Second-order nonlinear polarizability of ferrocene-BODIPY donor-acceptor adducts. Quantifying charge redistribution in the excited state

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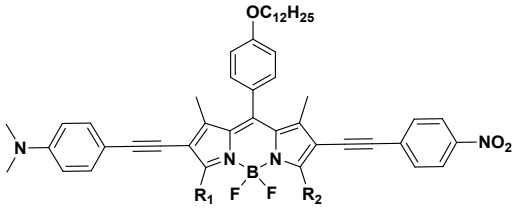
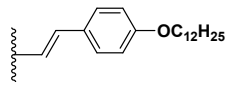
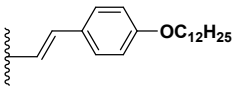
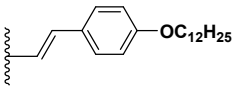
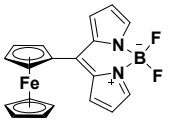
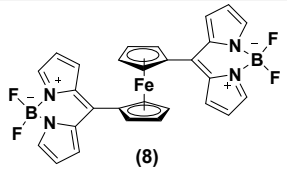
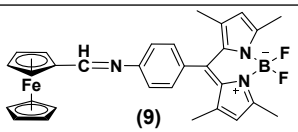
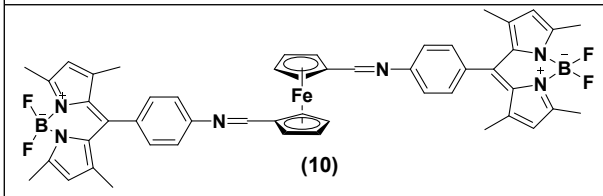
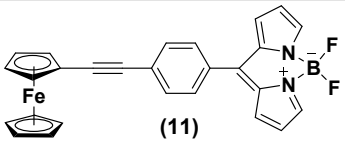
Table S1. Comparison of first hyperpolarisability β_{HRS} (x 10^{-30} esu) (Literature vs. current work)

COMPOUNDS	**β^a(x10^{-30}) esu**	
	R_1=R_2=CH_3	25
	R_1=  R_2=CH_3	30
	R_1= CH_3 R_2= 	12
	R_1=R_2= 	30
 (7)	**β (x10^{-30}) esu (present work)**	
	74	
 (8)	64	
 (9)	20	
 (10)	49	
 (11)	62	

[a] *Shi,W.-J.; Lo, P.-C.; Singh, A.; Ledoux.-Rak, I.; Ng, D.K.P. Tetrahedron, 68,* ***2012****,* 8712-8718.

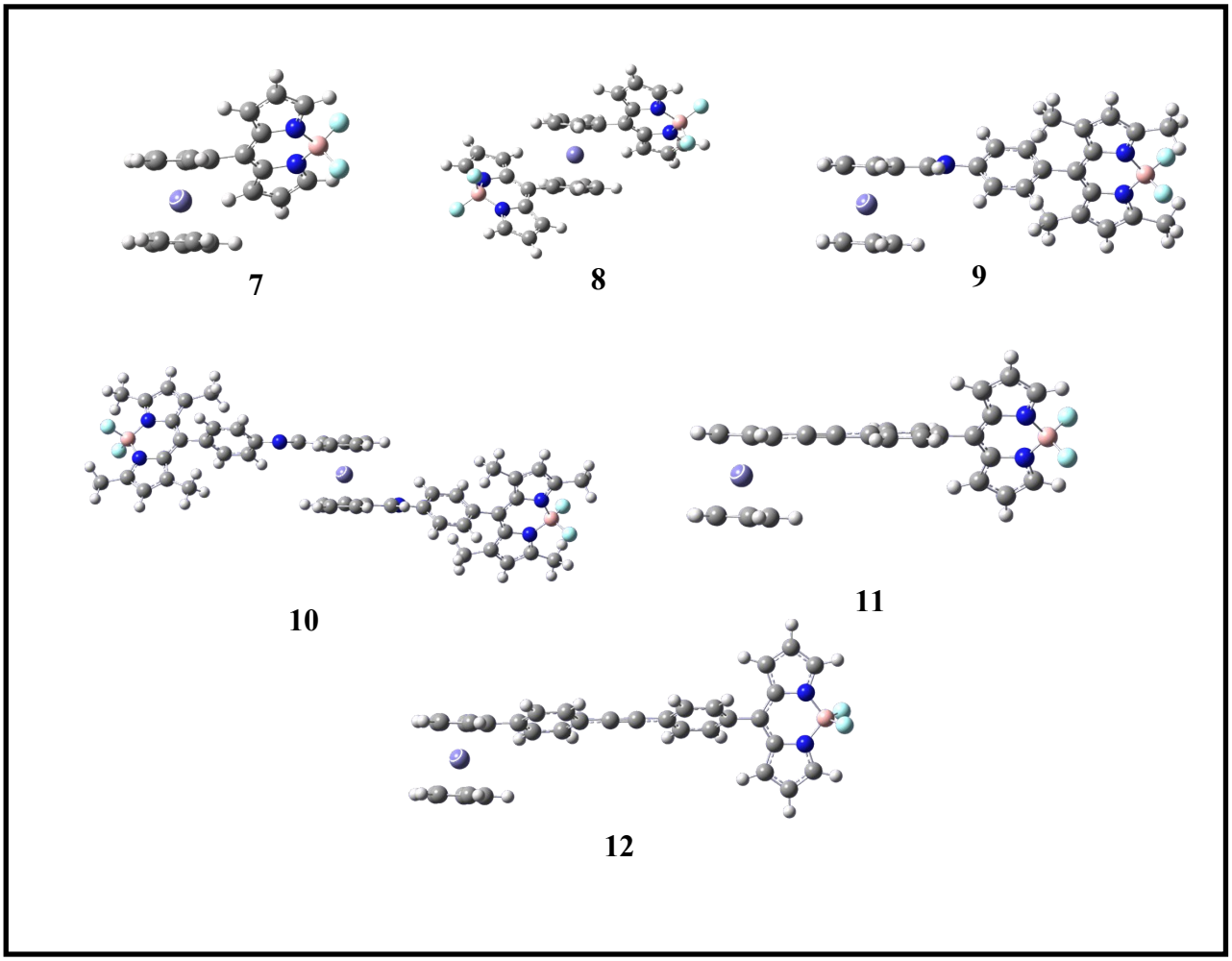


Fig. S1. Optimized structures of **7**-**12**.

Table S2. Cartesian coordinates of optimized structure of **7**.

Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z
1	26	-5.622920	-0.048728	0.281124
2	6	-4.085472	0.282892	-1.092489
3	6	-4.841000	-0.914550	-1.429398
4	1	-4.427944	-1.900525	-1.565796
5	6	-6.198055	-0.534573	-1.663741
6	1	-6.996071	-1.199969	-1.953227
7	6	-6.315272	0.879004	-1.448594
8	1	-7.221238	1.458766	-1.527893
9	6	-5.027243	1.384681	-1.092444
10	1	-4.797535	2.408201	-0.845542
11	6	-4.845674	-0.341679	2.194913
12	1	-3.796931	-0.394159	2.441994
13	6	-5.681282	-1.449301	1.827295
14	1	-5.380828	-2.483977	1.772522
15	6	-6.998517	-0.939885	1.563882
16	1	-7.855661	-1.523112	1.265607
17	6	-6.975202	0.480107	1.772022
18	1	-7.811352	1.151176	1.652482
19	6	-5.643816	0.850672	2.161668
20	1	-5.304215	1.848492	2.391173
21	6	-2.633655	0.376217	-0.944919
22	6	-2.257825	-1.883930	0.267315
23	6	-1.092331	-2.529817	0.694503
24	1	-3.266849	-2.244739	0.370851
25	6	-0.012699	-1.682279	0.386241
26	1	-1.022902	-3.492752	1.175447
27	1	1.040204	-1.820346	0.575789
28	6	-1.878643	-0.646552	-0.318856
29	7	-0.475167	-0.555417	-0.218442
30	6	-2.396406	2.560400	-2.315364
31	6	-0.161804	2.733468	-2.043623
32	6	-1.280936	3.334804	-2.649310
33	1	-3.408558	2.718882	-2.648106
34	1	0.875242	3.028180	-2.080582
35	1	-1.265583	4.218257	-3.267822
36	6	-1.949658	1.489154	-1.492314
37	7	-0.553646	1.628845	-1.355523
38	5	0.363551	0.681156	-0.571120
39	9	1.506810	0.316752	-1.360278
40	9	0.849945	1.316596	0.629333

Table S3. Cartesian coordinates of optimized structure of **8**.

Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z
1	26	0.267151	2.381821	0.405596
2	9	-5.331513	-2.214818	-0.798225
3	9	-3.099052	-2.612652	-1.371060
4	9	4.345218	-3.626702	-0.524821
5	9	3.681570	-2.771575	1.543881
6	5	-4.002552	-1.737968	-0.666215
7	5	3.709751	-2.536805	0.131918
8	7	-3.862293	-0.302414	-1.223521
9	7	-3.584798	-1.650681	0.815926
10	7	2.270140	-2.335982	-0.395817
11	7	4.447696	-1.213525	-0.174831
12	6	-4.343561	0.146328	-2.406945
13	1	-5.014879	-0.460279	-2.993882
14	6	-3.813396	1.425083	-2.677116
15	1	-4.030052	2.028601	-3.544578
16	6	-2.964299	1.751152	-1.615540
17	1	-2.387385	2.654071	-1.505417
18	6	-3.000053	0.672666	-0.688103
19	6	-2.405436	0.487431	0.583841
20	6	-2.752085	-0.648136	1.345841
21	6	-2.513880	-0.981601	2.712595
22	1	-1.945870	-0.390839	3.412484
23	6	-3.193545	-2.169527	2.980094
24	1	-3.237425	-2.695059	3.920855
25	6	-3.840917	-2.557550	1.785539
26	1	-4.463472	-3.415728	1.586907
27	6	1.340159	-3.304619	-0.559768
28	1	1.607155	-4.344314	-0.453448
29	6	0.085915	-2.721106	-0.849800
30	1	-0.844218	-3.232424	-1.040483
31	6	0.272372	-1.339877	-0.843350
32	1	-0.490170	-0.603425	-1.025322
33	6	1.649363	-1.082036	-0.571326
34	6	2.409439	0.105936	-0.538679
35	6	3.817633	0.021061	-0.404644
36	6	4.849175	0.987002	-0.591472
37	1	4.702867	2.024398	-0.843920
38	6	6.073539	0.327069	-0.461509
39	1	7.057262	0.758419	-0.560863
40	6	5.788240	-1.029943	-0.201997
41	1	6.459903	-1.859610	-0.048516
42	6	-1.467881	1.460435	1.155100
43	6	-1.600223	2.904234	1.154966
44	1	-2.389683	3.460860	0.676793
45	6	-0.572422	3.447025	1.986844

46	1	-0.426672	4.493253	2.205030
47	6	0.221493	2.362098	2.487426
48	1	1.082169	2.448840	3.131600
49	6	-0.319172	1.143860	1.973925
50	1	0.073866	0.153405	2.140134
51	6	0.520676	3.216677	-1.493574
52	1	-0.196039	3.790893	-2.058985
53	6	1.488603	3.746267	-0.577589
54	1	1.610126	4.784576	-0.311914
55	6	2.264989	2.655970	-0.076428
56	1	3.061279	2.724681	0.646301
57	6	1.793428	1.432979	-0.689029
58	6	0.693113	1.799357	-1.555492
59	1	0.140514	1.126722	-2.189895

Table S4. Cartesian coordinates of optimized structure of **9.**

Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z
1	26	-6.208677	0.109881	-0.226176
2	6	-3.343341	-1.138839	0.307330
3	1	-2.982770	-1.656340	-0.593354
4	6	-4.773155	-1.187272	0.538244
5	6	-5.500420	-0.548947	1.609818
6	1	-5.052321	0.051165	2.384262
7	6	-6.881033	-0.892712	1.473869
8	1	-7.678741	-0.579862	2.129190
9	6	-7.026609	-1.727834	0.313114
10	1	-7.949531	-2.151808	-0.049924
11	6	-5.732991	-1.907541	-0.269386
12	1	-5.502511	-2.500901	-1.141062
13	6	-5.251969	1.591133	-1.335531
14	1	-4.187188	1.691243	-1.476699
15	6	-6.015779	2.182107	-0.275326
16	1	-5.626687	2.805059	0.514417
17	6	-7.389424	1.805955	-0.457583
18	1	-8.216073	2.101255	0.169368
19	6	-7.472703	0.982251	-1.629857
20	1	-8.372748	0.549562	-2.037764
21	6	-6.150633	0.847626	-2.172418
22	1	-5.883062	0.298495	-3.061449
23	6	-1.148059	-0.440956	0.834697
24	6	-0.249086	-0.512038	1.915427
25	6	-0.636605	-0.218374	-0.459654
26	6	1.124814	-0.402163	1.704737
27	1	-0.652548	-0.658879	2.910843
28	6	0.739412	-0.093302	-0.664545
29	1	-1.317196	-0.112167	-1.298281
30	6	1.637499	-0.190884	0.411307
31	1	1.808309	-0.469561	2.545225

32	1	1.122334	0.088242	-1.664078
33	7	-2.528450	-0.544309	1.117204
34	6	3.110146	-0.057516	0.183570
35	6	3.179864	2.527017	0.482657
36	6	4.260885	3.408739	0.400525
37	6	5.430343	2.670788	0.107219
38	1	4.219853	4.479143	0.537860
39	6	3.709995	1.212524	0.231076
40	7	5.098155	1.355910	0.007105
41	6	3.532226	-2.598234	-0.188032
42	6	5.775109	-2.338102	-0.545727
43	6	4.720289	-3.276349	-0.473911
44	1	4.825283	-4.341489	-0.618088
45	6	3.877101	-1.204915	-0.082457
46	7	5.267710	-1.098440	-0.310665
47	5	6.079527	0.209972	-0.300824
48	9	7.110243	0.151099	0.702211
49	9	6.706665	0.419146	-1.579521
50	6	2.193221	-3.257845	-0.033369
51	6	7.220959	-2.575225	-0.826215
52	6	1.768157	2.938800	0.781422
53	6	6.825994	3.163294	-0.079149
54	1	7.837171	-2.217341	0.005776
55	1	7.413403	-3.638468	-0.986808
56	1	7.537512	-2.012330	-1.711145
57	1	1.770169	-3.105935	0.965899
58	1	1.456651	-2.871535	-0.746375
59	1	2.289281	-4.335551	-0.197381
60	1	1.722712	4.020590	0.940062
61	1	1.082341	2.689086	-0.035784
62	1	1.375439	2.449269	1.679126
63	1	7.502037	2.678121	0.633116
64	1	7.192973	2.906524	-1.078973
65	1	6.874579	4.246202	0.055899

Table S5. Cartesian coordinates of optimized structure of **10**.

Center	Atomic	Coordinates (Å)		
Number	Number	X	Y	Z
1	26	-0.028721	-2.147570	-0.672871
2	6	-2.767436	-1.599805	0.844748
3	1	-2.782086	-0.595418	1.291025
4	6	-1.478654	-2.265012	0.815512
5	6	-1.195570	-3.575277	0.280215
6	1	-1.925815	-4.221995	-0.177189
7	6	0.187661	-3.856403	0.505591
8	1	0.701445	-4.765033	0.233409
9	6	0.776186	-2.721978	1.163141
10	1	1.808420	-2.626734	1.461463
11	6	-0.243102	-1.737926	1.351263
12	1	-0.121714	-0.779100	1.831431
13	6	-0.752027	-0.903399	-2.186278
14	1	-1.707819	-0.403281	-2.195634
15	6	-0.493039	-2.218495	-2.702068
16	1	-1.215673	-2.868379	-3.169162
17	6	0.892135	-2.509382	-2.494134
18	1	1.405991	-3.411319	-2.789957
19	6	1.500683	-1.365328	-1.852738
20	6	0.465803	-0.379603	-1.652302
21	1	0.619399	0.589892	-1.208131
22	6	-5.084037	-1.485999	0.376393
23	6	-6.246171	-2.253353	0.578565
24	6	-5.216927	-0.107394	0.116498
25	6	-7.504993	-1.654061	0.560098
26	1	-6.135148	-3.317376	0.753605
27	6	-6.480566	0.486905	0.085398
28	1	-4.336416	0.492346	-0.090494
29	6	-7.638720	-0.275363	0.313246
30	1	-8.393143	-2.254799	0.728230
31	1	-6.573294	1.548088	-0.123936
32	7	-3.842748	-2.162335	0.398404
33	6	-8.989746	0.366913	0.279927
34	6	-9.380973	-0.002058	-2.266667
35	6	-10.471693	0.351897	-3.065077
36	6	-11.436614	0.998219	-2.259021
37	1	-10.570911	0.165839	-4.124237
38	6	-9.693629	0.443624	-0.934026
39	7	-10.968580	1.051545	-0.983386
40	6	-9.052012	0.942254	2.817548
41	6	-11.118005	1.914966	2.710085

42	6	-10.044142	1.580281	3.566559
43	1	-10.006101	1.788273	4.625601
44	6	-9.539097	0.887312	1.464116
45	7	-10.812900	1.499236	1.451794
46	5	-11.710070	1.676919	0.212659
47	9	-12.975905	1.022894	0.414200
48	9	-11.957775	3.074401	-0.028110
49	6	2.906557	-1.233120	-1.521881
50	1	3.542227	-2.097048	-1.763144
51	6	4.777631	-0.008627	-0.752699
52	6	5.179846	0.700126	0.394611
53	6	5.764329	-0.476641	-1.643476
54	6	6.532591	0.903667	0.665106
55	1	4.413273	1.081368	1.059704
56	6	7.117518	-0.257778	-1.376250
57	1	5.470706	-0.976912	-2.560474
58	6	7.519566	0.427953	-0.217620
59	1	6.830633	1.444955	1.557399
60	1	7.869627	-0.610857	-2.074904
61	7	3.391615	-0.164520	-0.979309
62	6	8.971091	0.665676	0.057020
63	6	9.098908	2.929287	-1.221631
64	6	10.185275	3.785624	-1.417788
65	6	11.321908	3.234086	-0.783081
66	1	10.169488	4.717442	-1.963408
67	6	9.591605	1.823003	-0.442616
68	7	10.963900	2.059220	-0.199620
69	6	9.325531	-1.516933	1.429294
70	6	11.544067	-1.112802	1.803340
71	6	10.480995	-2.014762	2.037449
72	1	10.559196	-2.935118	2.597000
73	6	9.698853	-0.274228	0.807000
74	7	11.072858	-0.071276	1.066637
75	5	11.906928	1.132682	0.590239
76	9	12.466207	1.830466	1.717337
77	9	12.989879	0.689468	-0.248630
78	6	7.716142	3.176793	-1.749371
79	1	7.387326	2.387469	-2.434428
80	1	6.969522	3.227032	-0.949360
81	1	7.691029	4.125878	-2.293390
82	6	12.709656	3.776642	-0.713038
83	1	12.998423	3.961974	-0.327571
84	1	13.425542	3.048073	-1.108282
85	1	12.789079	4.707103	-1.279714
86	6	7.987640	-2.195918	1.460323

87	1	7.221989	-1.577977	1.942578
88	1	7.617030	-2.426133	0.455331
89	1	8.060874	-3.135679	2.016340
90	6	12.965060	-1.205166	2.247405
91	1	13.638527	-1.191531	1.383528
92	1	13.231868	-0.338584	2.862121
93	1	13.131541	-2.119876	2.820863
94	6	-12.762714	1.556130	-2.652986
95	1	-13.565943	1.073557	-2.085609
96	1	-12.814813	2.624538	-2.416709
97	1	-12.939285	1.413547	-3.721504
98	6	-8.156417	-0.710534	-2.767060
99	1	-7.245148	-0.122366	-2.612050
100	1	-7.998425	-1.670555	-2.263353
101	1	-8.252868	-0.905270	-3.839552
102	6	-7.754803	0.438605	3.379221
103	1	-7.635749	-0.641841	3.242101
104	1	-6.887591	0.911657	2.905180
105	1	-7.708375	0.648670	4.452151
106	6	-12.399852	2.602601	3.040192
107	1	-12.517708	3.505255	2.431099
108	1	-13.253242	1.956821	2.805782
109	1	-12.431905	2.872761	4.098108

Table S6. Cartesian coordinates of optimized structure of **11**.

Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z
1	26	5.927127	0.106089	0.108301
2	6	3.021590	-0.913276	-0.639159
3	6	4.425692	-1.049726	-0.730799
4	6	5.276568	-0.496326	-1.765816
5	1	4.942131	0.138790	-2.570870
6	6	6.609177	-0.961955	-1.542573
7	1	7.470541	-0.726790	-2.147939
8	6	6.604089	-1.800926	-0.377660
9	1	7.460606	-2.305062	0.041804
10	6	5.268435	-1.858938	0.127706
11	1	4.926960	-2.419639	0.983473
12	6	5.023800	1.638033	1.188948
13	1	3.960517	1.795868	1.280590
14	6	5.872607	2.186590	0.170633
15	1	5.562770	2.842643	-0.627511
16	6	7.209175	1.719405	0.408916

17	1	8.080976	1.965476	-0.176831
18	6	7.185005	0.882111	1.574168
19	1	8.035457	0.388795	2.018013
20	6	5.833673	0.831981	2.056579
21	1	5.489673	0.292250	2.924738
22	6	0.403098	-0.610560	-0.436480
23	6	-0.324918	0.094717	-1.422638
24	6	-0.305714	-1.142670	0.665413
25	6	-1.700445	0.270033	-1.303670
26	1	0.201407	0.496320	-2.281269
27	6	-1.683238	-0.976575	0.774052
28	1	0.238897	-1.677872	1.435179
29	6	-2.406748	-0.262400	-0.204399
30	1	-2.243649	0.797342	-2.079849
31	1	-2.205203	-1.372137	1.638158
32	6	-3.869245	-0.072955	-0.077175
33	6	-3.831029	2.492598	-0.392033
34	6	-4.858505	3.436996	-0.415453
35	1	-2.772960	2.682198	-0.477177
36	6	-6.070581	2.736889	-0.229121
37	1	-4.759050	4.503971	-0.538809
38	1	-7.079017	3.114894	-0.170259
39	6	-4.430260	1.213112	-0.206232
40	7	-5.818941	1.412954	-0.101692
41	6	-4.430954	-2.571076	0.275647
42	6	-6.651487	-2.233873	0.516252
43	6	-5.644523	-3.223806	0.497287
44	1	-3.458253	-3.025210	0.174073
45	1	-7.716998	-2.342108	0.644208
46	1	-5.800369	-4.284160	0.619306
47	6	-4.707415	-1.176680	0.175797
48	7	-6.097253	-1.014202	0.322639
49	5	-6.876230	0.320542	0.201354
50	9	-7.828758	0.236163	-0.857365
51	9	-7.552021	0.620262	1.421872
52	6	1.812452	-0.771670	-0.544660

Table S7. Cartesian coordinates of optimized structure of **12**.

Center Number	Atomic Number	Coordinates (Å)		
		X	Y	Z
1	26	-7.967390	0.305360	-0.096932
2	6	-6.505747	-1.136445	0.290393
3	6	-7.368006	-0.952336	1.436247
4	1	-7.048476	-0.677794	2.429092
5	6	-8.711776	-1.259565	1.048331
6	1	-9.577379	-1.233878	1.691430
7	6	-8.701496	-1.624728	-0.338631
8	1	-9.559541	-1.913402	-0.925167
9	6	-7.350948	-1.544152	-0.807920
10	1	-7.023506	-1.754340	-1.813935
11	6	-7.003356	2.092231	-0.551687
12	1	-5.935326	2.243267	-0.571577
13	6	-7.859618	2.268252	0.586567
14	1	-7.551571	2.591806	1.568506
15	6	-9.202295	1.957623	0.183917
16	1	-10.079220	2.004472	0.810325
17	6	-9.175123	1.590239	-1.203217
18	1	-10.028153	1.312620	-1.802346
19	6	-7.815972	1.673912	-1.657810
20	1	-7.467456	1.468141	-2.657672
21	6	1.844793	-0.394716	0.133768
22	6	2.519889	0.424209	1.068353
23	6	2.613192	-1.072854	-0.840616
24	6	3.903570	0.566302	1.021859
25	1	1.946020	0.940670	1.829568
26	6	3.998152	-0.939403	-0.874874
27	1	2.109402	-1.696720	-1.570328
28	6	4.669405	-0.113808	0.051525
29	1	4.405163	1.184081	1.758290
30	1	4.568145	-1.450214	-1.642816
31	6	6.141418	0.037559	0.003856
32	6	6.138148	2.621924	-0.042303
33	6	7.182274	3.547467	-0.074976
34	1	5.081130	2.834298	-0.060169
35	6	8.388638	2.813224	-0.075577
36	1	7.098307	4.622390	-0.106710
37	1	9.406865	3.167003	-0.112824
38	6	6.720423	1.321686	-0.006900
39	7	8.117178	1.487701	-0.037622
40	6	6.668971	-2.492137	0.046712
41	6	8.908298	-2.220249	-0.072876

42	6	7.880073	-3.184805	0.010768
43	1	5.681231	-2.915096	0.137805
44	1	9.977482	-2.358836	-0.104779
45	1	8.019956	-4.253581	0.051730
46	6	6.969623	-1.101278	-0.030727
47	7	8.369688	-0.978657	-0.095449
48	5	9.167808	0.350263	-0.114119
49	9	10.051092	0.406577	1.004716
50	9	9.923786	0.464070	-1.319126
51	6	0.429124	-0.529333	0.170145
52	6	-2.204672	-0.765334	0.223775
53	6	-2.971443	-0.132756	1.229402
54	6	-2.885148	-1.523712	-0.754768
55	6	-4.356999	-0.250337	1.245878
56	1	-2.465994	0.453435	1.989286
57	6	-4.271938	-1.639833	-0.727571
58	1	-2.313058	-2.023570	-1.528922
59	6	-5.041931	-1.004034	0.268334
60	1	-4.920905	0.258149	2.020585
61	1	-4.766920	-2.247853	-1.476726
62	6	-0.787029	-0.640289	0.197186

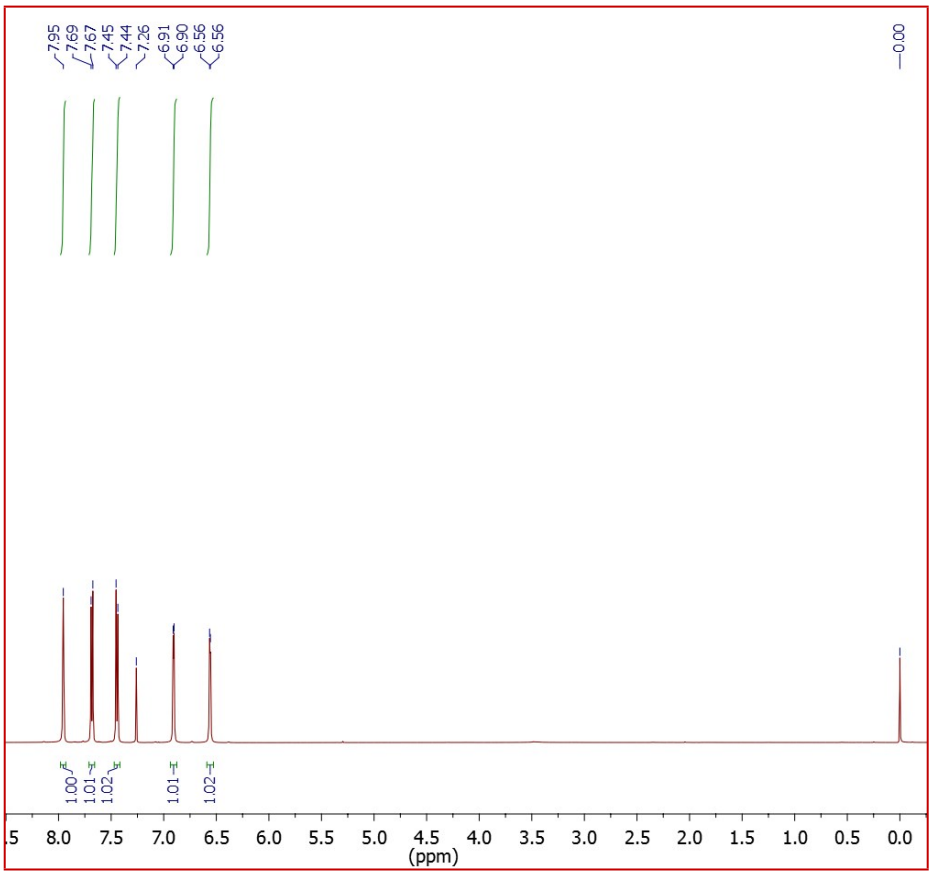


Fig. S2. ^{1}H NMR ($CDCl_3$) spectrum of **6**.

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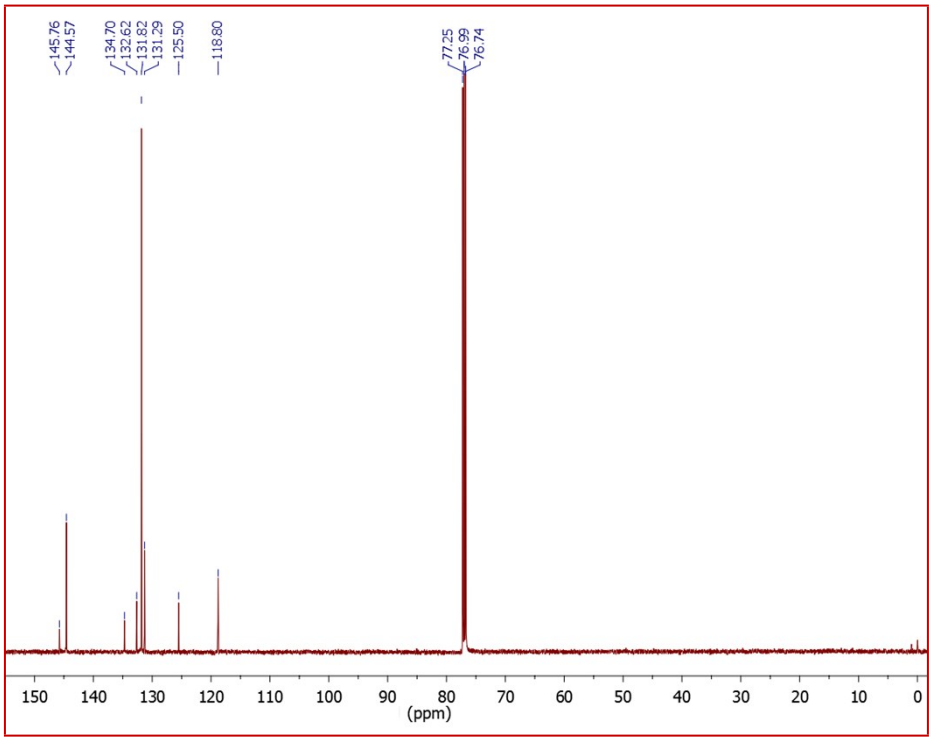

Fig. S3. ^{13}C NMR ($CDCl_3$) spectrum of **6**.

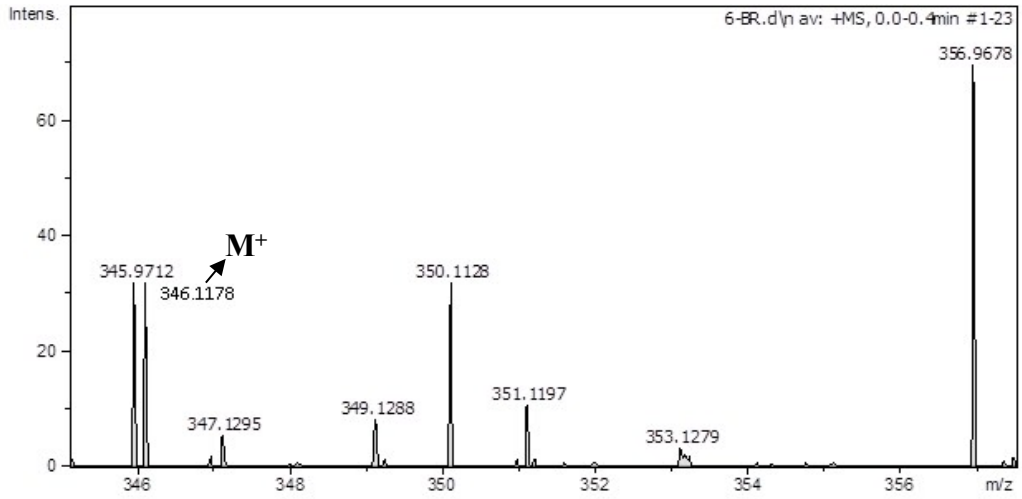

Fig. S4. HRMS spectrum of **6.**

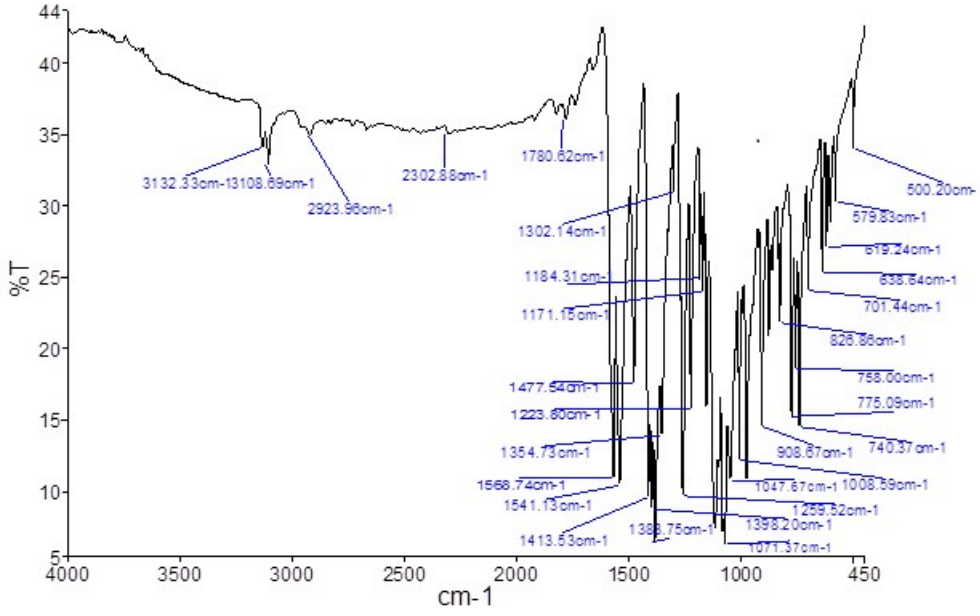

Fig. S5. FTIR spectrum of **6**.

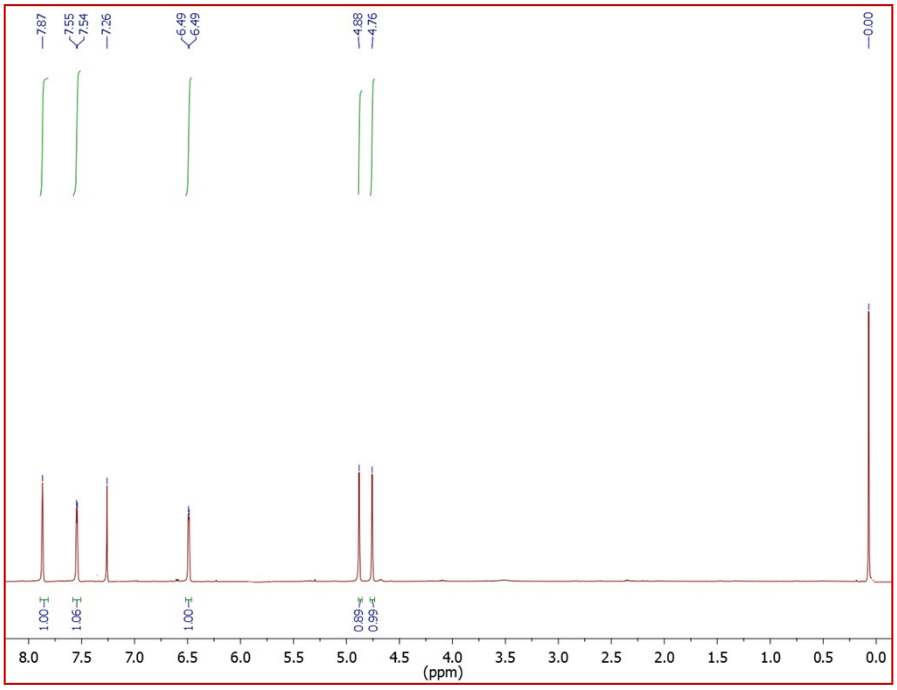

Fig. S6. ^{1}H NMR ($CDCl_3$) spectrum of **8**.

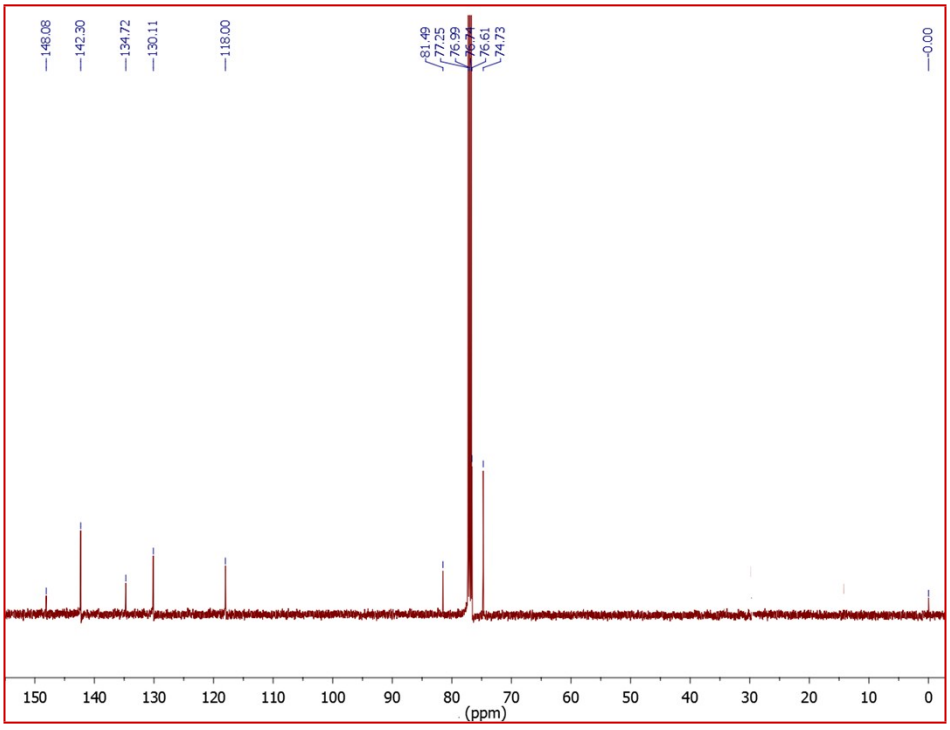

Fig. S7. ^{13}C NMR ($CDCl_3$) spectrum of **8**.

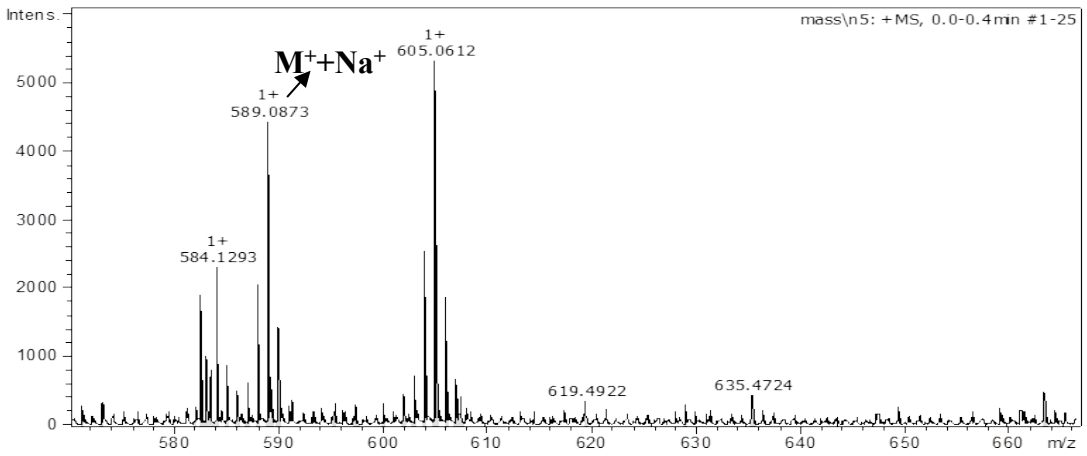

Fig. S8. HRMS spectrum of **8**.

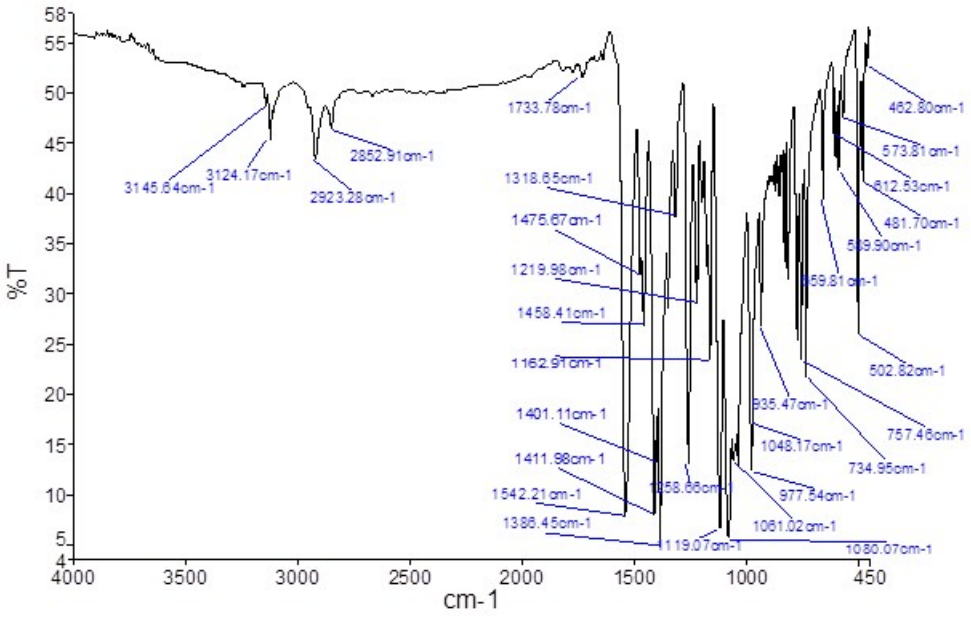

Fig. S9. FTIR spectrum of **8**.

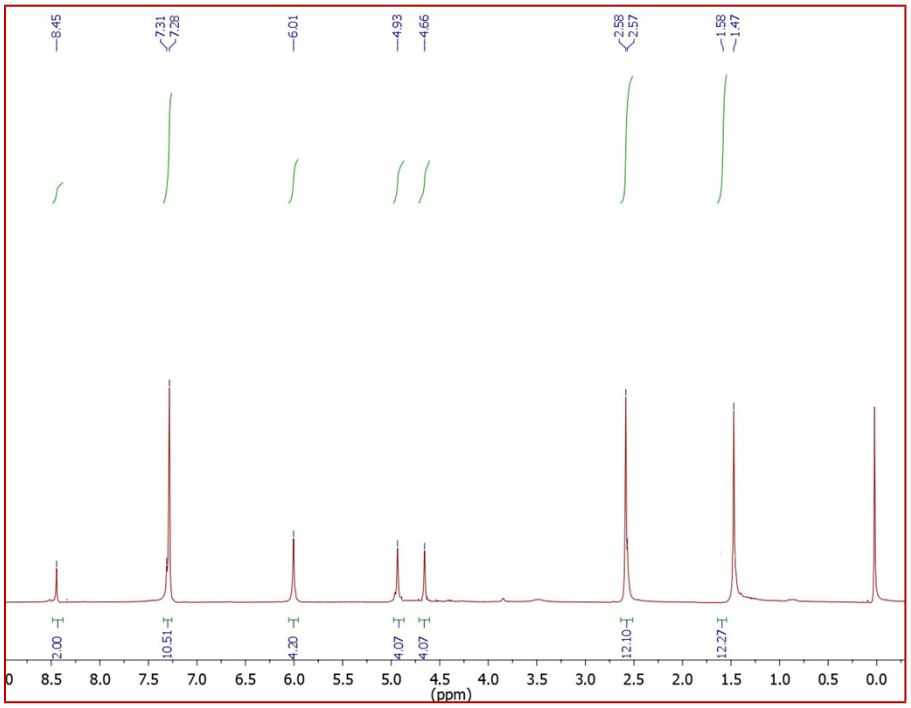

Fig. S10. ^{1}H NMR ($CDCl_3$) spectrum of **10**.

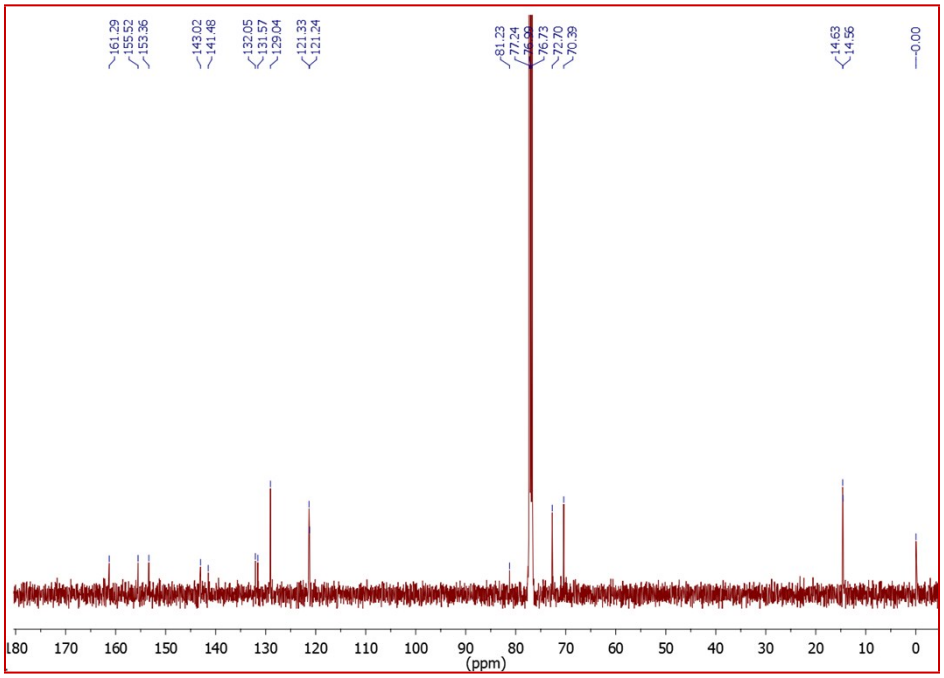

Fig. S11. ^{13}C NMR ($CDCl_3$) spectrum of **10**.

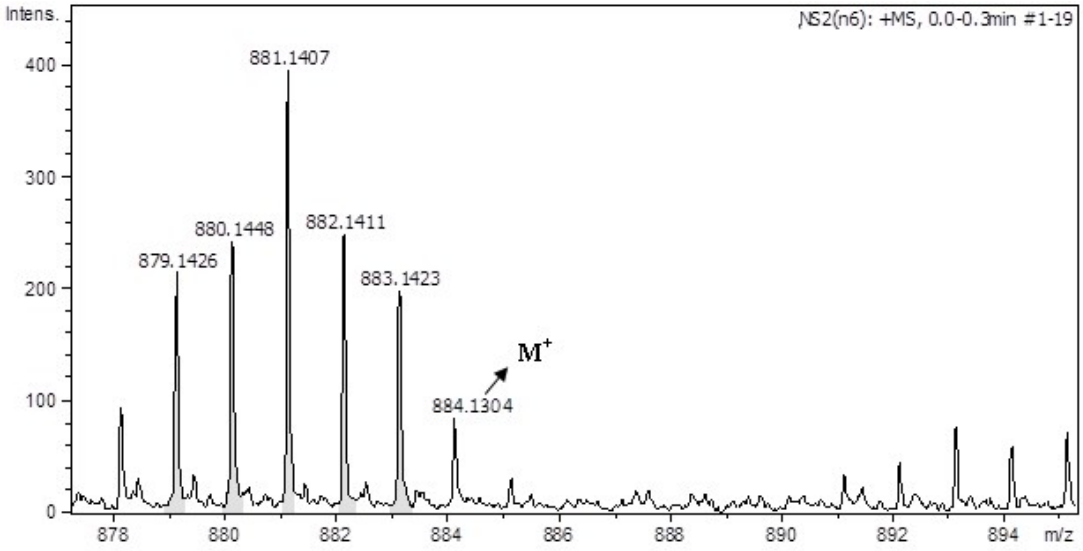

Fig. S12. HRMS spectrum of **10**.

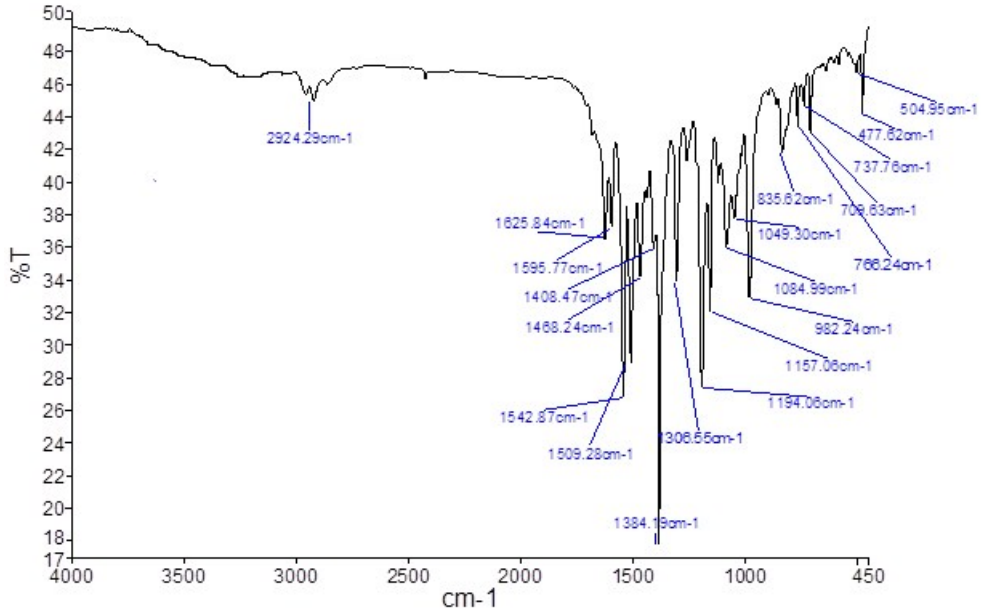

Fig. S13. FTIR spectrum of **10**.

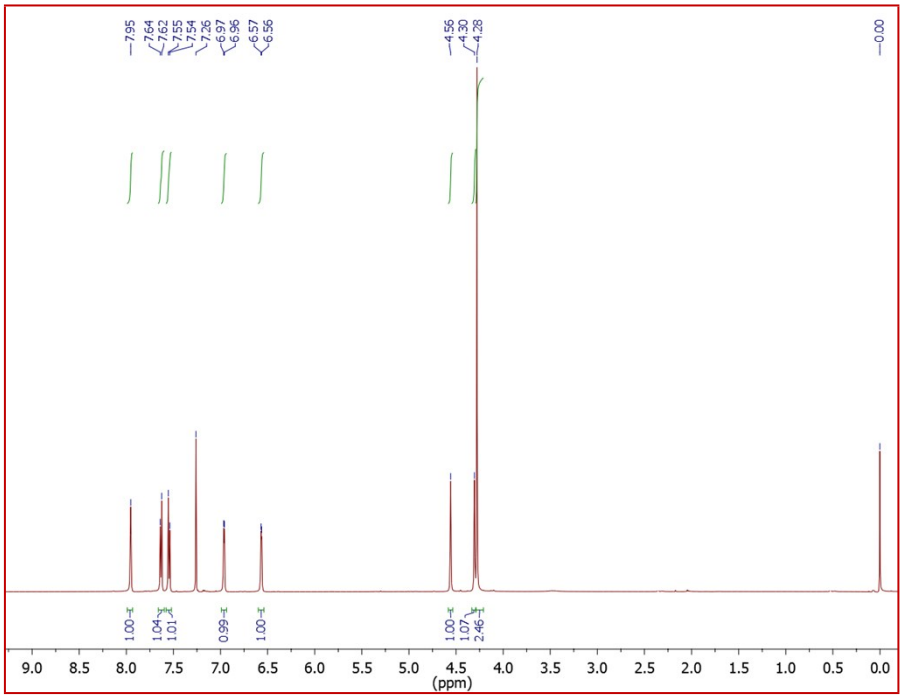

Fig. S14. ^{1}H NMR ($CDCl_3$) spectrum of **11**.

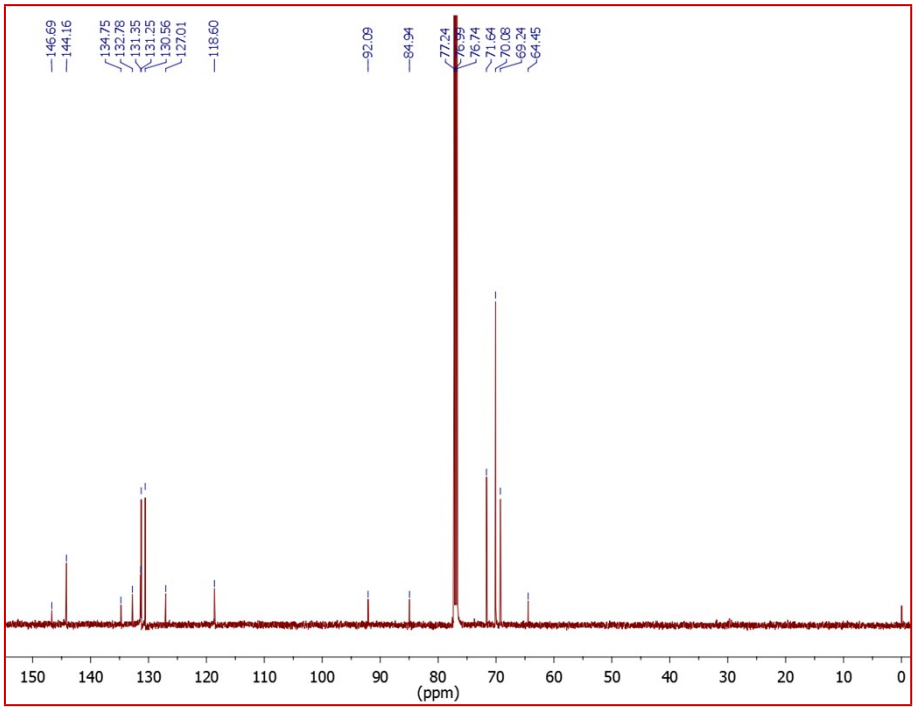

Fig. S15. ^{13}C NMR ($CDCl_3$) spectrum of **11**.

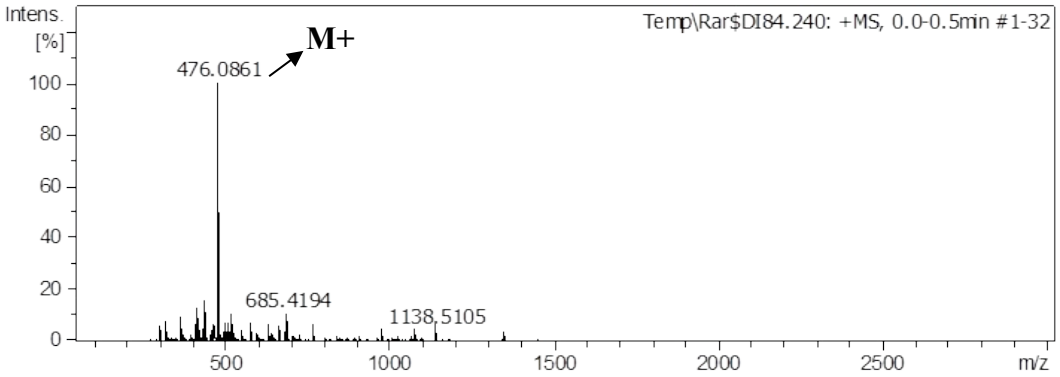

Fig. S16. HRMS spectrum of **11**.

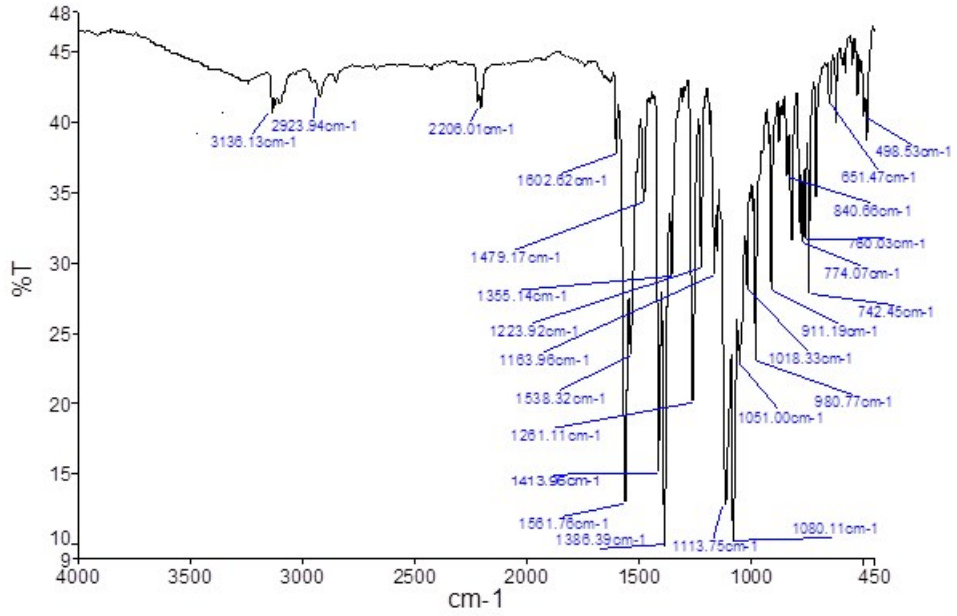

Fig. S17. FTIR spectrum of **11**.

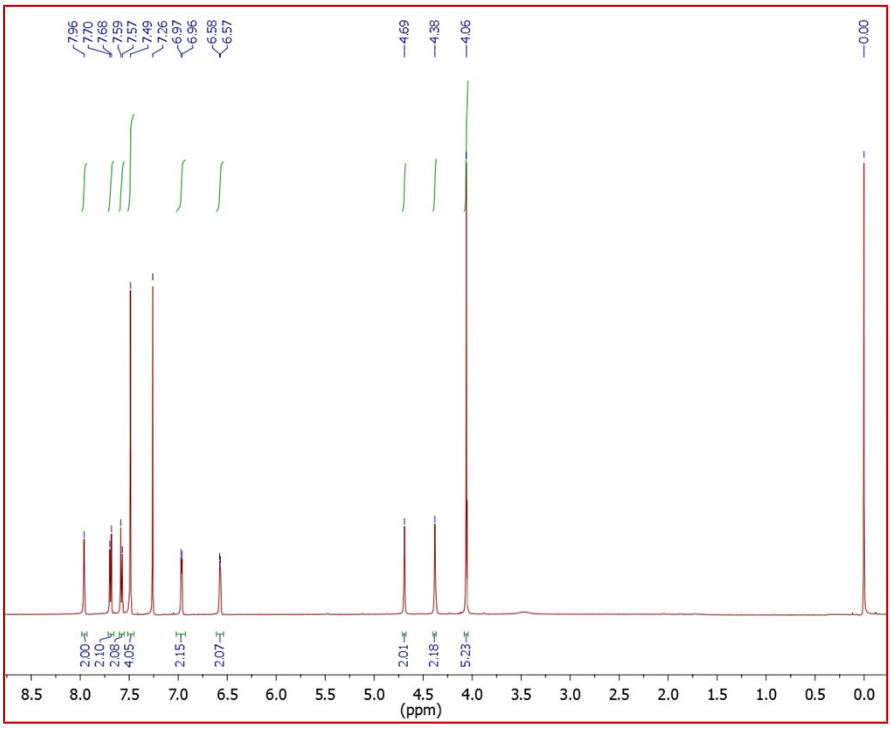

Fig. S18. ^{1}H NMR ($CDCl_3$) spectrum of **12**.

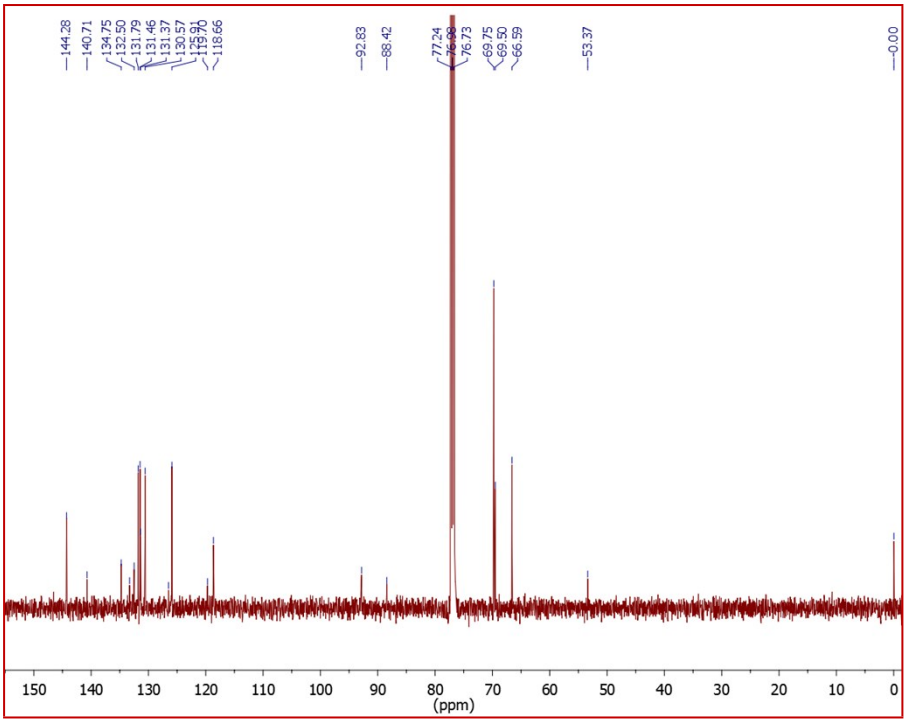

Fig. S19. ^{13}C NMR ($CDCl_3$) spectrum of **12**.

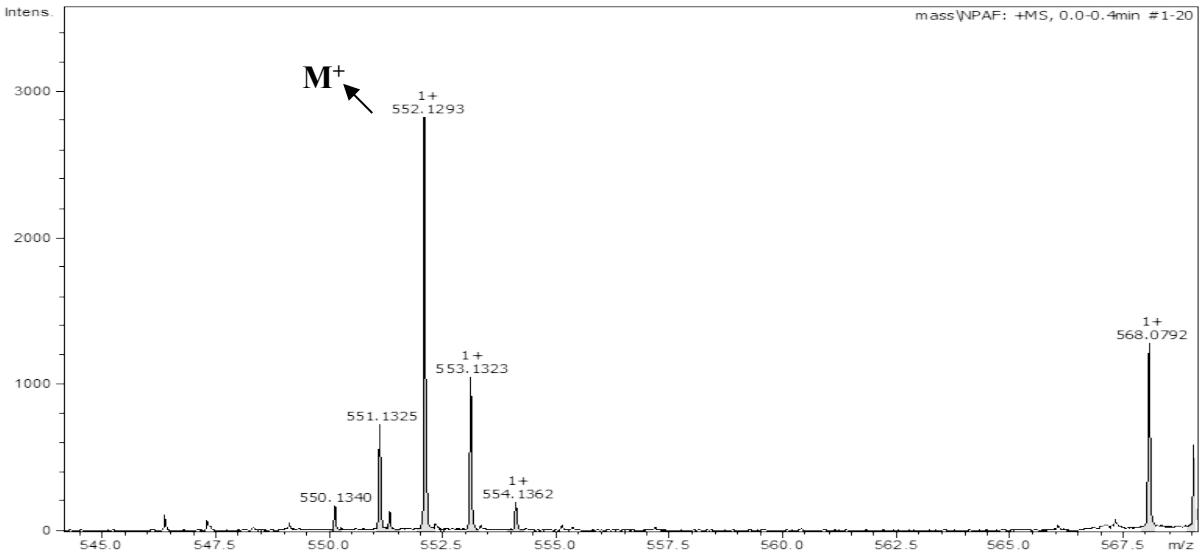

Fig. S20. HRMS spectrum of **12**.

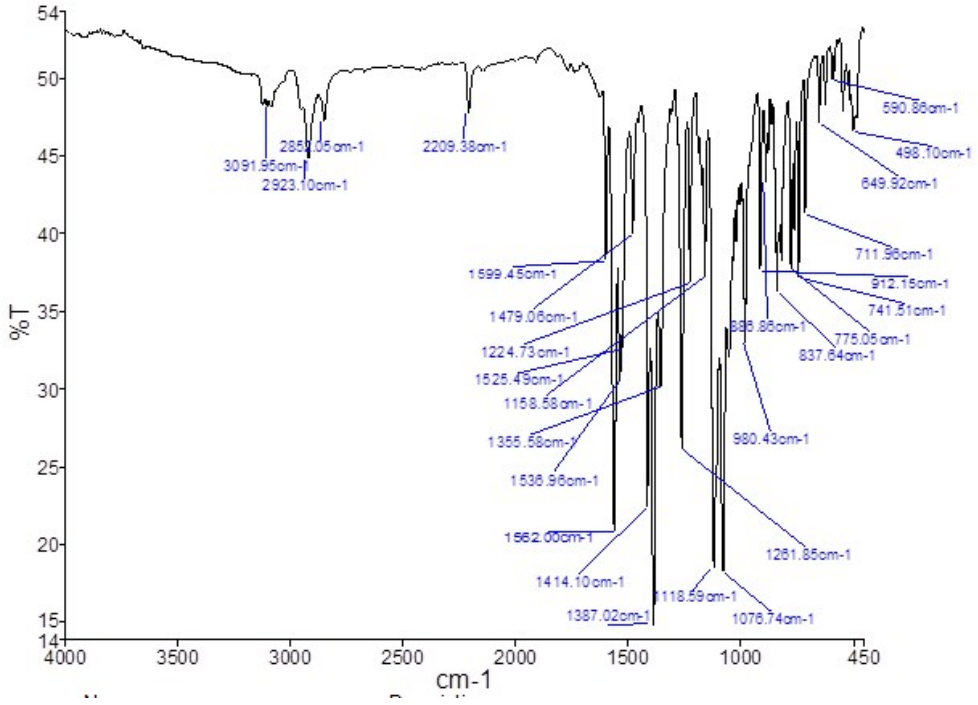

Fig. S21. FTIR spectrum of **12**.

Table S8. Crystal data and structure refinement for **8**.

Identification code	shelx
Empirical formula	$C_{28}H_{20}B_2F_4FeN_4$
Formula weight	565.95
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.0604(7) Å α = 65.087(8) deg. b = 11.0621(8) Å β = 86.182(6) deg. c = 11.2138(9) Å γ = 69.916(6) deg
Volume	1163.77(17) A^3
Z, Calculated density	2, 1.615 Mg/m^3
Absorption coefficient	0.708 mm^{-1}
F(000)	576
Crystal size	0.320 x 0.280 x 0.260 mm
Theta range for data collection	2.941 to 32.266 deg.
Limiting indices	-16<=h<=15, -16<=k<=15, -16<=l<=15
Reflections collected / unique	13094 / 7502 [R (int) = 0.0484]
Completeness to theta	25.242 99.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7502 / 0 / 353
Goodness-of-fit on F^2	1.102
Final R indices [I>2sigma(I)]	R1 = 0.0707, wR2 = 0.1734
R indices (all data)	R1 = 0.1068, wR2 = 0.2177
Extinction coefficient	0.154(9)
Largest diff. peak and hole	1.288 and -1.377 $e.A^{-3}$

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **8**. U (eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	X	y	Z	U(eq)
Fe(1)	2447(1)	4496(1)	2802(1)	35(1)
F(1)	1917(2)	11819(2)	-706(2)	61(1)
F(2)	3446(2)	10214(3)	967(2)	63(1)
F(3)	9083(2)	3010(2)	4377(2)	58(1)
F(4)	8767(2)	2572(2)	2667(2)	63(1)
B(1)	2460(3)	10399(4)	139(4)	41(1)
B(2)	8169(3)	2950(4)	3643(4)	41(1)
N(1)	1430(2)	9836(2)	949(3)	38(1)
N(2)	2995(2)	9497(3)	-640(3)	40(1)
N(3)	7055(2)	4395(3)	3032(3)	39(1)
N(4)	7535(2)	1876(3)	4548(3)	40(1)
C(1)	545(3)	10462(3)	1578(3)	41(1)
C(2)	-96(3)	9550(3)	2356(3)	44(1)
C(3)	431(3)	8313(3)	2201(3)	42(1)
C(4)	1383(3)	8482(3)	1296(3)	36(1)
C(5)	2122(3)	7642(3)	667(3)	34(1)
C(6)	2876(3)	8186(3)	-347(3)	37(1)
C(7)	3490(3)	7726(4)	-1290(3)	45(1)
C(8)	3968(4)	8731(4)	-2136(4)	56(1)
C(9)	3657(4)	9808(4)	-1705(4)	53(1)
C(10)	7172(4)	5621(4)	2170(4)	51(1)
C(11)	5970(3)	6704(4)	1787(4)	55(1)
C(12)	5073(3)	6109(3)	2438(3)	45(1)
C(13)	5741(3)	4658(3)	3225(3)	35(1)
C(14)	5314(3)	3551(3)	4061(3)	33(1)
C(15)	6236(3)	2179(3)	4769(3)	36(1)
C(16)	6108(3)	944(3)	5779(3)	43(1)
C(17)	7314(3)	-100(4)	6134(4)	51(1)
C(18)	8163(3)	514(4)	5363(4)	49(1)
C(19)	2079(3)	6227(3)	987(3)	39(1)
C(20)	983(3)	5781(3)	1318(3)	43(1)
C(21)	1359(3)	4355(3)	1472(4)	50(1)
C(22)	2682(3)	3891(3)	1270(3)	48(1)
C(23)	3136(3)	5033(3)	972(3)	41(1)
C(24)	1780(3)	4654(4)	4513(3)	47(1)
C(25)	2037(3)	3254(3)	4631(3)	47(1)
C(26)	3367(3)	2701(3)	4452(3)	40(1)
C(27)	3946(3)	3746(3)	4230(3)	35(1)
C(28)	2930(3)	4973(3)	4243(3)	40(1)

Table S10. Bond lengths [Å] and angles [deg] for **8**.

Fe(1)-C(26)	2.042(3)
Fe(1)-C(20)	2.048(3)
Fe(1)-C(28)	2.051(3)
Fe(1)-C(23)	2.054(3)
Fe(1)-C(25)	2.057(3)
Fe(1)-C(22)	2.062(3)
Fe(1)-C(21)	2.063(3)
Fe(1)-C(24)	2.065(3)
Fe(1)-C(19)	2.065(3)
Fe(1)-C(27)	2.072(3)
F(1)-B(1)	1.378(4)
F(2)-B(1)	1.384(4)
F(3)-B(2)	1.381(4)
F(4)-B(2)	1.382(4)
B(1)-N(2)	1.539(4)
B(1)-N(1)	1.544(4)
B(2)-N(3)	1.543(4)
B(2)-N(4)	1.547(4)
N(1)-C(1)	1.338(4)
N(1)-C(4)	1.399(3)
N(2)-C(9)	1.339(4)
N(2)-C(6)	1.398(4)
N(3)-C(10)	1.337(4)
N(3)-C(13)	1.402(4)
N(4)-C(18)	1.339(4)
N(4)-C(15)	1.390(3)
C(1)-C(2)	1.396(4)
C(1)-H(1)	0.9300
C(2)-C(3)	1.371(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.416(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.407(4)
C(5)-C(6)	1.412(4)
C(5)-C(19)	1.470(4)
C(6)-C(7)	1.399(4)
C(7)-C(8)	1.365(5)
C(7)-H(7)	0.9300
C(8)-C(9)	1.398(5)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(11)	1.391(5)
C(10)-H(10)	0.9300

C(11)-C(12)	1.377(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.407(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.404(4)
C(14)-C(15)	1.415(4)
C(14)-C(27)	1.464(4)
C(15)-C(16)	1.406(4)
C(16)-C(17)	1.378(4)
C(16)-H(16)	0.9300
C(17)-C(18)	1.388(5)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(20)	1.430(4)
C(19)-C(23)	1.438(4)
C(20)-C(21)	1.420(4)
C(20)-H(20)	0.9300
C(21)-C(22)	1.412(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.420(5)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-C(28)	1.414(4)
C(24)-C(25)	1.424(5)
C(24)-H(24)	0.9300
C(25)-C(26)	1.422(4)
C(25)-H(25)	0.9300
C(26)-C(27)	1.433(4)
C(26)-H(26)	0.9300
C(27)-C(28)	1.440(4)
C(28)-H(28)	0.9300
C(26)-Fe(1)-C(20)	154.04(12)
C(26)-Fe(1)-C(28)	68.37(12)
C(20)-Fe(1)-C(28)	126.06(12)
C(26)-Fe(1)-C(23)	124.57(12)
C(20)-Fe(1)-C(23)	68.27(13)
C(28)-Fe(1)-C(23)	124.59(12)
C(26)-Fe(1)-C(25)	40.60(12)
C(20)-Fe(1)-C(25)	119.42(13)
C(28)-Fe(1)-C(25)	68.28(13)
C(23)-Fe(1)-C(25)	159.45(13)
C(26)-Fe(1)-C(22)	106.08(13)
C(20)-Fe(1)-C(22)	68.02(13)
C(28)-Fe(1)-C(22)	158.57(14)
C(23)-Fe(1)-C(22)	40.37(13)

C(25)-Fe(1)-C(22)	121.83(14)
C(26)-Fe(1)-C(21)	118.86(13)
C(20)-Fe(1)-C(21)	40.42(12)
C(28)-Fe(1)-C(21)	161.02(14)
C(23)-Fe(1)-C(21)	67.64(14)
C(25)-Fe(1)-C(21)	105.01(14)
C(22)-Fe(1)-C(21)	40.05(14)
C(26)-Fe(1)-C(24)	67.87(13)
C(20)-Fe(1)-C(24)	107.98(13)
C(28)-Fe(1)-C(24)	40.19(12)
C(23)-Fe(1)-C(24)	159.50(13)
C(25)-Fe(1)-C(24)	40.42(13)
C(22)-Fe(1)-C(24)	158.77(14)
C(21)-Fe(1)-C(24)	123.46(14)
C(26)-Fe(1)-C(19)	162.81(12)
C(20)-Fe(1)-C(19)	40.70(12)
C(28)-Fe(1)-C(19)	110.50(12)
C(23)-Fe(1)-C(19)	40.86(11)
C(25)-Fe(1)-C(19)	156.25(13)
C(22)-Fe(1)-C(19)	68.36(12)
C(21)-Fe(1)-C(19)	68.08(13)
C(24)-Fe(1)-C(19)	123.16(13)
C(26)-Fe(1)-C(27)	40.77(11)
C(20)-Fe(1)-C(27)	163.72(12)
C(28)-Fe(1)-C(27)	40.86(11)
C(23)-Fe(1)-C(27)	109.51(12)
C(25)-Fe(1)-C(27)	68.59(12)
C(22)-Fe(1)-C(27)	121.51(13)
C(21)-Fe(1)-C(27)	155.11(13)
C(24)-Fe(1)-C(27)	68.09(12)
C(19)-Fe(1)-C(27)	127.10(11)
F(1)-B(1)-F(2)	109.5(3)
F(1)-B(1)-N(2)	110.7(3)
F(2)-B(1)-N(2)	109.8(3)
F(1)-B(1)-N(1)	110.8(3)
F(2)-B(1)-N(1)	110.6(3)
N(2)-B(1)-N(1)	105.4(2)
F(3)-B(2)-F(4)	108.5(3)
F(3)-B(2)-N(3)	110.7(2)
F(4)-B(2)-N(3)	110.6(3)
F(3)-B(2)-N(4)	110.1(3)
F(4)-B(2)-N(4)	111.4(3)
N(3)-B(2)-N(4)	105.5(2)
C(1)-N(1)-C(4)	108.1(2)
C(1)-N(1)-B(1)	126.5(2)

C(4)-N(1)-B(1)	124.9(2)
C(9)-N(2)-C(6)	107.5(3)
C(9)-N(2)-B(1)	126.9(3)
C(6)-N(2)-B(1)	125.6(3)
C(10)-N(3)-C(13)	107.6(3)
C(10)-N(3)-B(2)	125.5(3)
C(13)-N(3)-B(2)	126.8(2)
C(18)-N(4)-C(15)	107.4(3)
C(18)-N(4)-B(2)	125.8(3)
C(15)-N(4)-B(2)	126.4(2)
N(1)-C(1)-C(2)	110.2(2)
N(1)-C(1)-H(1)	124.9
C(2)-C(1)-H(1)	124.9
C(3)-C(2)-C(1)	107.0(3)
C(3)-C(2)-H(2)	126.5
C(1)-C(2)-H(2)	126.5
C(2)-C(3)-C(4)	107.9(3)
C(2)-C(3)-H(3)	126.0
C(4)-C(3)-H(3)	126.0
N(1)-C(4)-C(5)	120.1(3)
N(1)-C(4)-C(3)	106.7(2)
C(5)-C(4)-C(3)	132.9(3)
C(4)-C(5)-C(6)	120.0(2)
C(4)-C(5)-C(19)	121.6(3)
C(6)-C(5)-C(19)	118.3(3)
N(2)-C(6)-C(7)	107.5(3)
N(2)-C(6)-C(5)	120.1(3)
C(7)-C(6)-C(5)	132.1(3)
C(8)-C(7)-C(6)	108.1(3)
C(8)-C(7)-H(7)	126.0
C(6)-C(7)-H(7)	126.0
C(7)-C(8)-C(9)	107.0(3)
C(7)-C(8)-H(8)	126.5
C(9)-C(8)-H(8)	126.5
N(2)-C(9)-C(8)	110.0(3)
N(2)-C(9)-H(9)	125.0
C(8)-C(9)-H(9)	125.0
N(3)-C(10)-C(11)	110.5(3)
N(3)-C(10)-H(10)	124.8
C(11)-C(10)-H(10)	124.8
C(12)-C(11)-C(10)	107.0(3)
C(12)-C(11)-H(11)	126.5
C(10)-C(11)-H(11)	126.5
C(11)-C(12)-C(13)	107.6(3)
C(11)-C(12)-H(12)	126.2

C(13)-C(12)-H(12)	126.2
N(3)-C(13)-C(14)	120.6(2)
N(3)-C(13)-C(12)	107.3(2)
C(14)-C(13)-C(12)	132.0(3)
C(13)-C(14)-C(15)	119.2(2)
C(13)-C(14)-C(27)	122.8(2)
C(15)-C(14)-C(27)	118.0(2)
N(4)-C(15)-C(16)	107.6(3)
N(4)-C(15)-C(14)	121.1(3)
C(16)-C(15)-C(14)	131.3(3)
C(17)-C(16)-C(15)	107.6(3)
C(17)-C(16)-H(16)	126.2
C(15)-C(16)-H(16)	126.2
C(16)-C(17)-C(18)	106.6(3)
C(16)-C(17)-H(17)	126.7
C(18)-C(17)-H(17)	126.7
N(4)-C(18)-C(17)	110.7(3)
N(4)-C(18)-H(18)	124.6
C(17)-C(18)-H(18)	124.6
C(20)-C(19)-C(23)	106.8(2)
C(20)-C(19)-C(5)	127.3(3)
C(23)-C(19)-C(5)	125.9(3)
C(20)-C(19)-Fe(1)	69.04(18)
C(23)-C(19)-Fe(1)	69.17(17)
C(5)-C(19)-Fe(1)	128.6(2)
C(21)-C(20)-C(19)	108.3(3)
C(21)-C(20)-Fe(1)	70.34(18)
C(19)-C(20)-Fe(1)	70.27(17)
C(21)-C(20)-H(20)	125.8
C(19)-C(20)-H(20)	125.8
Fe(1)-C(20)-H(20)	125.1
C(22)-C(21)-C(20)	108.5(3)
C(22)-C(21)-Fe(1)	69.94(19)
C(20)-C(21)-Fe(1)	69.24(18)
C(22)-C(21)-H(21)	125.7
C(20)-C(21)-H(21)	125.7
Fe(1)-C(21)-H(21)	126.7
C(21)-C(22)-C(23)	108.0(3)
C(21)-C(22)-Fe(1)	70.02(19)
C(23)-C(22)-Fe(1)	69.52(18)
C(21)-C(22)-H(22)	126.0
C(23)-C(22)-H(22)	126.0
Fe(1)-C(22)-H(22)	126.0
C(22)-C(23)-C(19)	108.4(3)
C(22)-C(23)-Fe(1)	70.1(2)

C(19)-C(23)-Fe(1)	69.97(18)
C(22)-C(23)-H(23)	125.8
C(19)-C(23)-H(23)	125.8
Fe(1)-C(23)-H(23)	125.7
C(28)-C(24)-C(25)	108.7(3)
C(28)-C(24)-Fe(1)	69.38(17)
C(25)-C(24)-Fe(1)	69.49(19)
C(28)-C(24)-H(24)	125.7
C(25)-C(24)-H(24)	125.7
Fe(1)-C(24)-H(24)	127.0
C(26)-C(25)-C(24)	107.3(3)
C(26)-C(25)-Fe(1)	69.14(17)
C(24)-C(25)-Fe(1)	70.09(19)
C(26)-C(25)-H(25)	126.3
C(24)-C(25)-H(25)	126.3
Fe(1)-C(25)-H(25)	126.0
C(25)-C(26)-C(27)	109.1(3)
C(25)-C(26)-Fe(1)	70.26(18)
C(27)-C(26)-Fe(1)	70.76(17)
C(25)-C(26)-H(26)	125.4
C(27)-C(26)-H(26)	125.4
Fe(1)-C(26)-H(26)	125.1
C(26)-C(27)-C(28)	106.4(2)
C(26)-C(27)-C(14)	125.5(3)
C(28)-C(27)-C(14)	128.2(2)
C(26)-C(27)-Fe(1)	68.47(17)
C(28)-C(27)-Fe(1)	68.77(16)
C(14)-C(27)-Fe(1)	128.6(2)
C(24)-C(28)-C(27)	108.5(3)
C(24)-C(28)-Fe(1)	70.42(18)
C(27)-C(28)-Fe(1)	70.37(16)
C(24)-C(28)-H(28)	125.8
C(27)-C(28)-H(28)	125.8
Fe(1)-C(28)-H(28)	125.0

Symmetry transformations used to generate equivalent atoms:

Table S11. Anisotropic displacement parameters ($A^2 \times 10^3$) for **8**. The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12]$

	U11	U22	U33	U23	U13	U12
Fe(1)	29(1)	34(1)	46(1)	-18(1)	6(1)	-13(1)
F(1)	56(1)	37(1)	84(2)	-19(1)	22(1)	-21(1)
F(2)	48(1)	95(2)	72(2)	-52(1)	11(1)	-34(1)
F(3)	38(1)	65(1)	81(2)	-33(1)	0(1)	-25(1)
F(4)	64(1)	68(1)	75(2)	-46(1)	37(1)	-31(1)
B(1)	36(2)	39(2)	51(2)	-21(2)	10(1)	-17(1)
B(2)	33(2)	46(2)	54(2)	-27(2)	11(1)	-17(1)
N(1)	37(1)	33(1)	45(1)	-18(1)	7(1)	-11(1)
N(2)	38(1)	40(1)	44(1)	-19(1)	9(1)	-17(1)
N(3)	35(1)	42(1)	46(1)	-18(1)	11(1)	-22(1)
N(4)	30(1)	42(1)	49(2)	-20(1)	7(1)	-14(1)
C(1)	40(1)	39(1)	46(2)	-21(1)	6(1)	-13(1)
C(2)	38(1)	46(2)	49(2)	-25(1)	11(1)	-11(1)
C(3)	38(1)	39(1)	48(2)	-19(1)	10(1)	-15(1)
C(4)	33(1)	32(1)	41(2)	-15(1)	5(1)	-12(1)
C(5)	28(1)	32(1)	41(2)	-15(1)	2(1)	-9(1)
C(6)	35(1)	36(1)	40(2)	-17(1)	3(1)	-12(1)
C(7)	46(2)	49(2)	45(2)	-24(2)	9(1)	-18(1)
C(8)	66(2)	67(2)	52(2)	-35(2)	27(2)	-32(2)
C(9)	59(2)	57(2)	52(2)	-25(2)	21(2)	-33(2)
C(10)	50(2)	53(2)	56(2)	-18(2)	12(2)	-33(2)
C(11)	52(2)	43(2)	64(2)	-9(2)	3(2)	-28(2)
C(12)	40(2)	41(2)	54(2)	-14(1)	1(1)	-19(1)
C(13)	31(1)	38(1)	39(2)	-16(1)	6(1)	-18(1)
C(14)	32(1)	37(1)	35(1)	-17(1)	6(1)	-17(1)
C(15)	31(1)	40(1)	40(2)	-17(1)	6(1)	-14(1)
C(16)	40(2)	44(2)	40(2)	-11(1)	4(1)	-19(1)
C(17)	48(2)	40(2)	52(2)	-9(1)	-6(2)	-15(1)
C(18)	33(1)	46(2)	61(2)	-19(2)	0(1)	-10(1)
C(19)	36(1)	36(1)	44(2)	-18(1)	2(1)	-11(1)
C(20)	36(1)	37(1)	57(2)	-19(1)	-1(1)	-13(1)
C(21)	52(2)	43(2)	62(2)	-24(2)	-6(2)	-20(1)
C(22)	56(2)	37(2)	52(2)	-23(1)	1(2)	-11(1)
C(23)	43(2)	38(1)	44(2)	-21(1)	7(1)	-11(1)
C(24)	33(1)	54(2)	54(2)	-26(2)	16(1)	-14(1)
C(25)	34(1)	50(2)	53(2)	-15(2)	-12(1)	22(1)
C(26)	35(1)	35(1)	47(2)	-14(1)	6(1)	-16(1)
C(27)	31(1)	38(1)	36(1)	-13(1)	7(1)	-15(1)
C(28)	38(1)	42(2)	47(2)	-25(1)	12(1)	-16(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **8**.

	x	y	z	U(eq)
H(1)	381	11374	1507	49
H(2)	-755	9744	2880	53
H(3)	204	7507	2617	50
H(7)	3560	6883	-1333	54
H(8)	4415	8704	-2862	68
H(9)	3878	10621	-2100	63
H(10)	7947	5733	1868	61
H(11)	5803	7650	1202	65
H(12)	4186	6581	2370	54
H(16)	5346	849	6143	51
H(17)	7519	-1034	6765	61
H(18)	9048	45	5407	59
H(20)	165	6330	1415	52
H(21)	823	3819	1673	60
H(22)	3170	2995	1324	57
H(23)	3975	5012	796	50
H(24)	987	5259	4598	56
H(25)	1446	2787	4795	56
H(26)	3792	1805	4475	47
H(28)	3015	5831	4099	47

Table S13. Torsion angles [deg] for **8**.

F(1)	B(1)	N(1)	C(1)	46.7(4)
F(2)	B(1)	N(1)	C(1)	74.9(4)
N(2)	B(1)	N(1)	C(1)	166.5(3)
F(1)	B(1)	N(1)	C(4)	142.5(3)
F(2)	B(1)	N(1)	C(4)	95.9(3)
N(2)	B(1)	N(1)	C(4)	22.7(4)
F(1)	B(1)	N(2)	C(9)	42.1(4)
F(2)	B(1)	N(2)	C(9)	78.9(4)
N(1)	B(1)	N(2)	C(9)	162.0(3)
F(1)	B(1)	N(2)	C(6)	138.2(3)
F(2)	B(1)	N(2)	C(6)	100.8(3)
N(1)	B(1)	N(2)	C(6)	18.4(4)
F(3)	B(2)	N(3)	C(10)	61.9(4)
F(4)	B(2)	N(3)	C(10)	58.3(4)
N(4)	B(2)	N(3)	C(10)	179.0(3)
F(3)	B(2)	N(3)	C(13)	121.3(3)

F(4)	B(2)	N(3)	C(13)	118.4(3)
N(4)	B(2)	N(3)	C(13)	2.2(4)
F(3)	B(2)	N(4)	C(18)	54.3(4)
F(4)	B(2)	N(4)	C(18)	66.1(4)
N(3)	B(2)	N(4)	C(18)	173.8(3)
F(3)	B(2)	N(4)	C(15)	118.4(3)
F(4)	B(2)	N(4)	C(15)	121.2(3)
N(3)	B(2)	N(4)	C(15)	1.1(4)
C(4)	N(1)	C(1)	C(2)	0.5(4)
B(1)	N(1)	C(1)	C(2)	171.6(3)
N(1)	C(1)	C(2)	C(3)	0.5(4)
C(1)	C(2)	C(3)	C(4)	1.3(4)
C(1)	N(1)	C(4)	C(5)	173.4(3)
B(1)	N(1)	C(4)	C(5)	14.4(4)
C(1)	N(1)	C(4)	C(3)	1.3(3)
B(1)	N(1)	C(4)	C(3)	170.9(3)
C(2)	C(3)	C(4)	N(1)	1.6(4)
C(2)	C(3)	C(4)	C(5)	172.1(3)
N(1)	C(4)	C(5)	C(6)	2.3(4)
C(3)	C(4)	C(5)	C(6)	170.8(3)
N(1)	C(4)	C(5)	C(19)	178.8(3)
C(3)	C(4)	C(5)	C(19)	5.8(5)
C(9)	N(2)	C(6)	C(7)	0.4(4)
B(1)	N(2)	C(6)	C(7)	179.9(3)
C(9)	N(2)	C(6)	C(5)	174.5(3)
B(1)	N(2)	C(6)	C(5)	5.7(4)
C(4)	C(5)	C(6)	N(2)	6.4(4)
C(19)	C(5)	C(6)	N(2)	176.9(3)
C(4)	C(5)	C(6)	C(7)	166.1(3)
C(19)	C(5)	C(6)	C(7)	10.6(5)
N(2)	C(6)	C(7)	C(8)	0.1(4)
C(5)	C(6)	C(7)	C(8)	173.1(3)
C(6)	C(7)	C(8)	C(9)	0.6(4)
C(6)	N(2)	C(9)	C(8)	0.7(4)
B(1)	N(2)	C(9)	C(8)	179.6(3)
C(7)	C(8)	C(9)	N(2)	0.8(5)
C(13)	N(3)	C(10)	C(11)	0.6(4)
B(2)	N(3)	C(10)	C(11)	177.9(3)
N(3)	C(10)	C(11)	C(12)	0.6(4)
C(10)	C(11)	C(12)	C(13)	0.3(4)
C(10)	N(3)	C(13)	C(14)	178.3(3)
B(2)	N(3)	C(13)	C(14)	1.0(4)
C(10)	N(3)	C(13)	C(12)	0.4(3)
B(2)	N(3)	C(13)	C(12)	177.7(3)
C(11)	C(12)	C(13)	N(3)	0.0(4)

C(11)	C(12)	C(13)	C(14)	178.5(3)
N(3)	C(13)	C(14)	C(15)	3.6(4)
C(12)	C(13)	C(14)	C(15)	178.1(3)
N(3)	C(13)	C(14)	C(27)	175.9(3)
C(12)	C(13)	C(14)	C(27)	2.4(5)
C(18)	N(4)	C(15)	C(16)	1.2(3)
B(2)	N(4)	C(15)	C(16)	172.5(3)
C(18)	N(4)	C(15)	C(14)	179.4(3)
B(2)	N(4)	C(15)	C(14)	5.6(4)
C(13)	C(14)	C(15)	N(4)	6.7(4)
C(27)	C(14)	C(15)	N(4)	172.8(3)
C(13)	C(14)	C(15)	C(16)	170.9(3)
C(27)	C(14)	C(15)	C(16)	9.6(5)
N(4)	C(15)	C(16)	C(17)	1.6(4)
C(14)	C(15)	C(16)	C(17)	179.5(3)
C(15)	C(16)	C(17)	C(18)	1.4(4)
C(15)	N(4)	C(18)	C(17)	0.4(4)
B(2)	N(4)	C(18)	C(17)	173.4(3)
C(16)	C(17)	C(18)	N(4)	0.6(4)
C(4)	C(5)	C(19)	C(20)	35.7(5)
C(6)	C(5)	C(19)	C(20)	140.9(3)
C(4)	C(5)	C(19)	C(23)	147.1(3)
C(6)	C(5)	C(19)	C(23)	36.3(4)
C(4)	C(5)	C(19)	Fe(1)	56.2(4)
C(6)	C(5)	C(19)	Fe(1)	127.2(3)
C(23)	C(19)	C(20)	C(21)	1.2(4)
C(5)	C(19)	C(20)	C(21)	176.4(3)
Fe(1)	C(19)	C(20)	C(21)	60.3(2)
C(23)	C(19)	C(20)	Fe(1)	59.1(2)
C(5)	C(19)	C(20)	Fe(1)	123.2(3)
C(19)	C(20)	C(21)	C(22)	1.2(4)
Fe(1)	C(20)	C(21)	C(22)	59.1(2)
C(19)	C(20)	C(21)	Fe(1)	60.3(2)
C(20)	C(21)	C(22)	C(23)	0.7(4)
Fe(1)	C(21)	C(22)	C(23)	59.4(2)
C(20)	C(21)	C(22)	Fe(1)	58.6(2)
C(21)	C(22)	C(23)	C(19)	0.0(4)
Fe(1)	C(22)	C(23)	C(19)	59.7(2)
C(21)	C(22)	C(23)	Fe(1)	59.7(2)
C(20)	C(19)	C(23)	C(22)	0.8(4)
C(5)	C(19)	C(23)	C(22)	176.9(3)
Fe(1)	C(19)	C(23)	C(22)	59.8(2)
C(20)	C(19)	C(23)	Fe(1)	59.0(2)
C(5)	C(19)	C(23)	Fe(1)	123.3(3)
C(28)	C(24)	C(25)	C(26)	0.9(4)

Fe(1)	C(24)	C(25)	C(26)	59.4(2)
C(28)	C(24)	C(25)	Fe(1)	58.5(2)
C(24)	C(25)	C(26)	C(27)	0.4(4)
Fe(1)	C(25)	C(26)	C(27)	60.3(2)
C(24)	C(25)	C(26)	Fe(1)	60.0(2)
C(25)	C(26)	C(27)	C(28)	1.4(4)
Fe(1)	C(26)	C(27)	C(28)	58.6(2)
C(25)	C(26)	C(27)	C(14)	177.2(3)
Fe(1)	C(26)	C(27)	C(14)	122.8(3)
C(25)	C(26)	C(27)	Fe(1)	60.0(2)
C(13)	C(14)	C(27)	C(26)	146.0(3)
C(15)	C(14)	C(27)	C(26)	33.5(4)
C(13)	C(14)	C(27)	C(28)	35.7(5)
C(15)	C(14)	C(27)	C(28)	144.8(3)
C(13)	C(14)	C(27)	Fe(1)	56.5(4)
C(15)	C(14)	C(27)	Fe(1)	123.0(3)
C(25)	C(24)	C(28)	C(27)	1.8(4)
Fe(1)	C(24)	C(28)	C(27)	60.3(2)
C(25)	C(24)	C(28)	Fe(1)	58.5(2)
C(26)	C(27)	C(28)	C(24)	2.0(4)
C(14)	C(27)	C(28)	C(24)	176.6(3)
Fe(1)	C(27)	C(28)	C(24)	60.4(2)
C(26)	C(27)	C(28)	Fe(1)	58.4(2)
C(14)	C(27)	C(28)	Fe(1)	123.1(3)

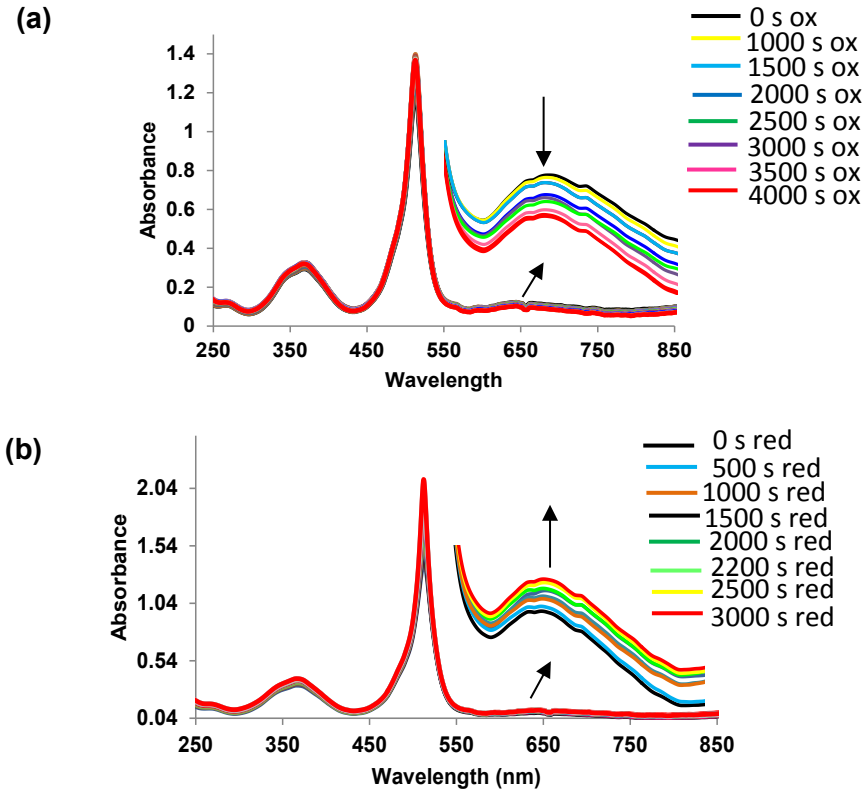

Fig. S22. Spectroelectrochemistry of **8** was performed in DCM by recording time dependent absorption changes in the UV-visible absorption spectra of **8** (1 x 10^{-5} M) upon varying the potential: oxidation (a, 1.2 V) as well as reduction (b, 1.0 V).

Table S14**.** Effect of change of solvent polarity on the low energy absorption band of **7** and **8**.

Compounds	**Hexane**	**Toluene**	**THF**	**DCM**	**Methanol**	**DMF**	**DMSO**
7	646 nm	678 nm	694 nm	698 nm	700 nm	710 nm	710 nm
8	--	--	656 nm	666 nm	688 nm	690 nm	692 nm

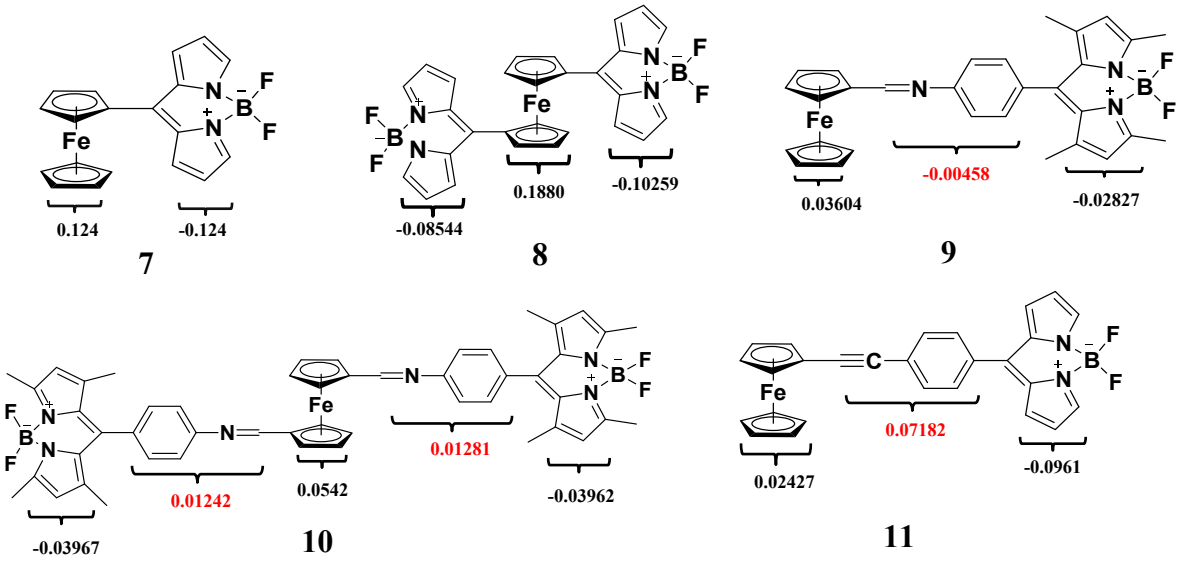

Fig. S23. The estimated Natural Bond Orbital (NBO) charge distribution.

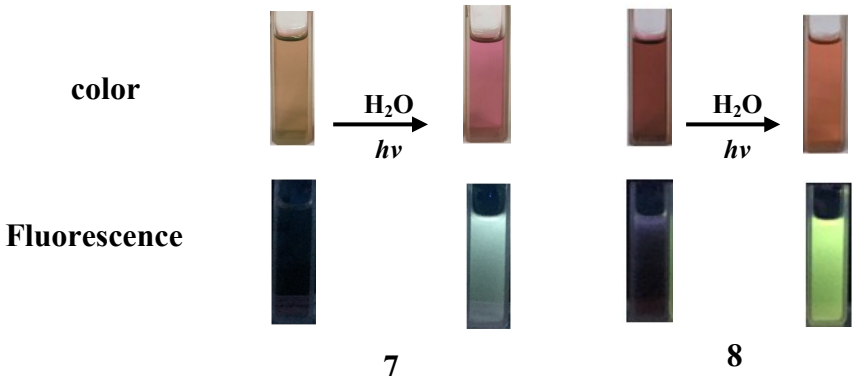

Fig. S24. Color and fluorescence changes of **7** and **8** upon reacting with water.

Complete reference 71.

Gaussian 09, Revision B.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.