348
23	6	0	2.570515	0.107332	-0.945998
24	1	0	2.854349	0.212417	-1.981242
25	6	0	3.375132	-0.107279	0.183380
26	6	0	2.455899	-0.167119	1.241900
27	1	0	2.631616	-0.316061	2.295544
28	6	0	-0.037678	1.276157	2.712192
29	1	0	0.791671	1.091934	3.413395
30	1	0	-0.938896	1.234960	3.344332
31	6	0	-0.243523	-1.385575	2.486838
32	1	0	-1.141637	-1.316361	3.120842
33	1	0	0.586587	-1.443673	3.208592
34	6	0	0.103254	2.696837	2.149020
35	1	0	1.006333	2.762077	1.526085
36	1	0	-0.737876	2.916974	1.476887
37	5	0	-0.097276	0.019958	1.674420
38	6	0	-0.299531	-2.701702	1.698754
39	1	0	-1.147552	-2.683340	1.000122
40	1	0	0.598690	-2.799869	1.073153
41	6	0	-0.204195	-3.408915	-3.148214
42	1	0	-1.047207	-3.194274	-3.819715
43	1	0	0.698362	-3.353215	-3.772860
44	6	0	-0.419845	-3.947205	2.589005
45	1	0	0.427660	-3.972503	3.288203
46	1	0	-1.320338	-3.858195	3.212766
47	6	0	-0.471981	-5.260359	1.801518
48	1	0	0.433257	-5.397547	1.198798
49	1	0	-0.561950	-6.125789	2.466898
50	1	0	-1.327184	-5.277700	1.116081
51	6	0	-0.348153	-4.826192	-2.584351
52	1	0	0.495838	-5.081516	-1.933171
53	1	0	-1.262811	-4.924901	-1.988351
54	1	0	-0.389907	-5.574990	-3.382687
55	6	0	0.394933	4.321998	-2.498407
56	1	0	-0.452096	4.348713	-3.198138
57	1	0	1.295696	4.232108	-3.121647
58	6	0	0.169882	3.785393	3.230029
59	1	0	1.011998	3.571977	3.903052
60	1	0	-0.733598	3.729657	3.853330
61	6	0	0.313725	5.202246	2.665083
62	1	0	0.353854	5.951794	3.462801
63	1	0	1.229145	5.301031	2.070267
64	1	0	-0.529512	5.456440	2.012488
65	6	0	0.448294	5.634752	-1.710348
66	1	0	0.539701	6.500335	-2.375337
67	1	0	-0.457069	5.772851	-1.108022

68	1	0	1.303169	5.650761	-1.024472
69	6	0	4.780103	-0.247515	0.243312
70	6	0	5.987731	-0.380783	0.300316
71	6	0	-4.815279	0.560284	-0.160903
72	6	0	-6.026578	0.655365	-0.216221
73	6	0	7.397596	-0.553737	0.373250
74	6	0	8.022582	-0.885718	1.591566
75	6	0	8.208010	-0.405495	-0.773597
76	6	0	9.397333	-1.067880	1.650923
77	1	0	7.416671	-1.001823	2.484416
78	6	0	9.580222	-0.588215	-0.702932
79	1	0	7.742082	-0.145484	-1.718770
80	6	0	10.213681	-0.930809	0.510434
81	1	0	9.858483	-1.328601	2.600146
82	1	0	10.170335	-0.462703	-1.605351
83	6	0	-7.442825	0.767481	-0.284838
84	6	0	-8.082009	1.146032	-1.481926
85	6	0	-8.246667	0.501544	0.845342
86	6	0	-9.464932	1.252150	-1.538657
87	1	0	-7.481177	1.355257	-2.361153
88	6	0	-9.626809	0.608729	0.777345
89	1	0	-7.769199	0.208462	1.774957
90	6	0	-10.275922	0.987680	-0.416915
91	1	0	-9.937498	1.547050	-2.472145
92	1	0	-10.210875	0.394084	1.666844
93	6	0	-11.726908	1.117937	-0.547146
94	1	0	-12.069665	1.421971	-1.535202
95	6	0	-12.654298	0.908589	0.410824
96	1	0	-12.338880	0.628640	1.414288
97	6	0	11.652798	-1.156517	0.641234
98	1	0	11.987434	-1.384184	1.652352
99	6	0	12.576849	-1.132894	-0.342200
100	1	0	12.268382	-0.942779	-1.368664
101	6	0	14.000768	-1.385262	-0.166494
102	26	0	15.540141	0.039499	-0.191297
103	6	0	14.756591	-1.423681	1.056085
104	6	0	14.927971	-1.641752	-1.236061
105	6	0	16.112196	-1.729448	0.740521
106	6	0	16.219271	-1.863191	-0.677249
107	6	0	14.706864	1.929033	-0.445849
108	6	0	15.625026	1.650625	-1.503645
109	6	0	16.909993	1.423447	-0.923834
110	6	0	16.785348	1.558739	0.491905
111	6	0	15.423320	1.871071	0.787167
112	1	0	14.368702	-1.227103	2.045874
113	1	0	14.677059	-1.656674	-2.288334
114	1	0	16.925805	-1.805082	1.448810
115	1	0	17.126353	-2.063669	-1.230542
116	1	0	13.646123	2.109056	-0.554326
117	1	0	15.384276	1.594957	-2.556378
118	1	0	17.811884	1.161256	-1.459954
119	1	0	17.576309	1.417841	1.215767

120	1	0	15.001988	2.010441	1.773225
121	6	0	-14.094358	1.047236	0.239893
122	26	0	-15.470570	-0.521752	0.038383
123	6	0	-15.051253	1.057247	1.314184
124	6	0	-14.841603	1.173102	-0.982158
125	6	0	-16.354977	1.214459	0.762756
126	6	0	-16.224328	1.287209	-0.657337
127	6	0	-14.440078	-2.329117	0.068896
128	6	0	-15.131041	-2.178968	-1.170848
129	6	0	-16.525487	-2.056741	-0.886705
130	6	0	-16.695477	-2.130812	0.528824
131	6	0	-15.406373	-2.297265	1.119878
132	1	0	-14.811155	0.954384	2.364102
133	1	0	-14.428681	1.157883	-1.981036
134	1	0	-17.282040	1.239932	1.318714
135	1	0	-17.036531	1.371671	-1.366303
136	1	0	-13.368562	-2.407563	0.191334
137	1	0	-14.675230	-2.134859	-2.150302
138	1	0	-17.311328	-1.903794	-1.613743
139	1	0	-17.632407	-2.042440	1.061538
140	1	0	-15.196550	-2.361529	2.178796

Total Energy (HF) = -2920.4247373 Hartree

III. Copies of ^{1}H NMR, ^{13}C NMR and HRMS Spectra of the New Compounds.



11a

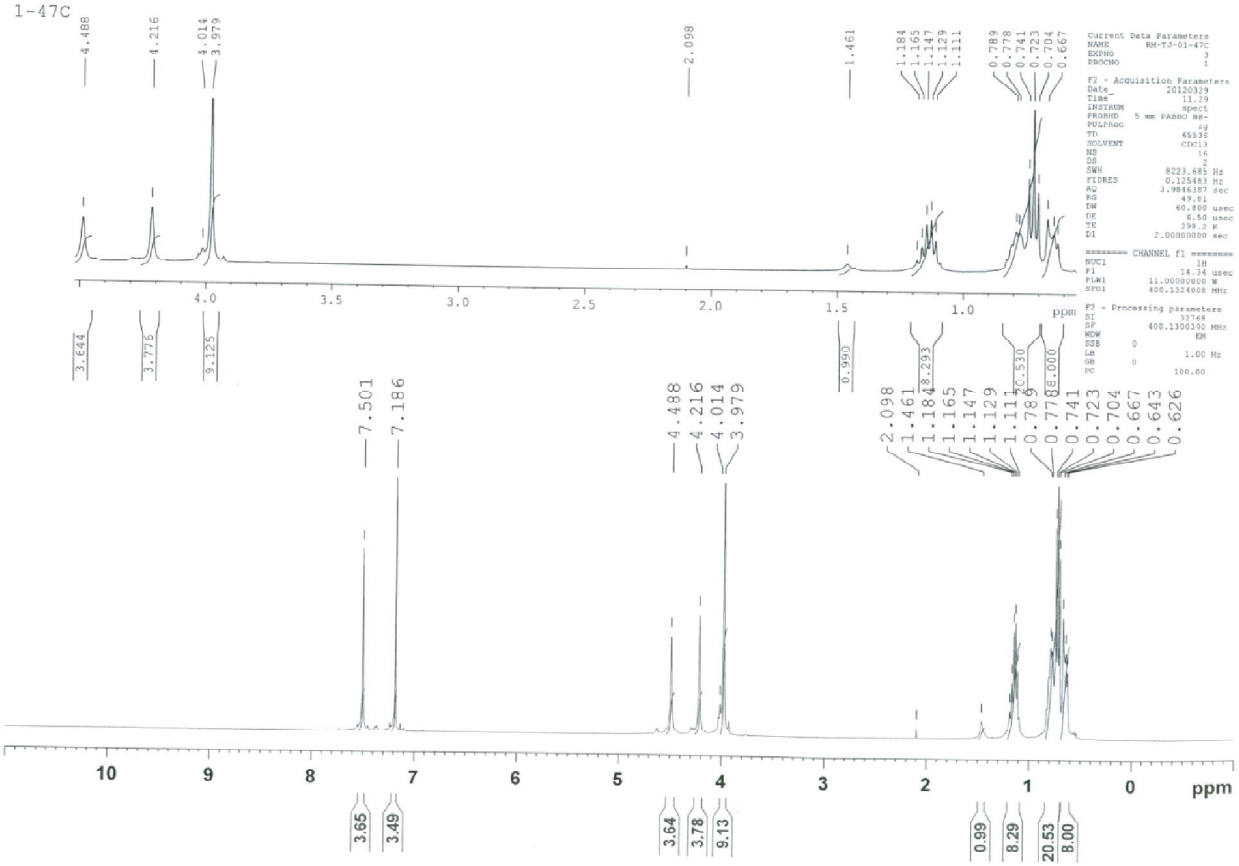
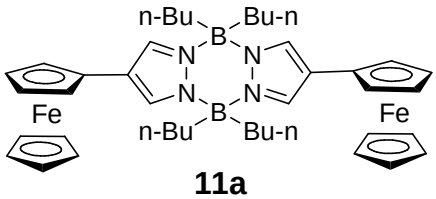


Figure S-6: ^{1}H-NMR spectrum of compound **11a.**



11a

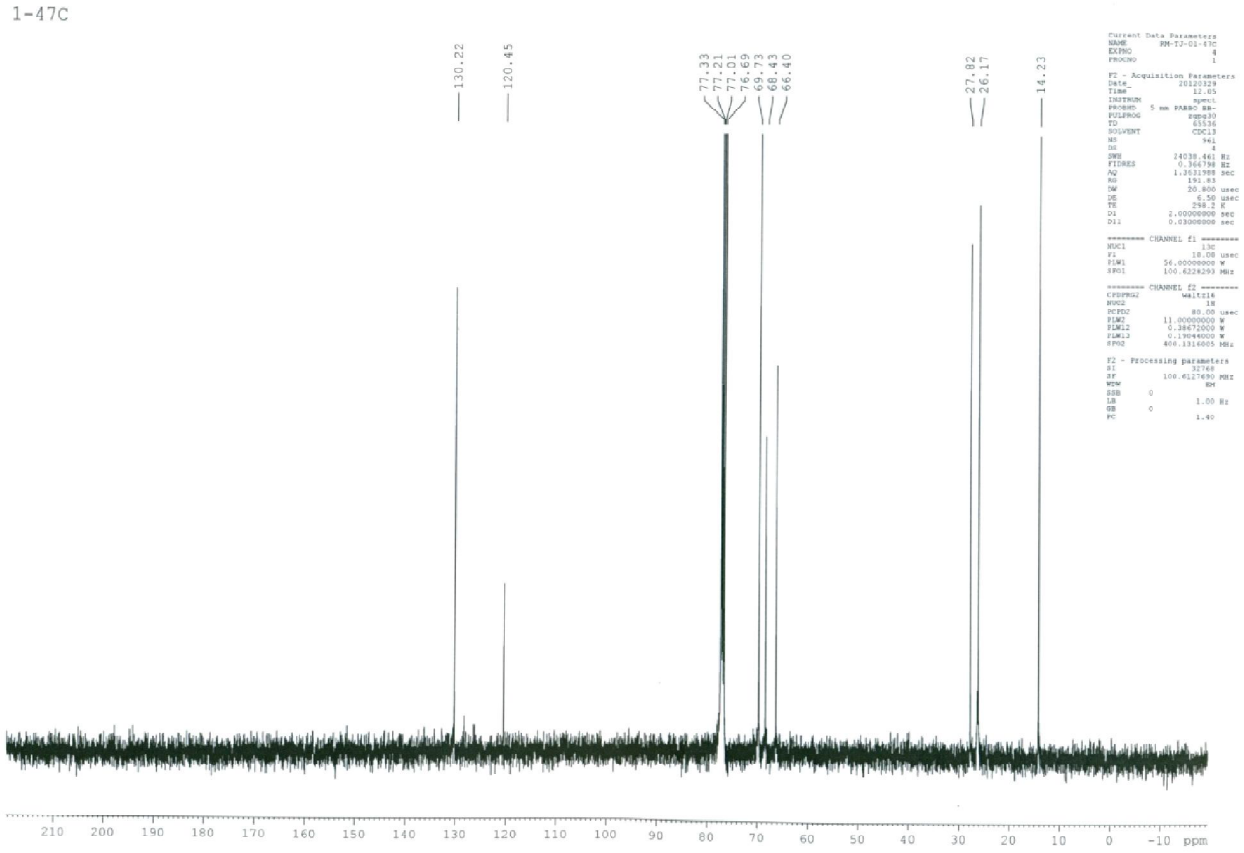
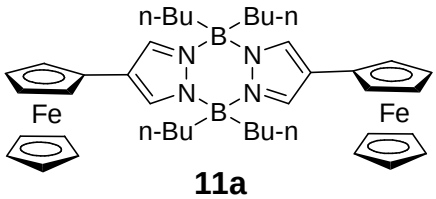


Figure S-7: ^{13}C-NMR spectrum of compound **11a.**



11a

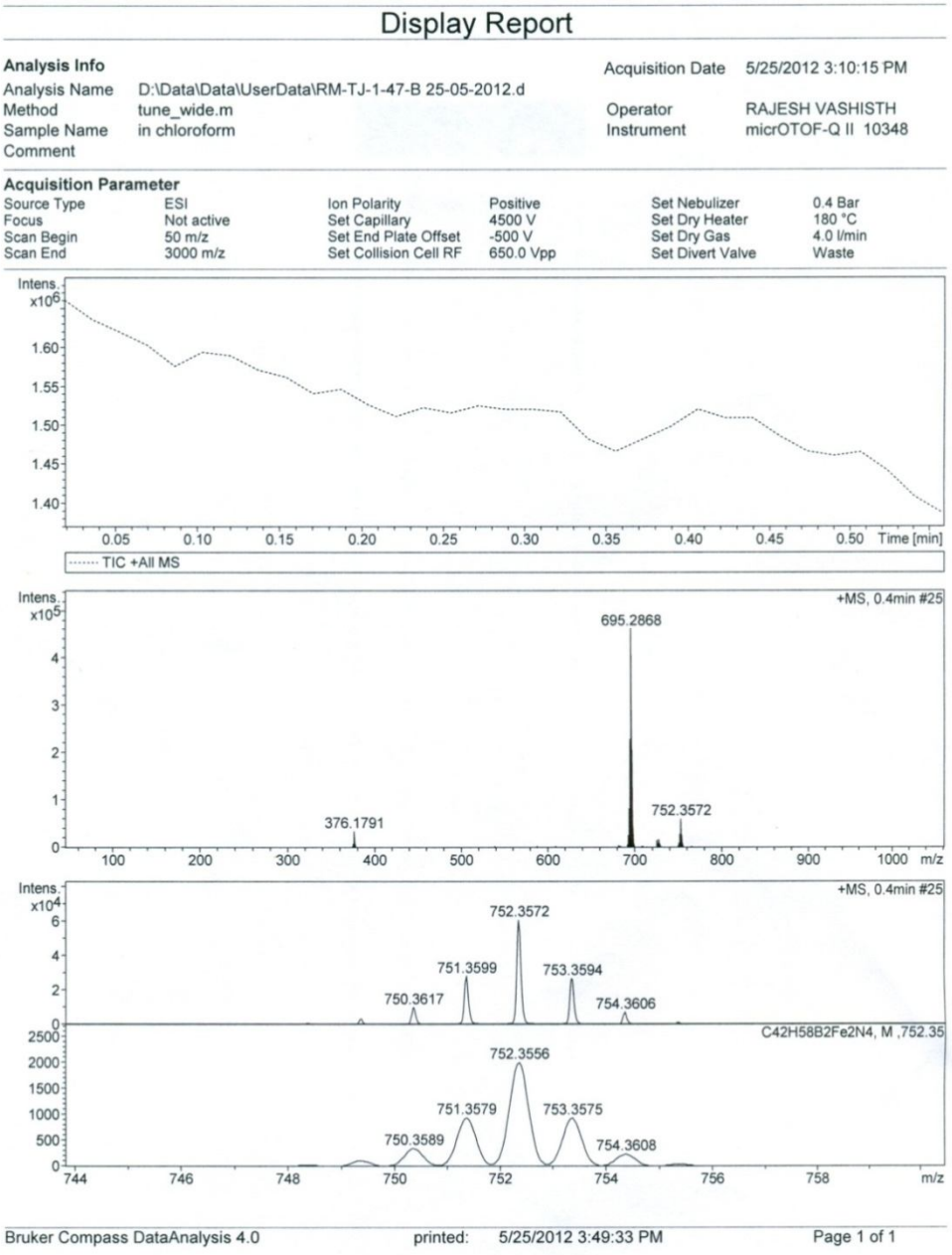


Figure S-8: HRMS spectrum of compound **11a.**

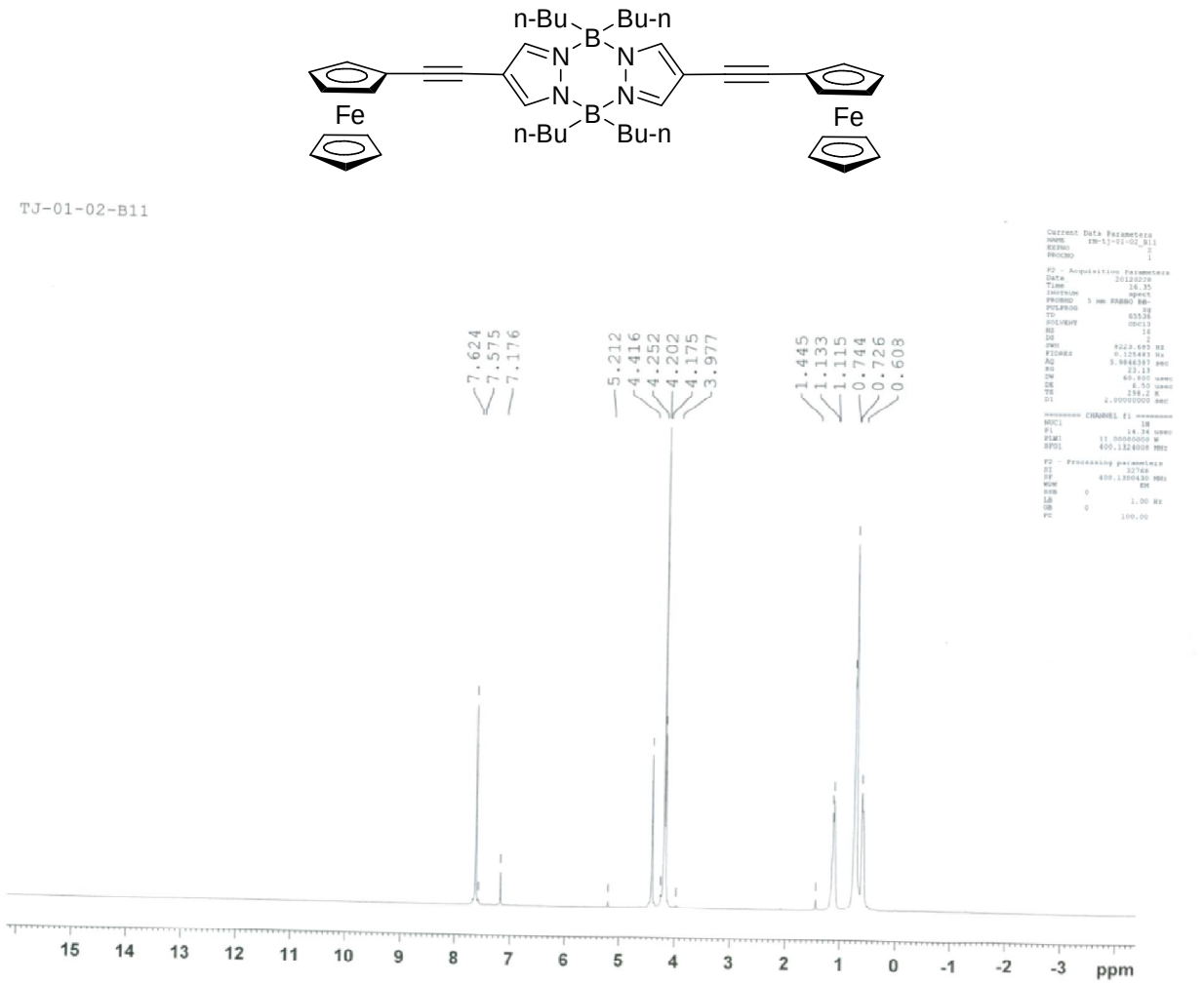
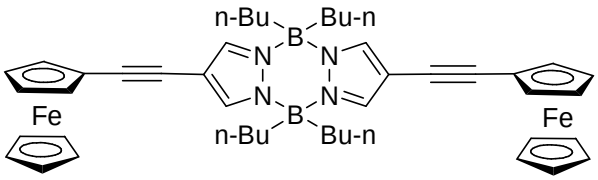


Figure S-9: ^{1}H-NMR spectrum of compound **11b.**



11b

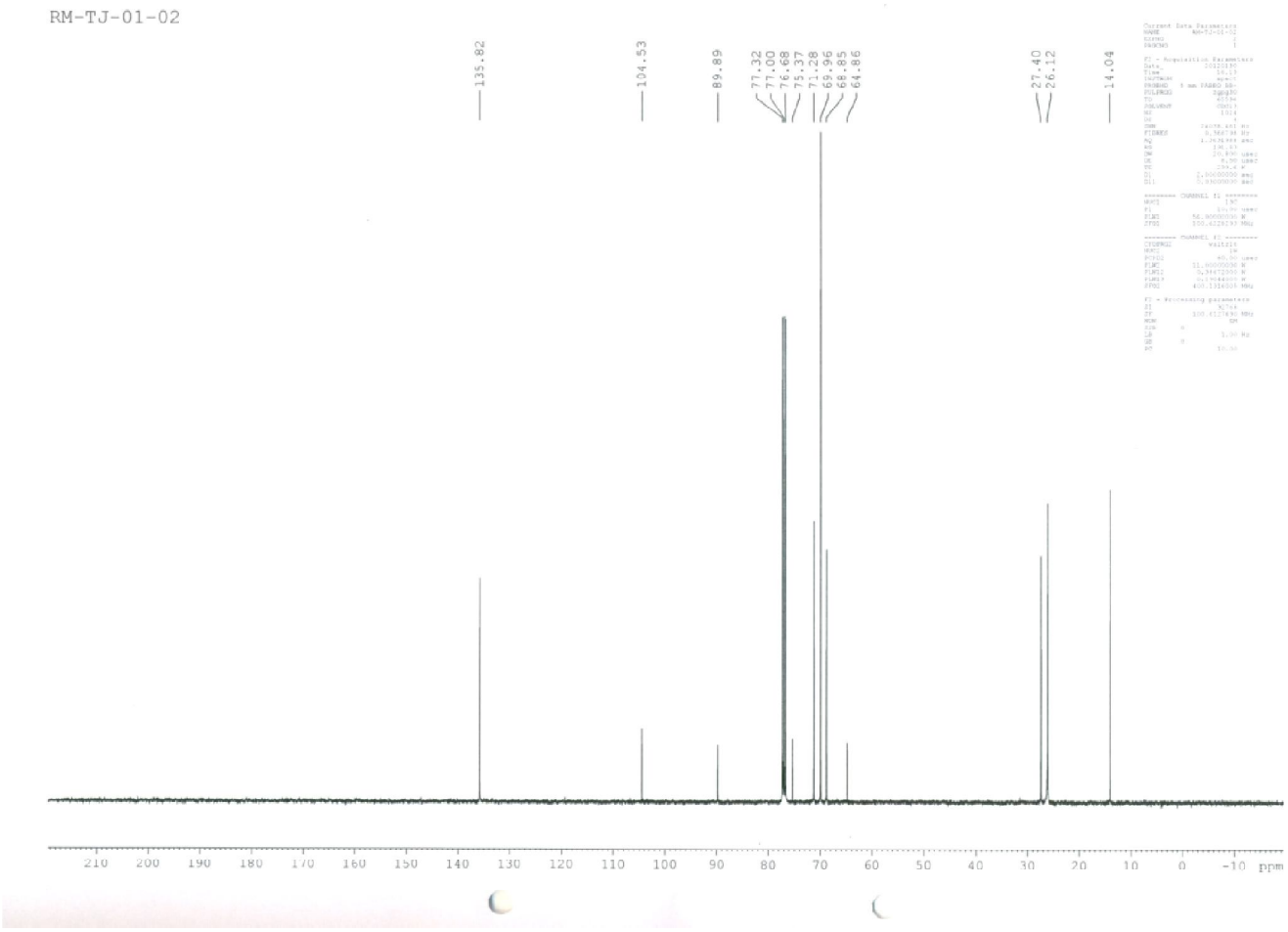
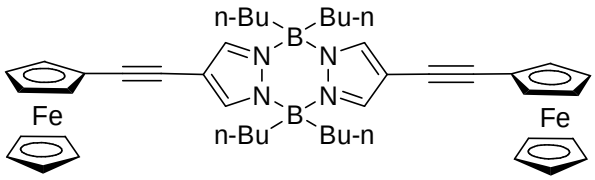


Figure S-10: ^{13}C-NMR spectrum of compound **11b.**



11b

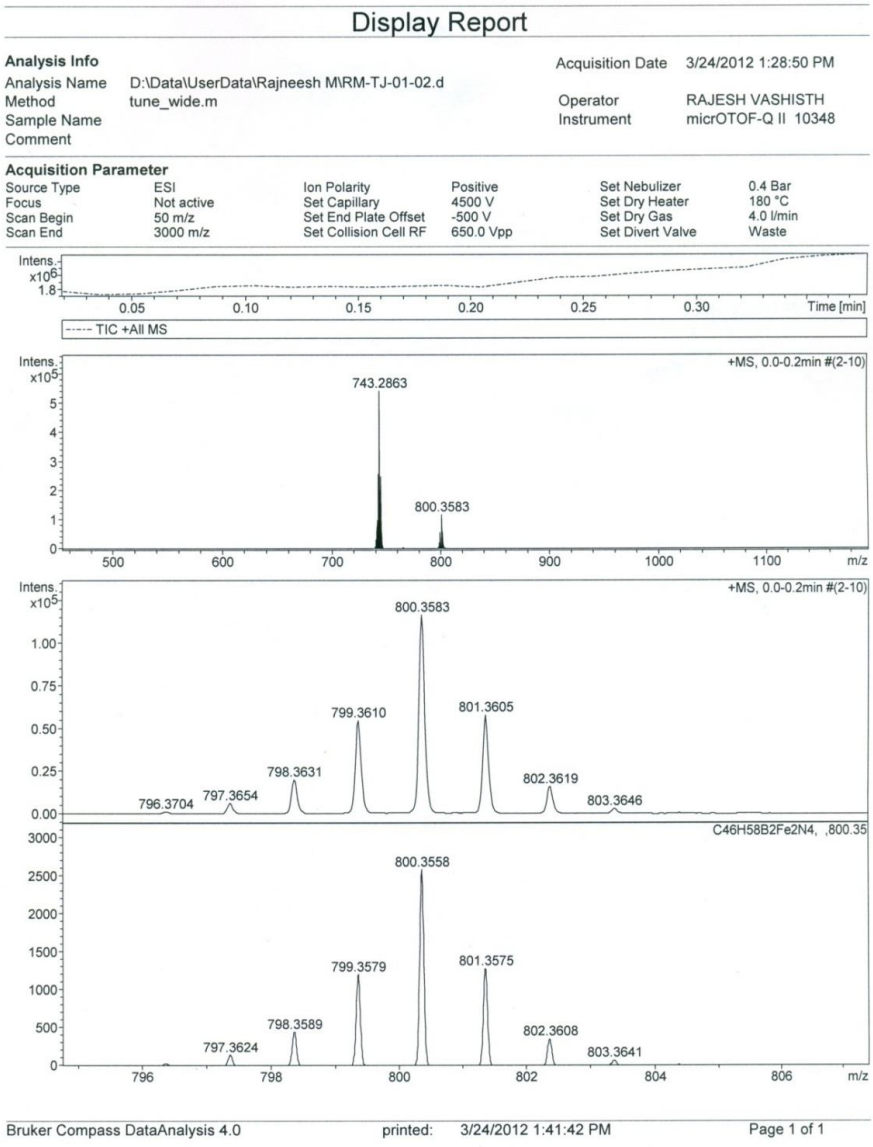
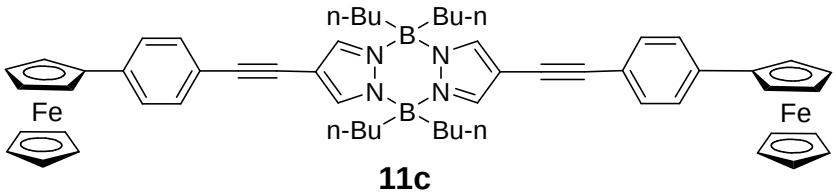


Figure S-11: HRMS spectrum of compound **11b.**



11c

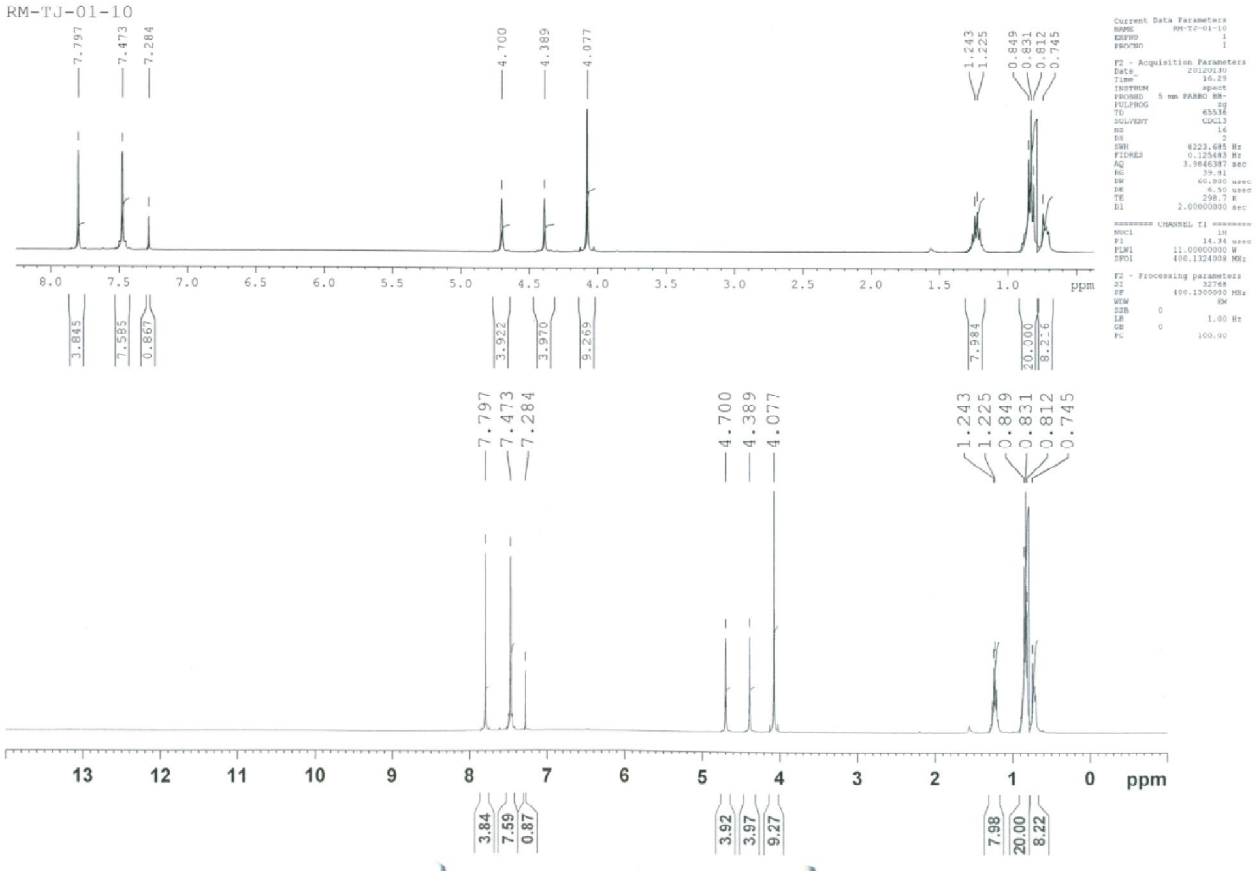
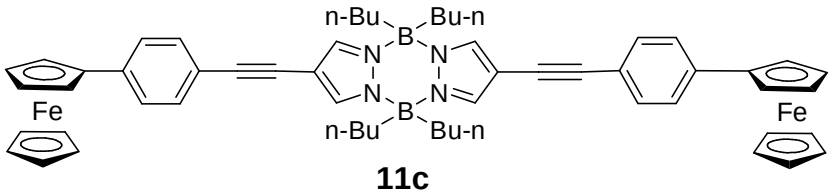


Figure S-12: ^{1}H-NMR spectrum of compound **11c.**



11c

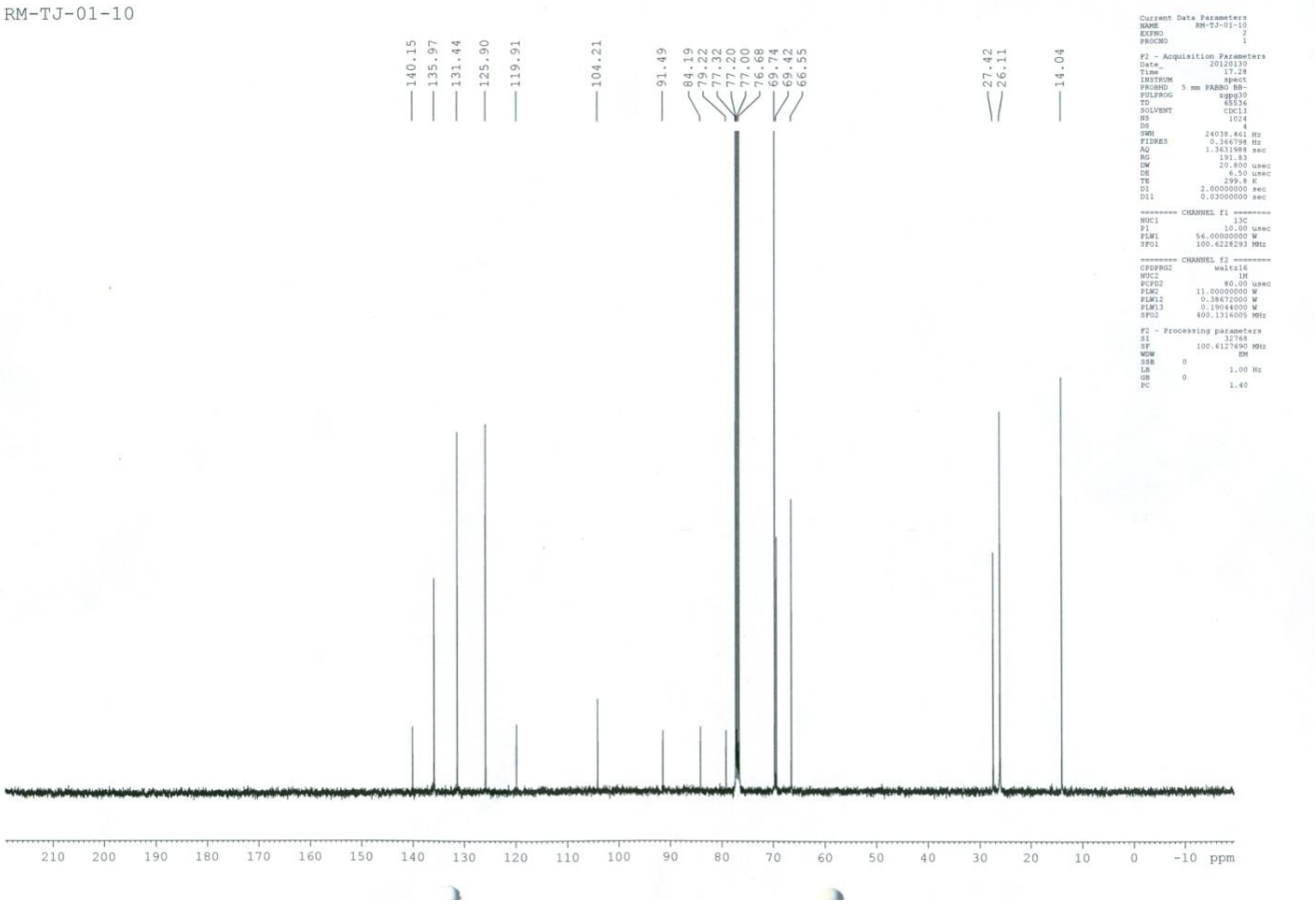
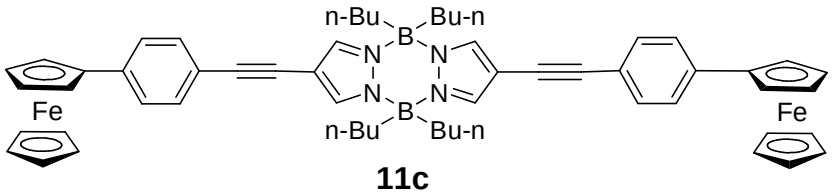


Figure S-13: ^{13}C-NMR spectrum of compound **11c.**



11c

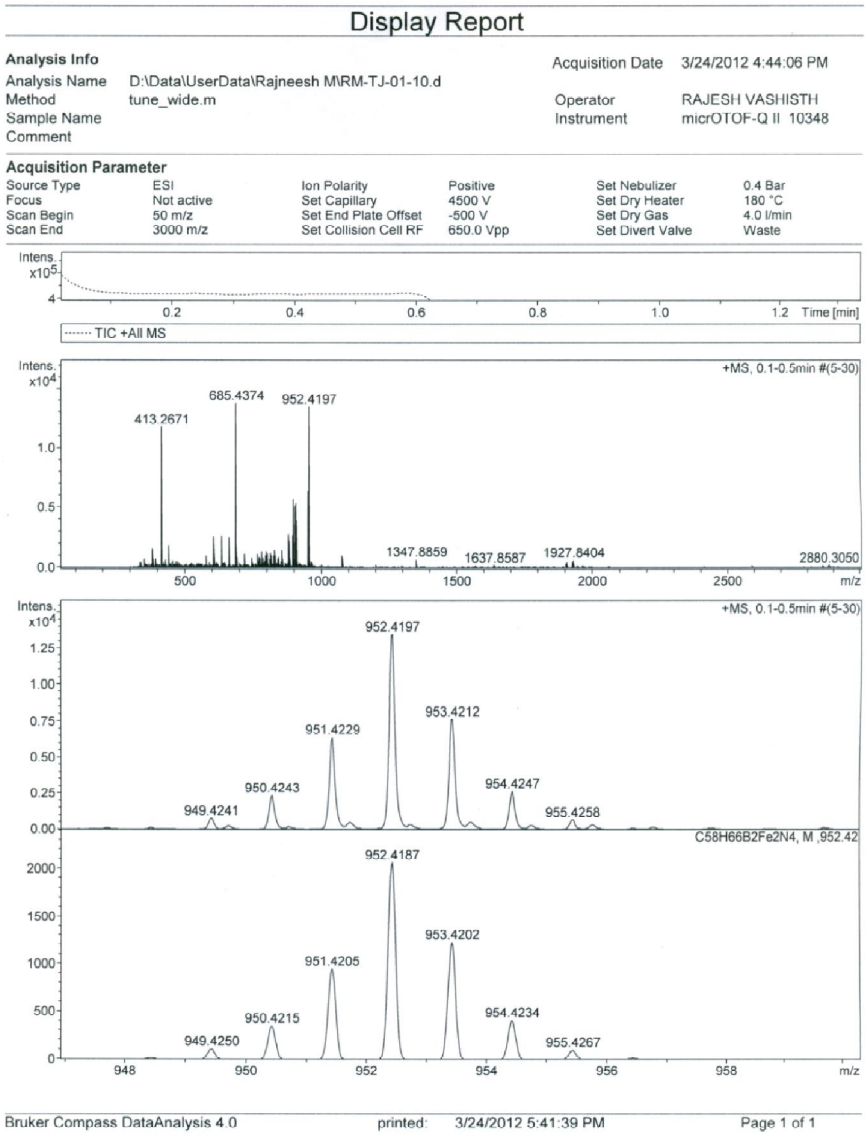
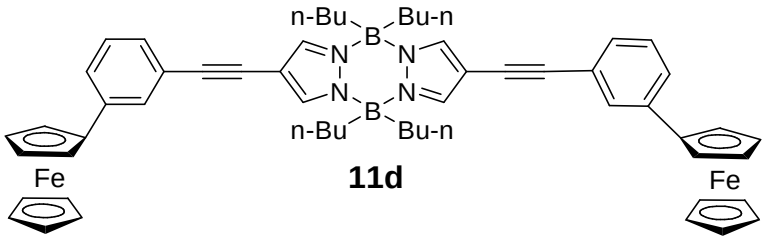


Figure S-14: HRMS spectrum of compound **11c.**



11d

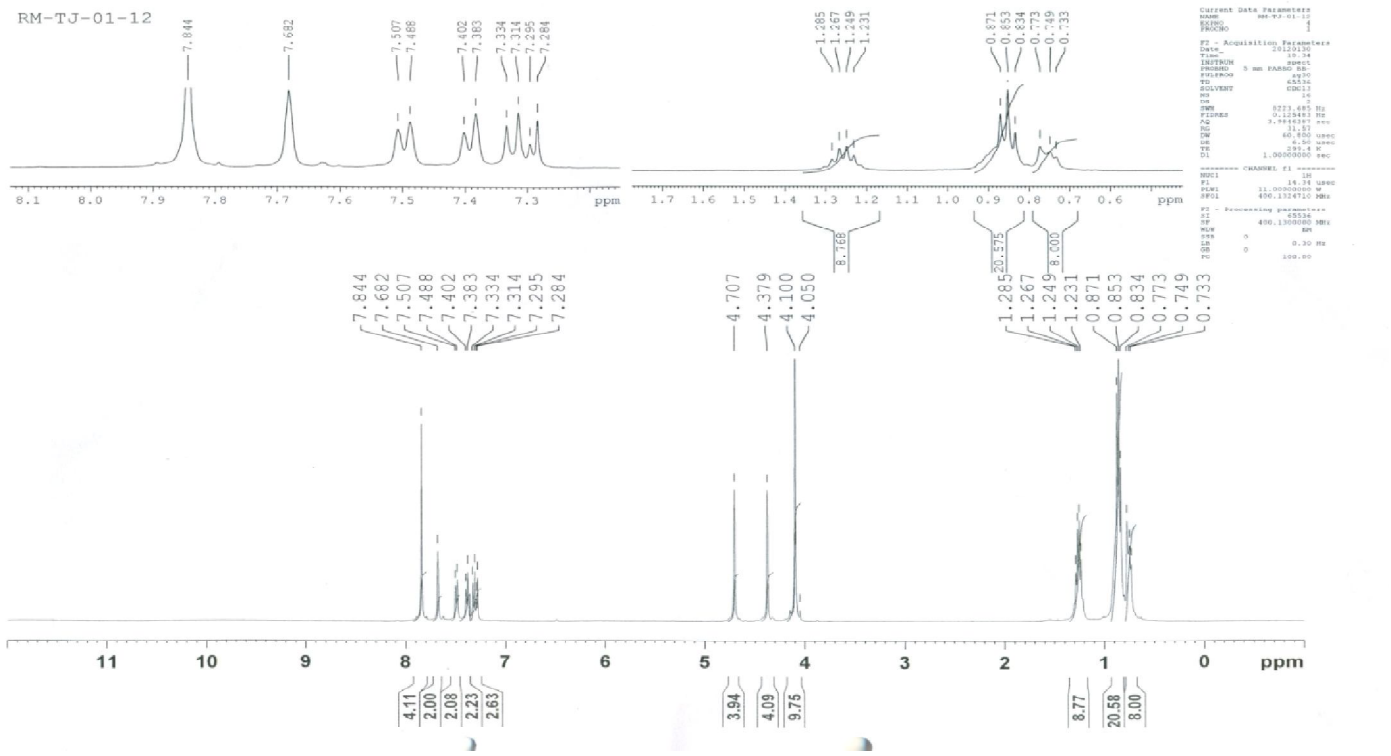
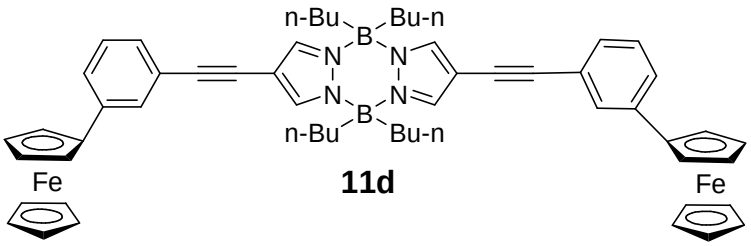


Figure S-15: ^{1}H-NMR spectrum of compound **11d.**



11d

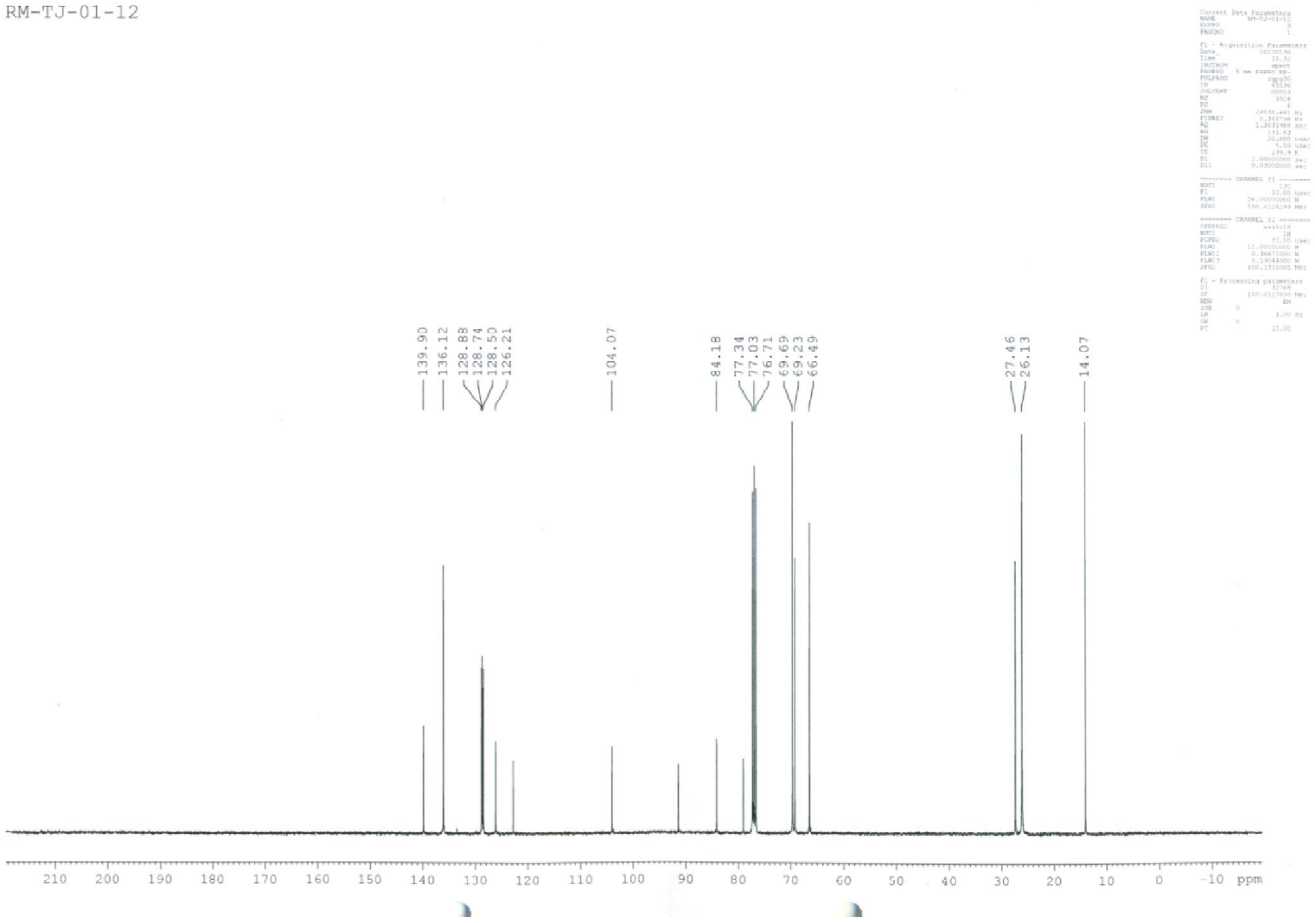
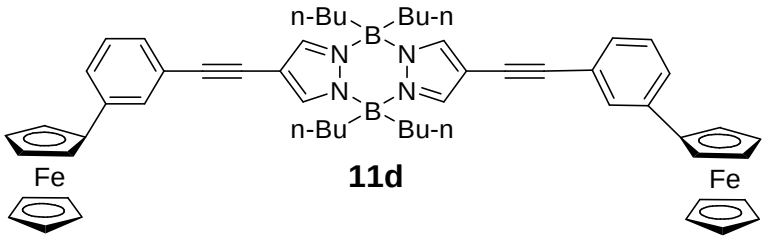


Figure S-16: ^{13}C-NMR spectrum of compound **11d.**



11d

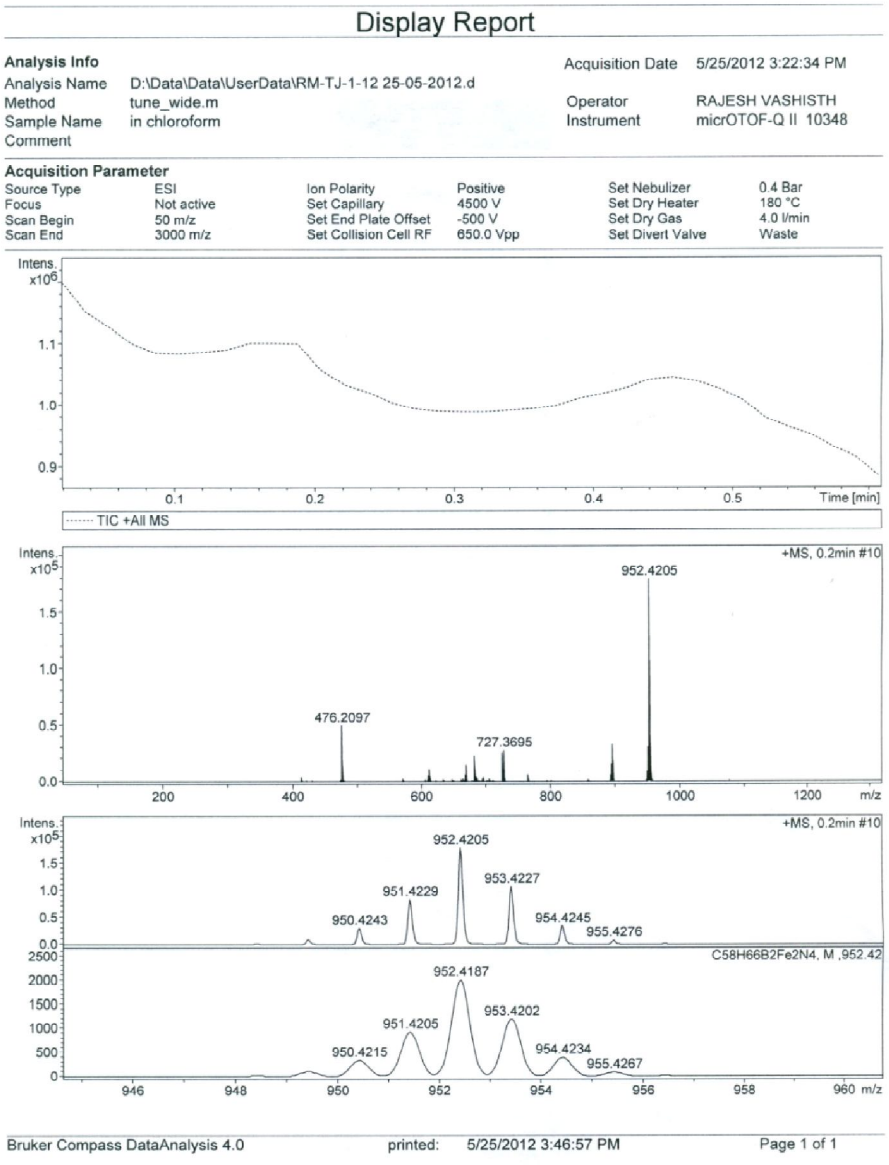
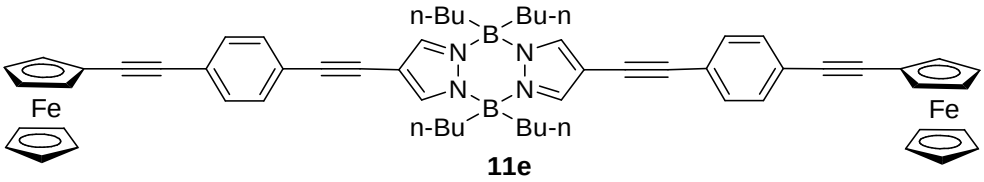


Figure S-17: HRMS spectrum of compound **11d.**



11e

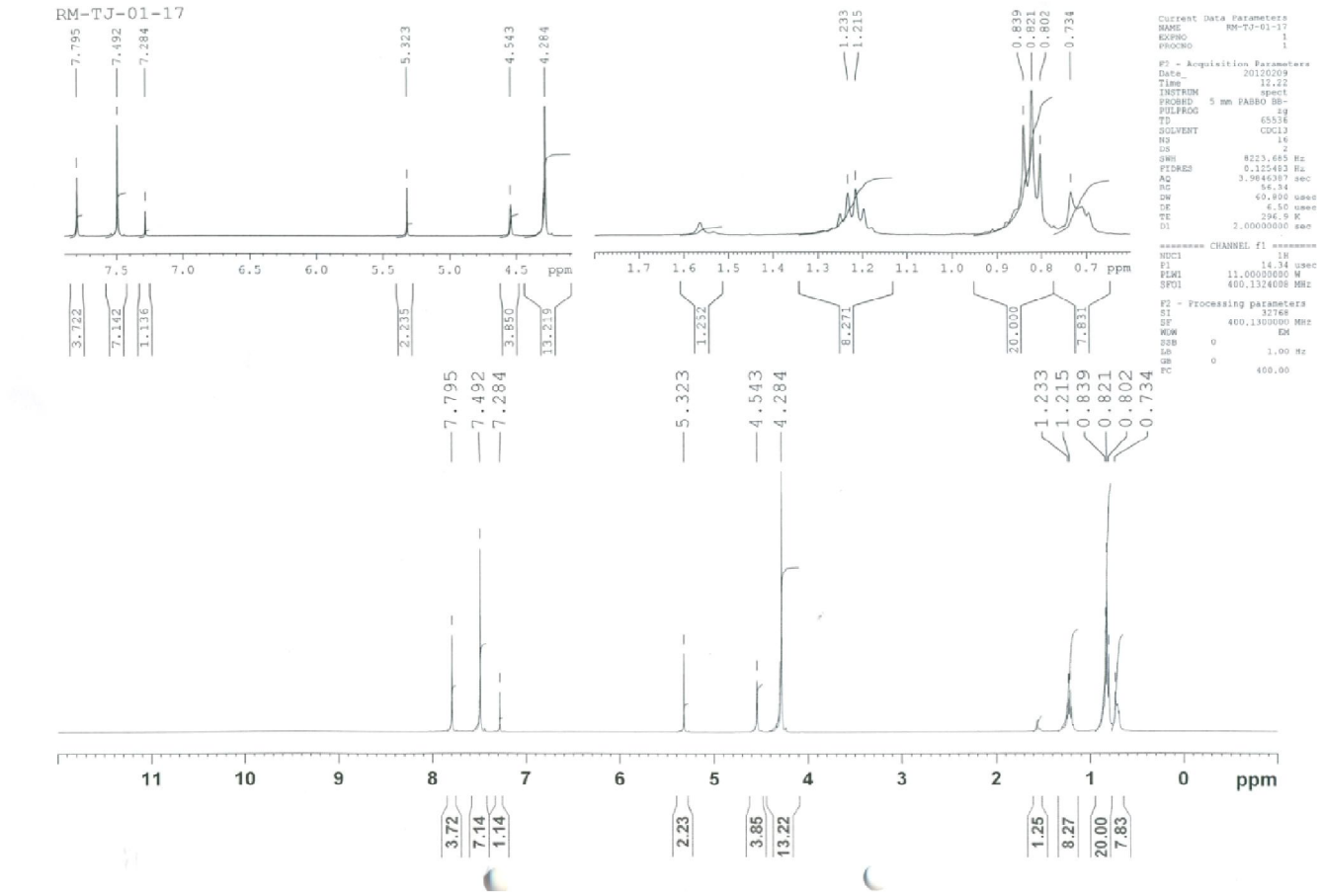
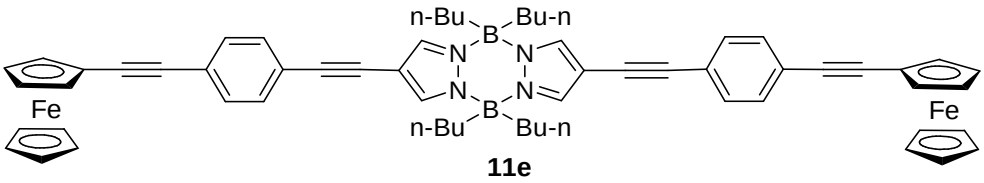


Figure S-18: ^{1}H-NMR spectrum of compound **11e.**



11e

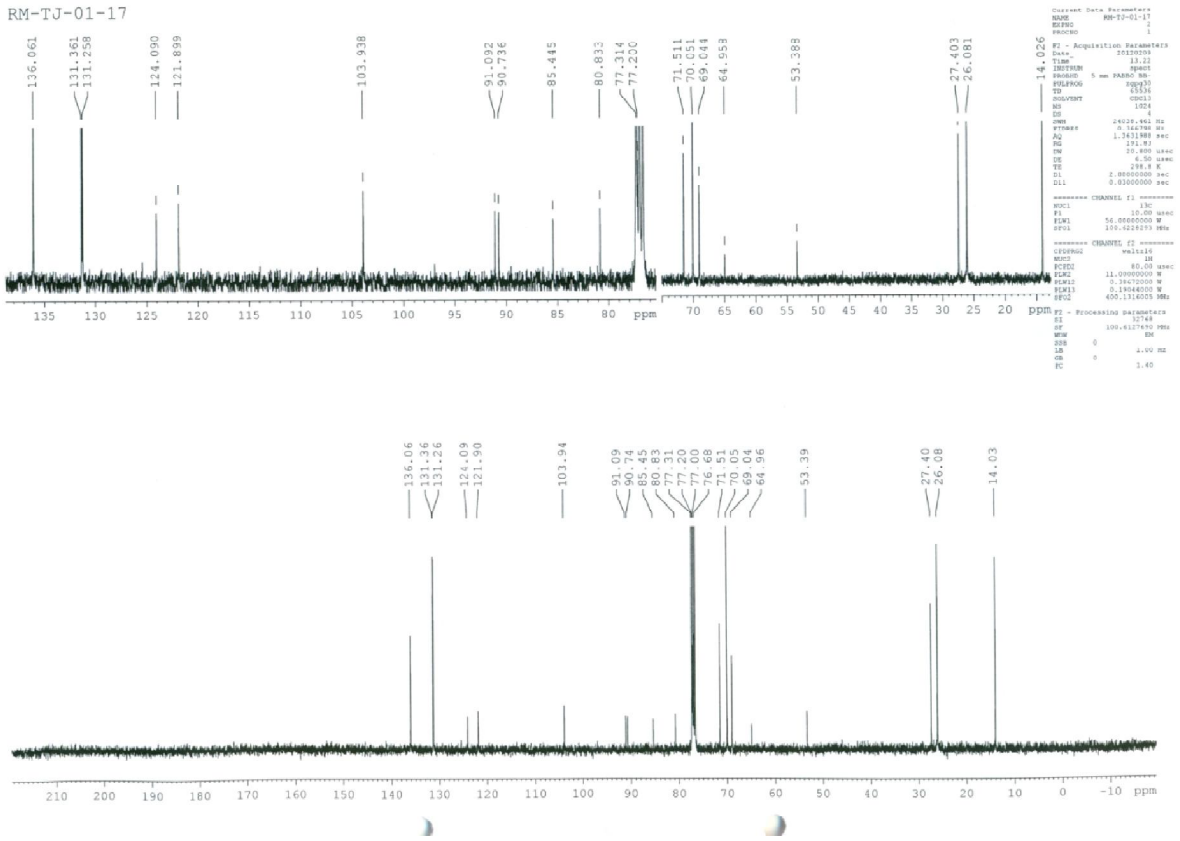
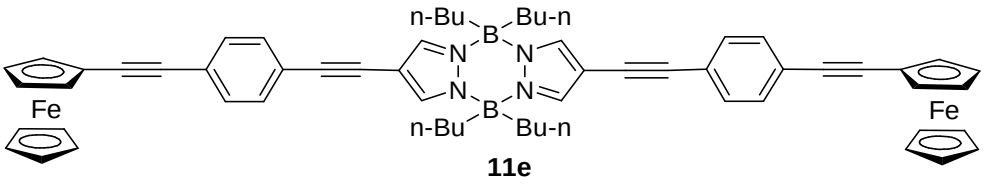


Figure S-19: ^{13}C-NMR spectrum of compound **11e.**



11e

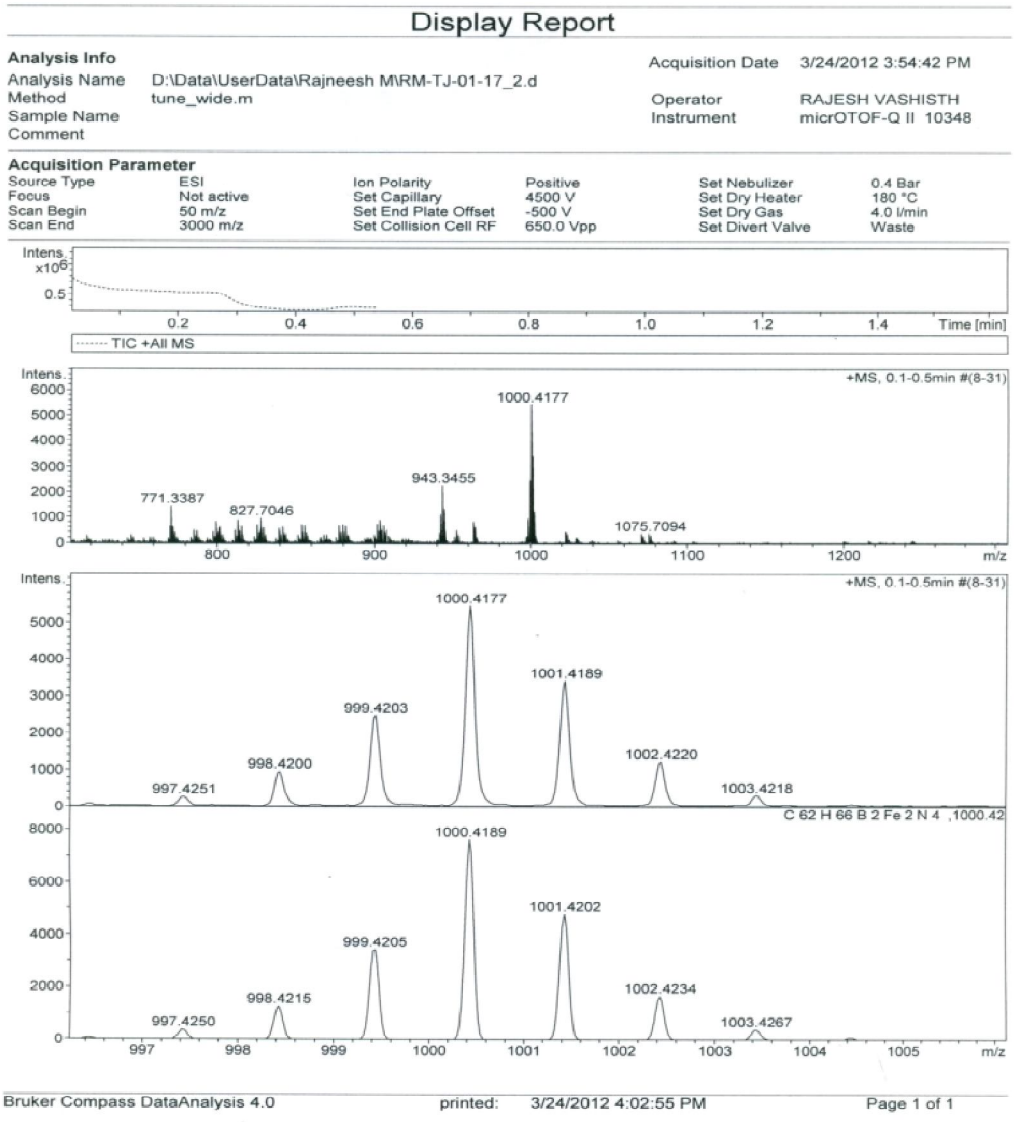


Figure S-20: HRMS spectrum of compound **11e.**

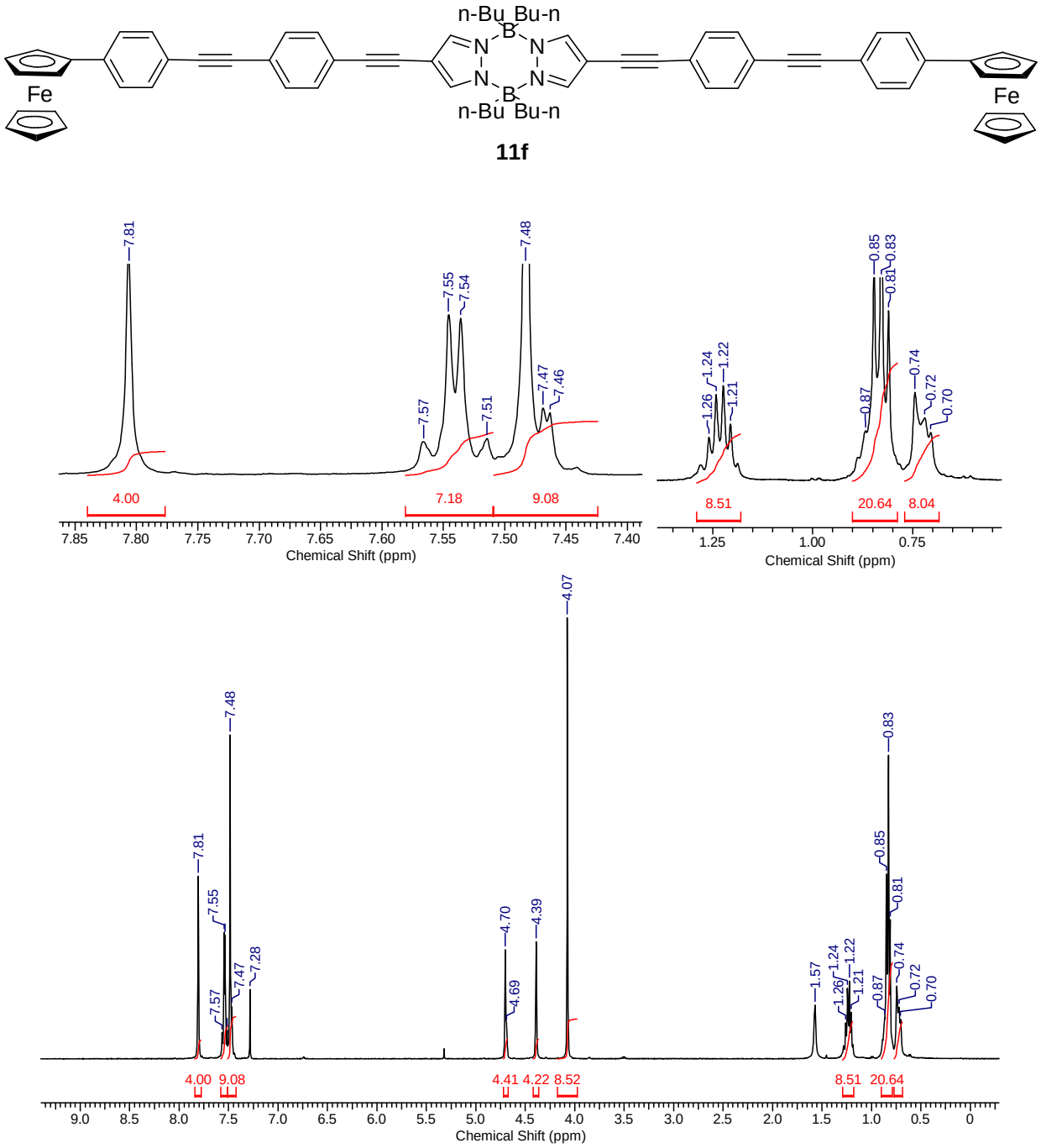
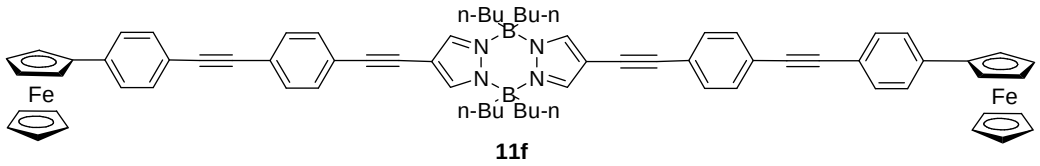


Figure S-21: ^{1}H-NMR spectrum of compound **11f.**



11f

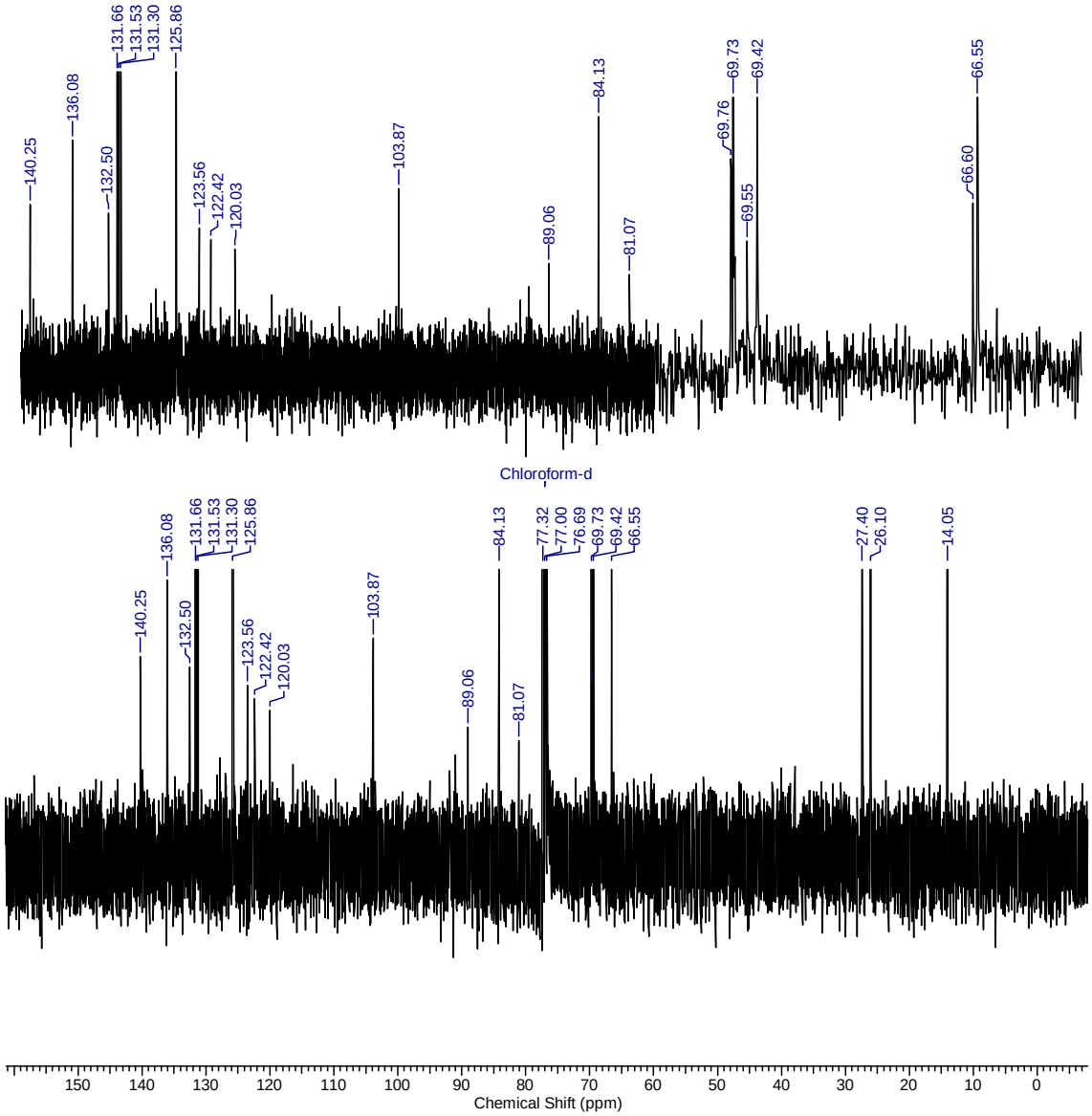
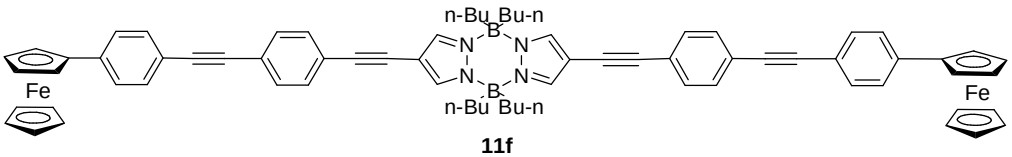


Figure S-22: ^{13}C-NMR spectrum of compound **11f.**



11f

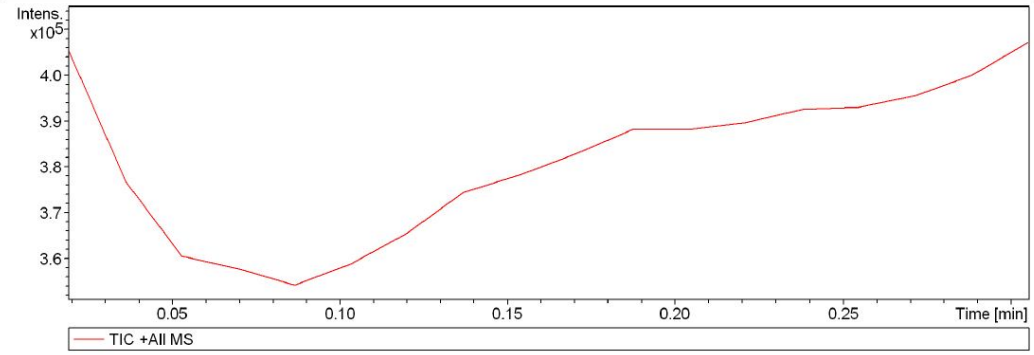
Display Report

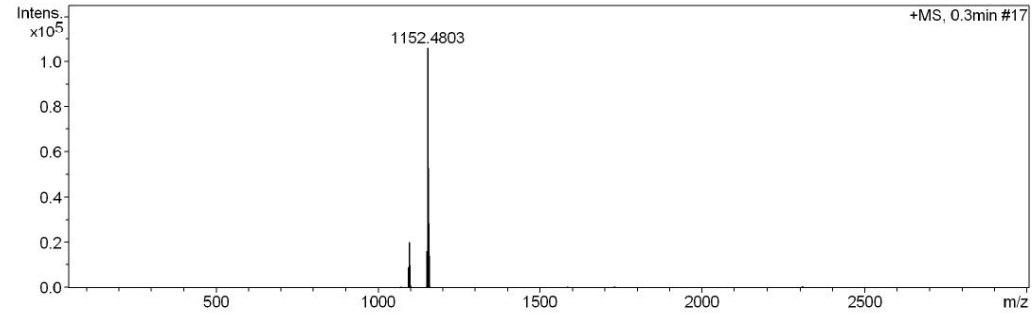
Analysis Info

Analysis Name	D:\Data\UserData\RM-TJ-01-71 26-06-2012.d	Acquisition Date	6/26/2012 5:31:54 PM
Method	tune_high.m	Operator	RAJESH VASHISTH
Sample Name	in chloroform	Instrument	micrOTOF-Q II 10348
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	1600.0 Vpp	Set Divert Valve	Waste





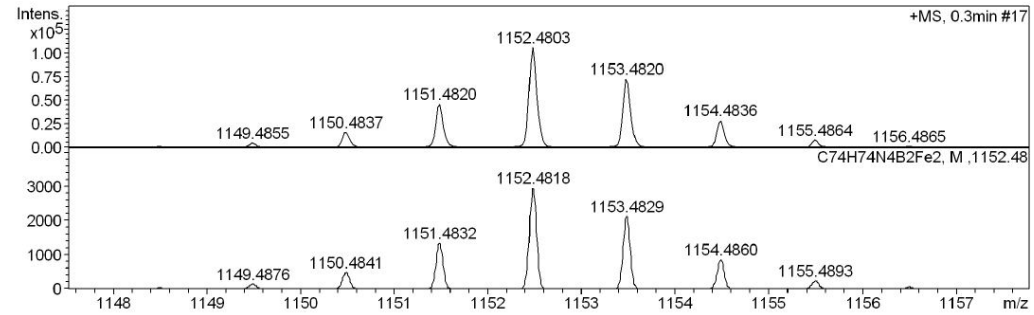
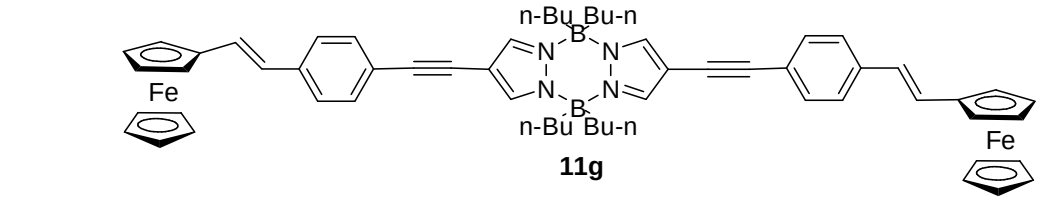


Figure S-23: HRMS spectrum of compound **11f.**



11g

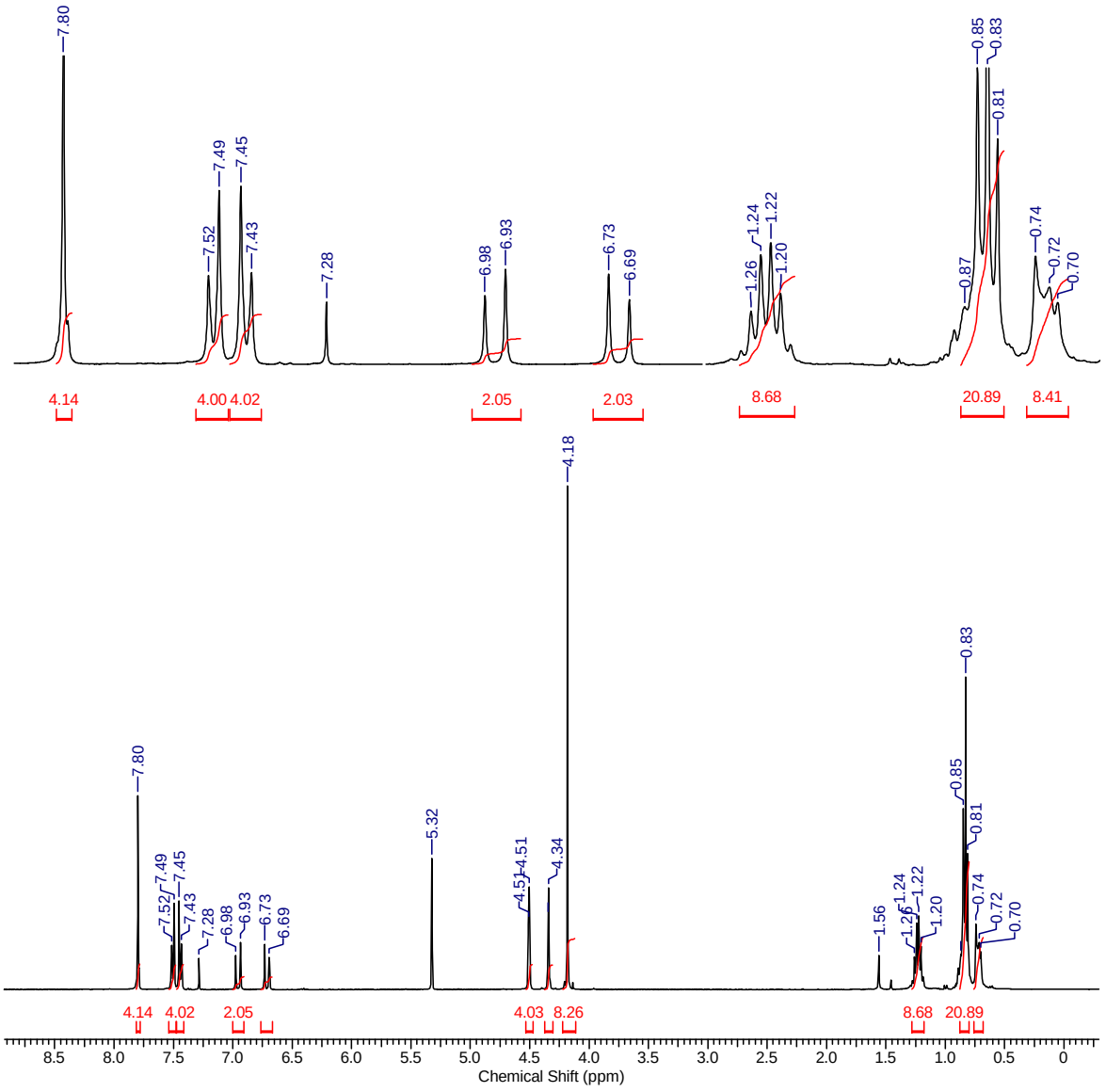
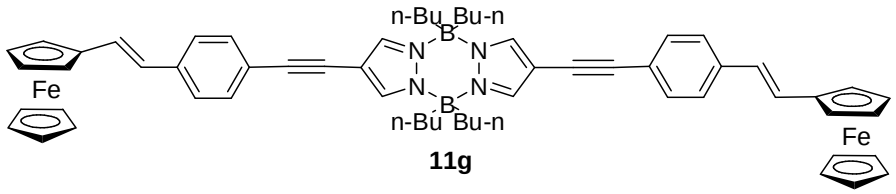


Figure S-24: ^{1}H-NMR spectrum of compound **11g.**



11g

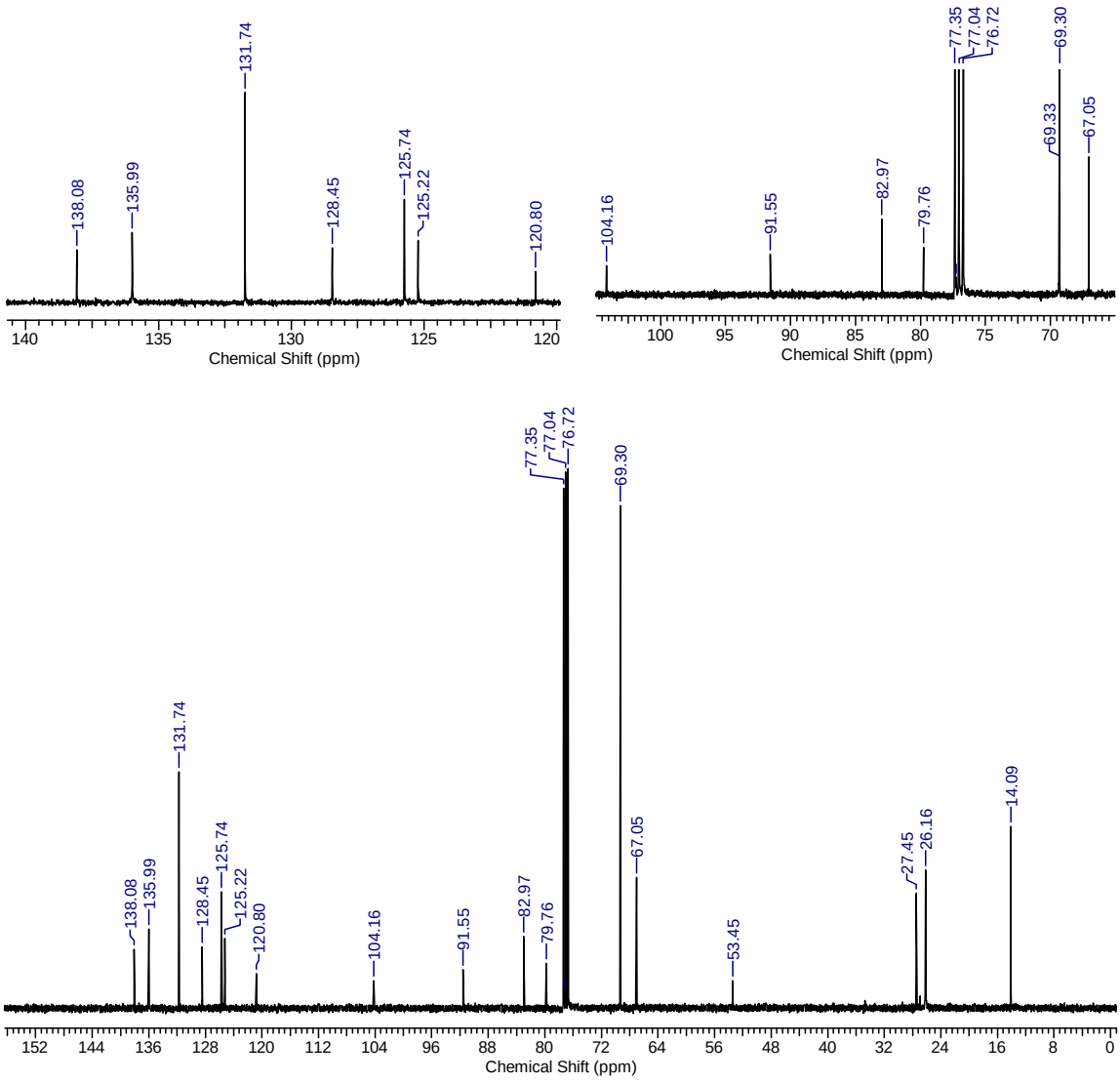
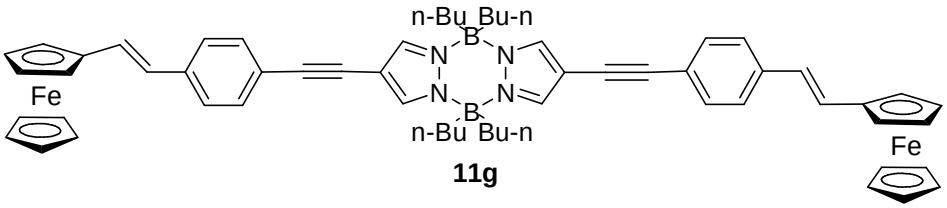


Figure S-25: ^{13}C-NMR spectrum of compound **11g.**



11g

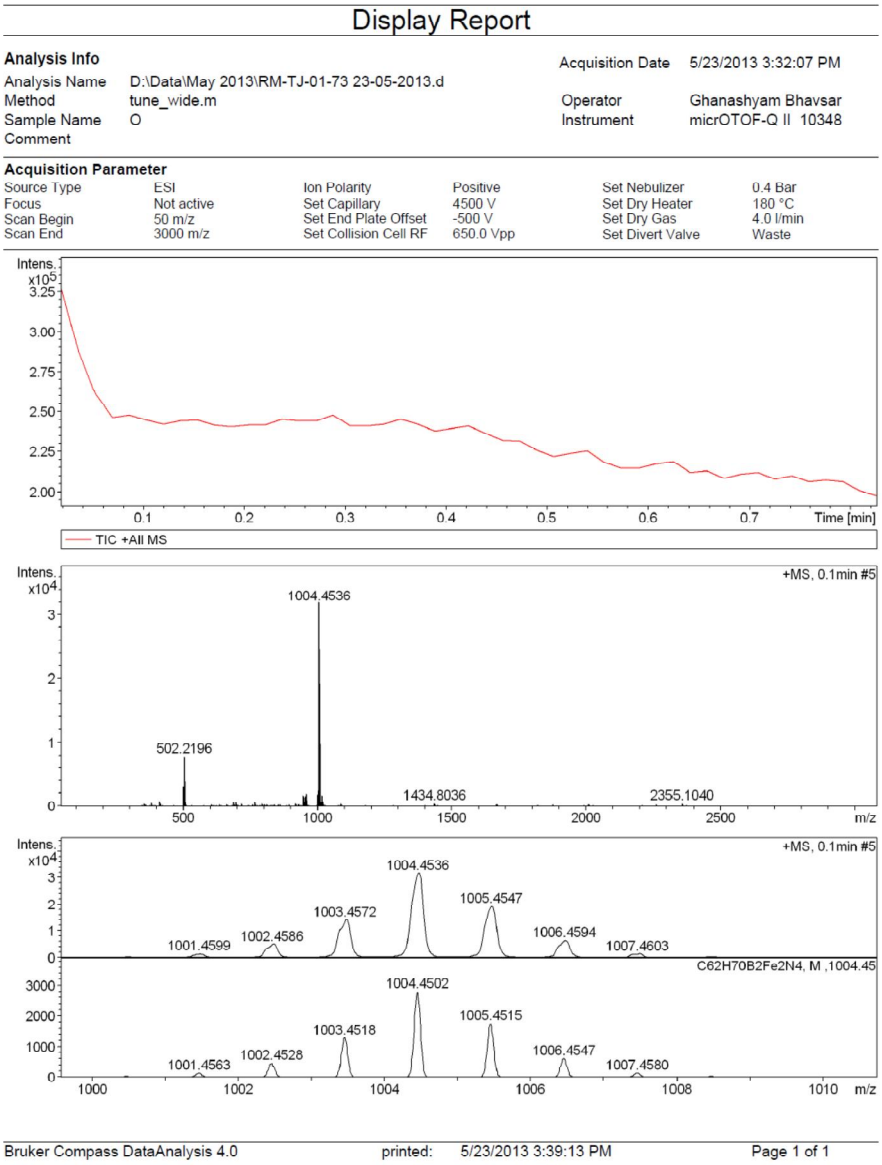


Figure S-26: HRMS spectrum of compound **11g.**