

Carborane Bridged Ferrocenyl Conjugated Molecules: Synthesis, Structure, Electrochemistry and Photophysics Properties

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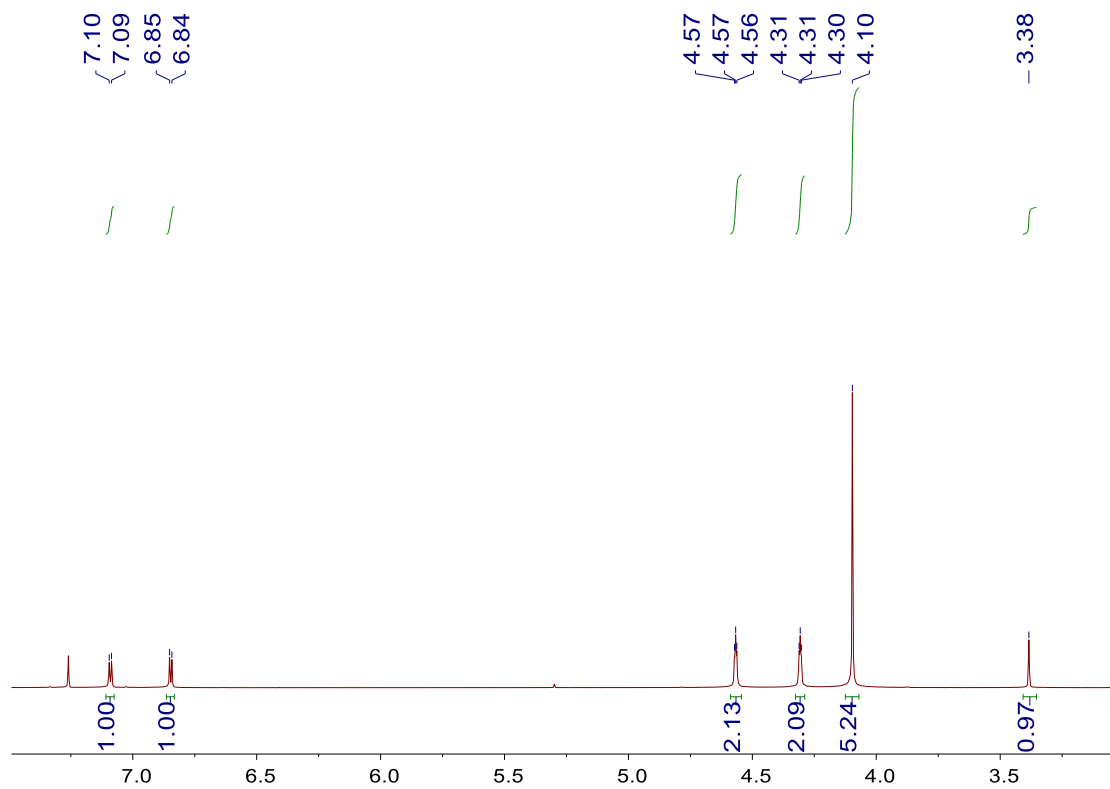


Figure S1. ^1H NMR spectrum of **3** (CDCl_3)

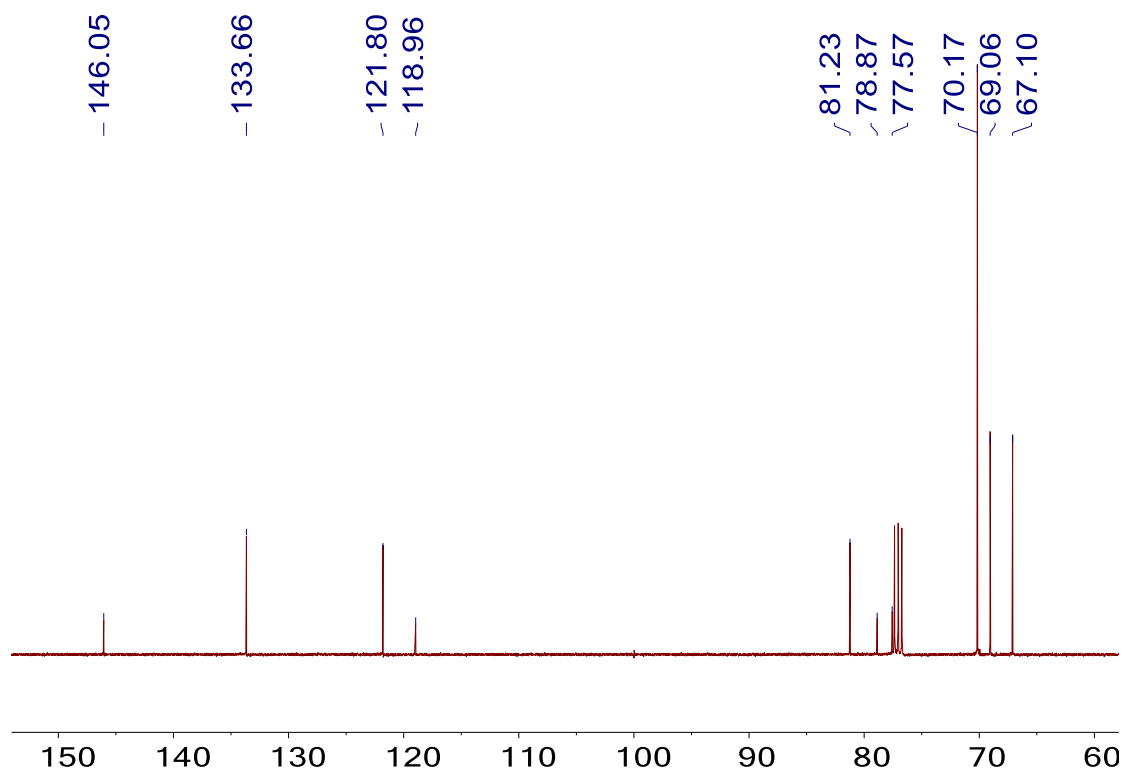


Figure S2. ^{13}C NMR spectrum of **3** (CDCl_3)

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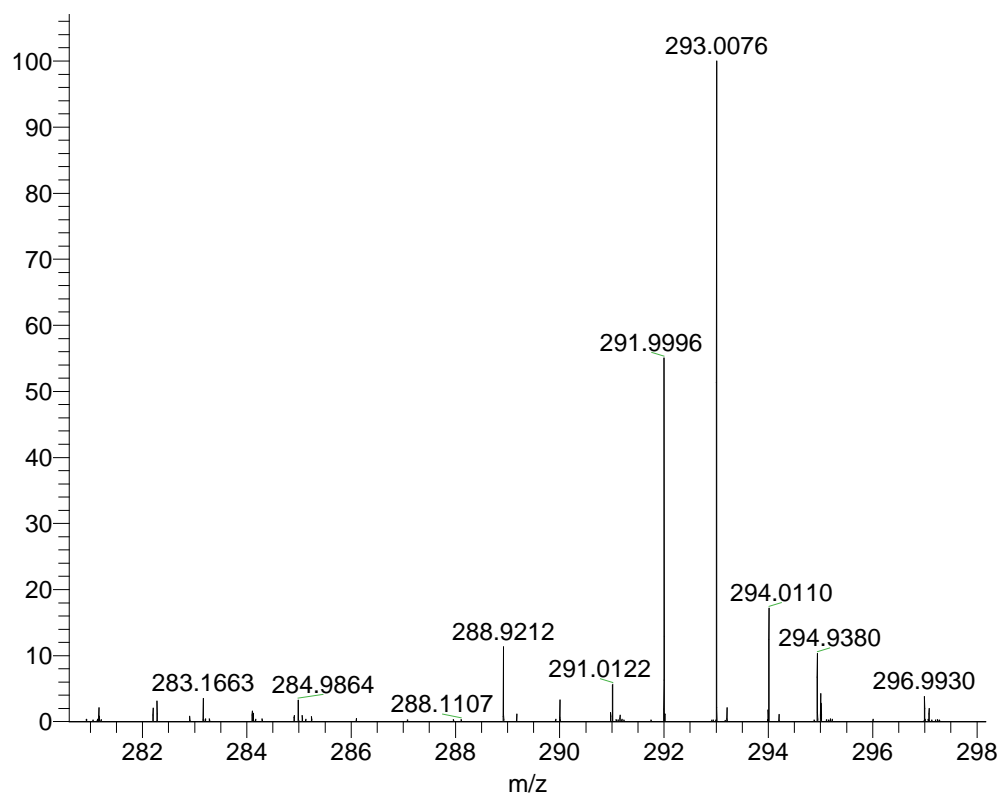


Figure S3. HRMS spectrum of **3**

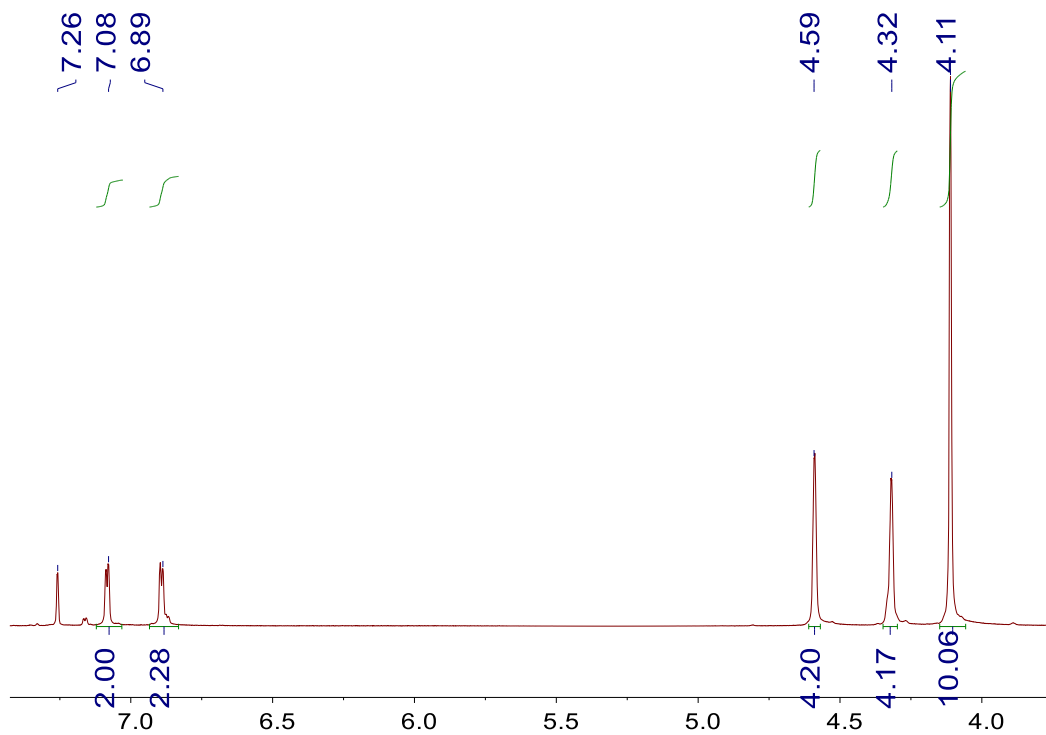


Figure S4. ¹H NMR spectrum of **5** (CDCl₃)

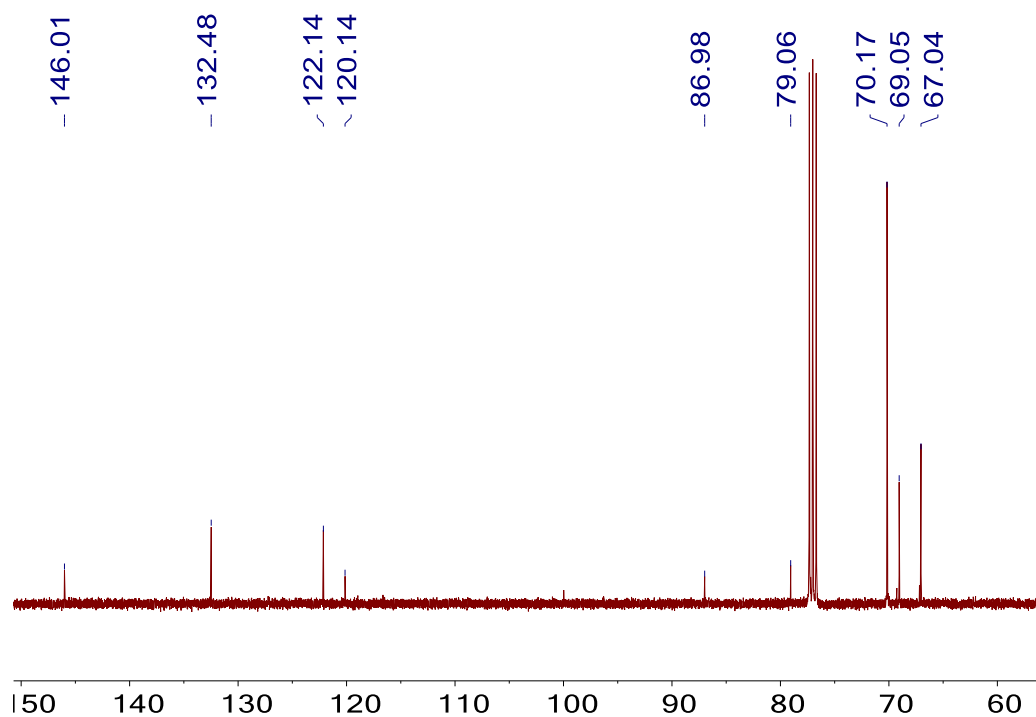


Figure S5. ^{13}C NMR spectrum of **5** (CDCl_3)

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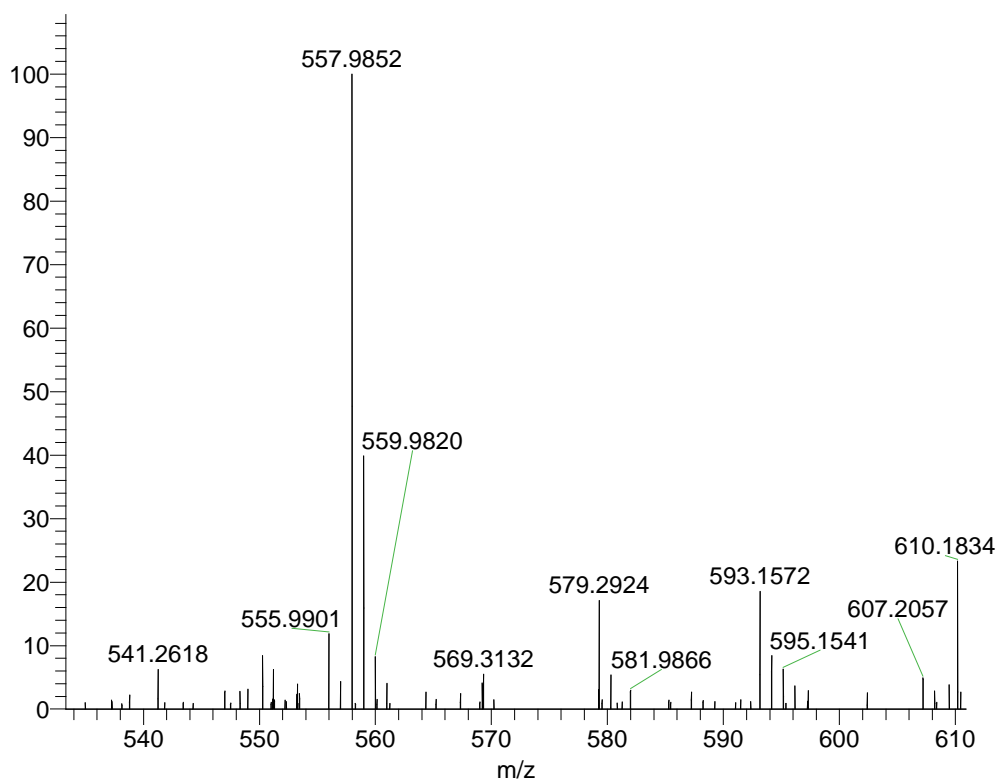


Figure S6. HRMS spectrum of **5**

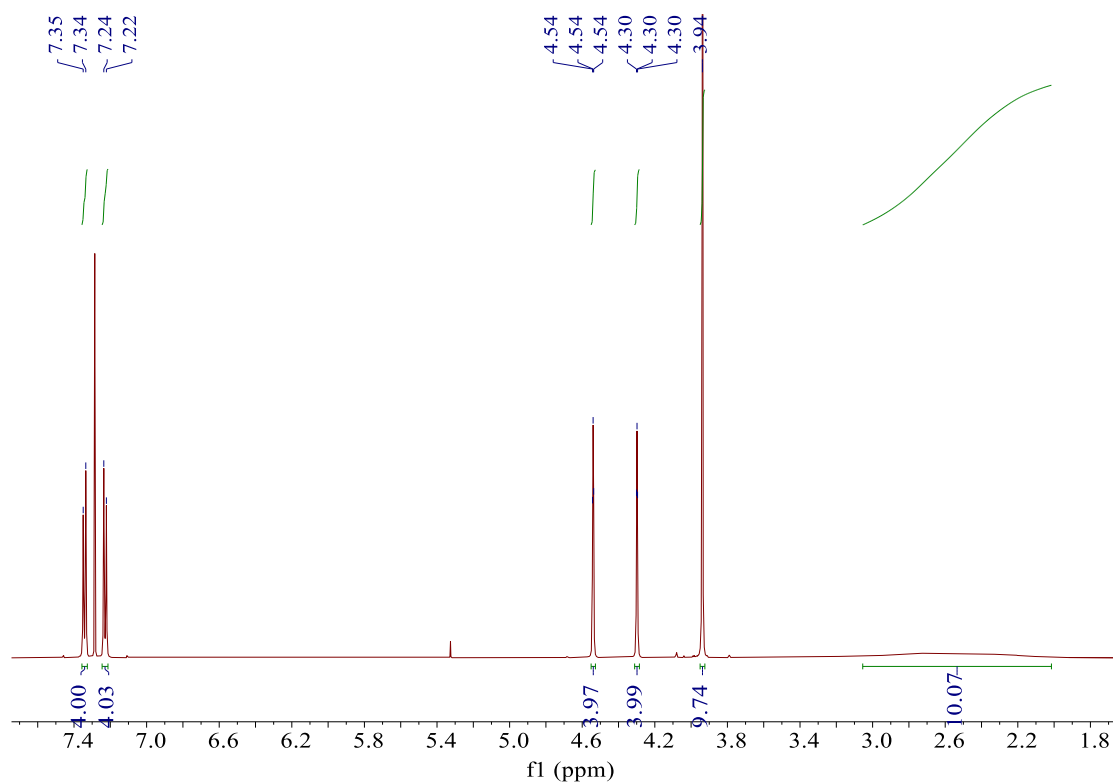


Figure S7. ^1H NMR spectrum of **8** (CDCl_3)

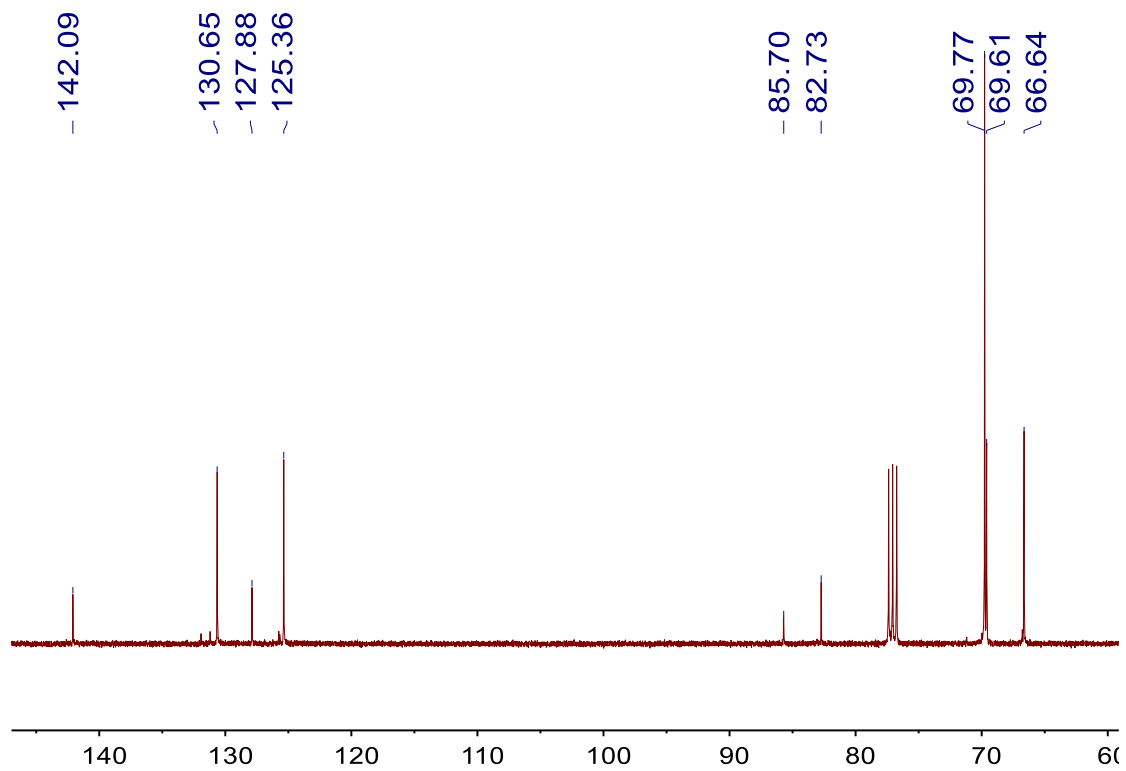


Figure S8. ^{13}C NMR spectrum of **8** (CDCl_3)

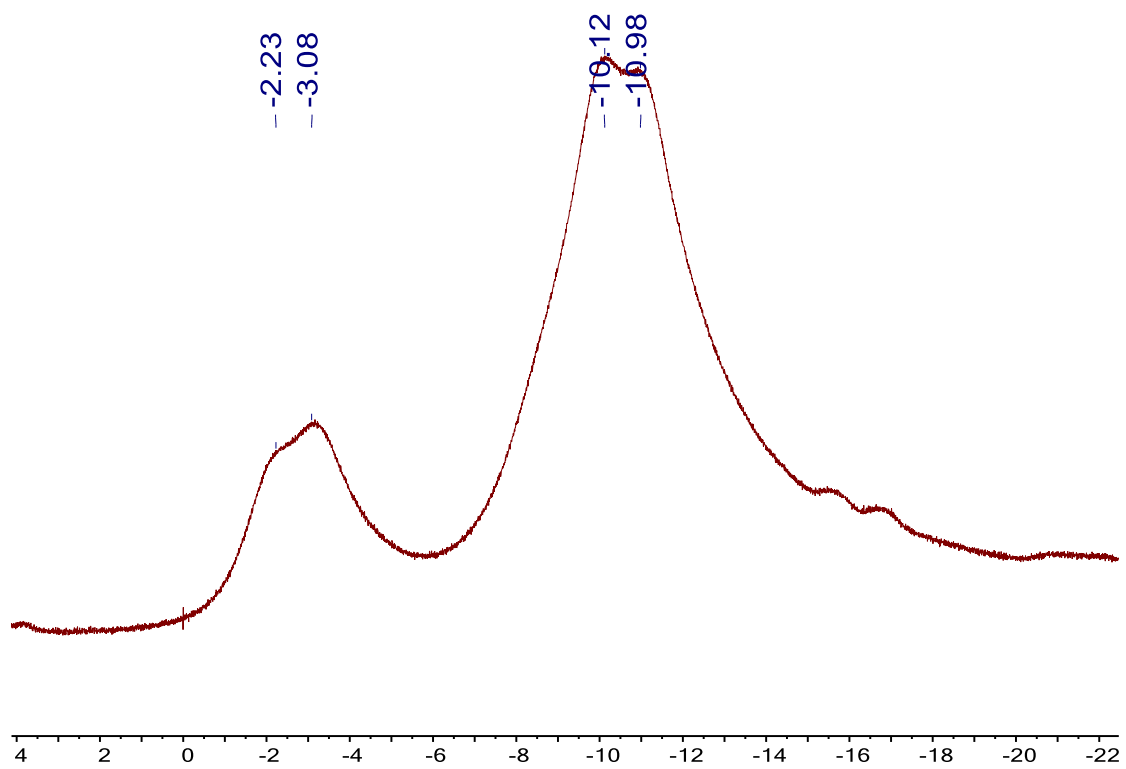


Figure S9. ^{11}B NMR spectrum of **8** (CDCl_3)

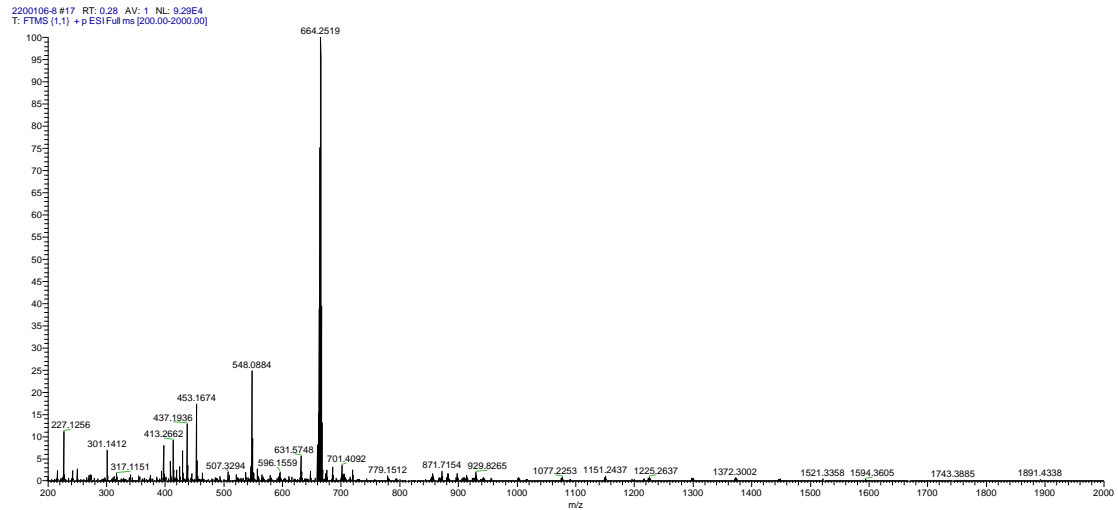


Figure S10. HRMS spectrum of **8**

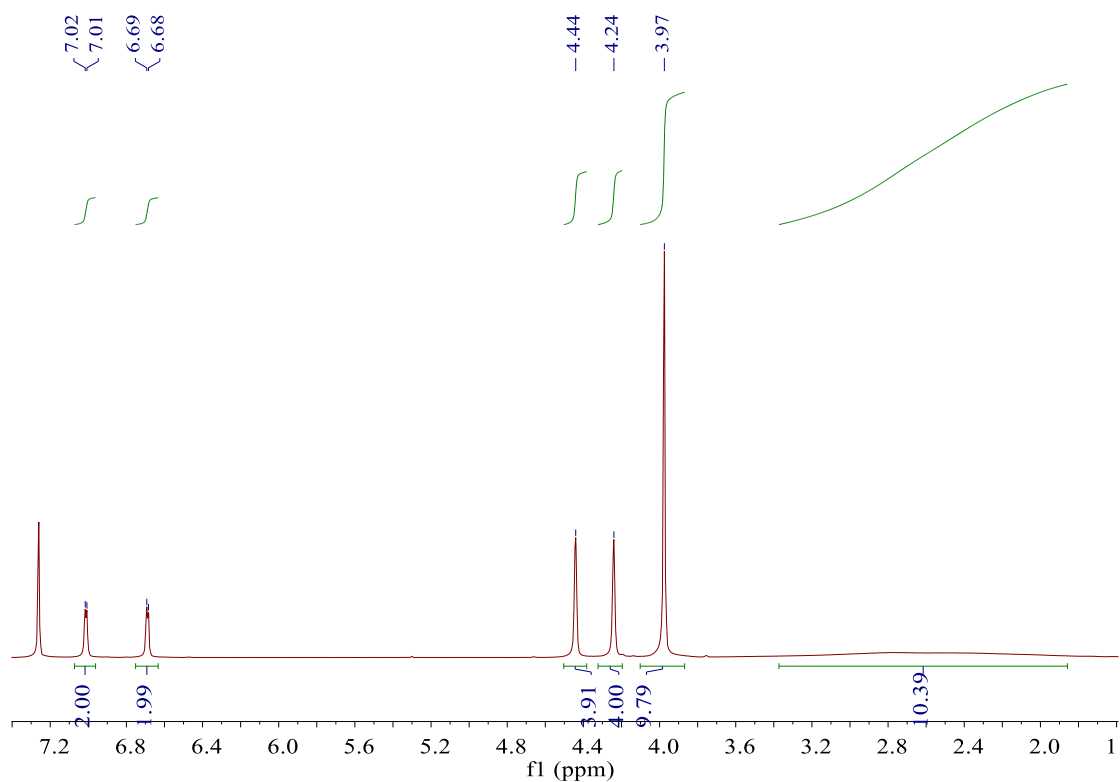


Figure S11. ^1H NMR spectrum of **9** (CDCl_3)

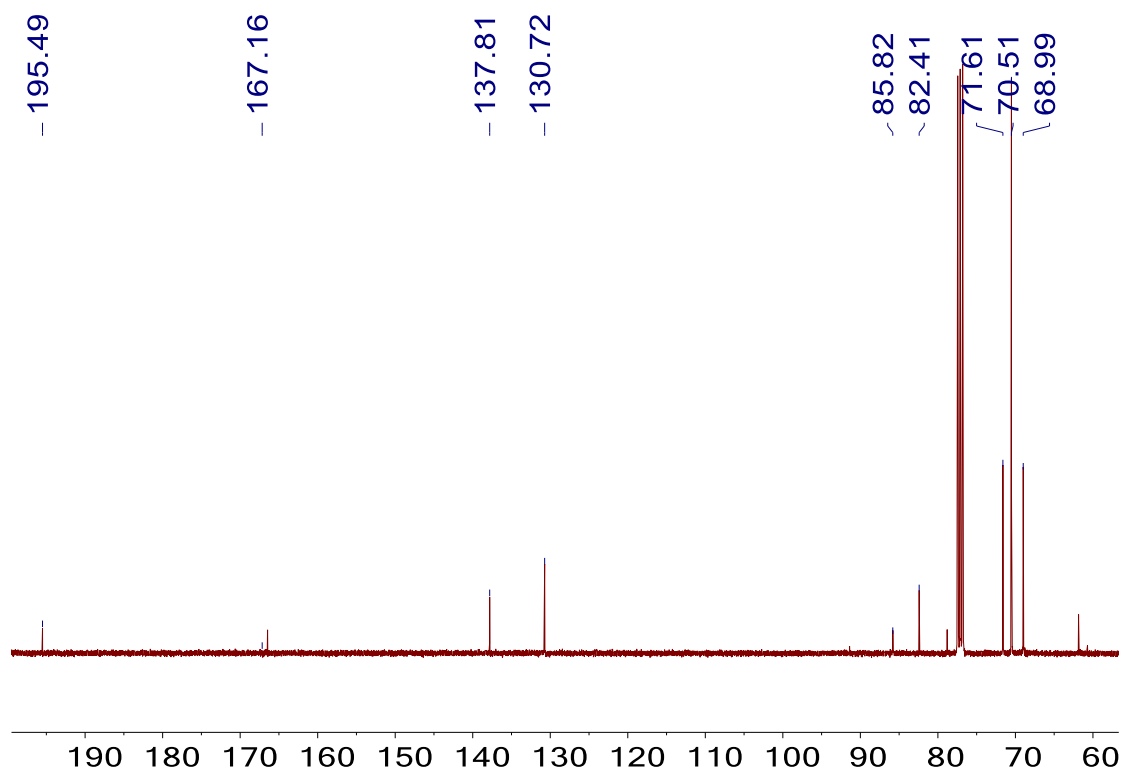


Figure S12. ^{13}C NMR spectrum of **9** (CDCl_3)

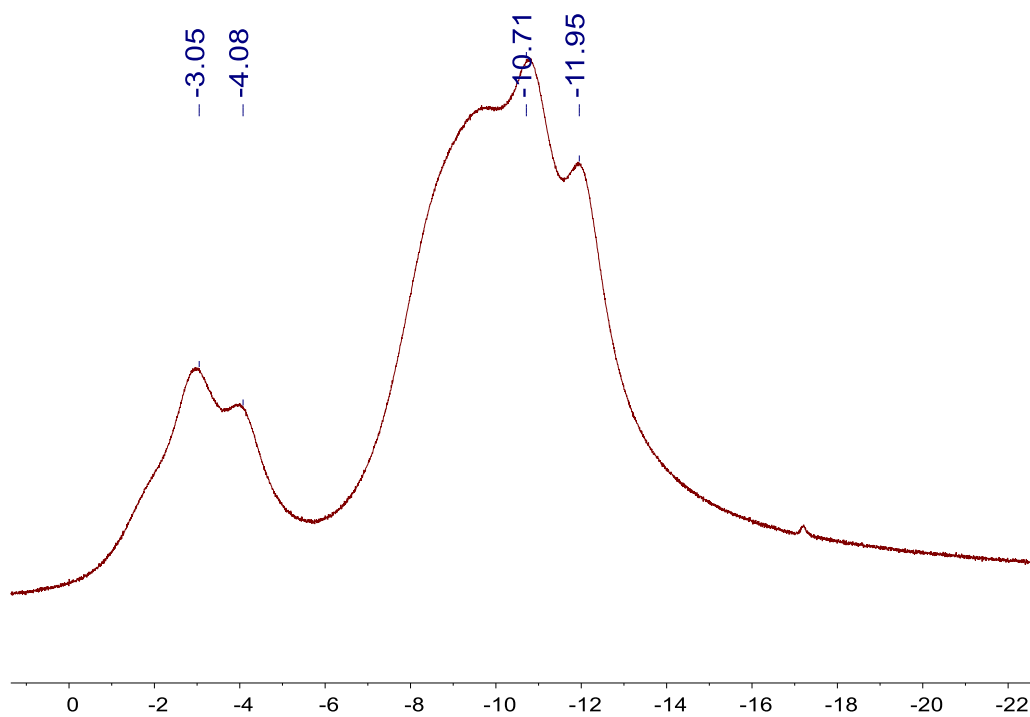


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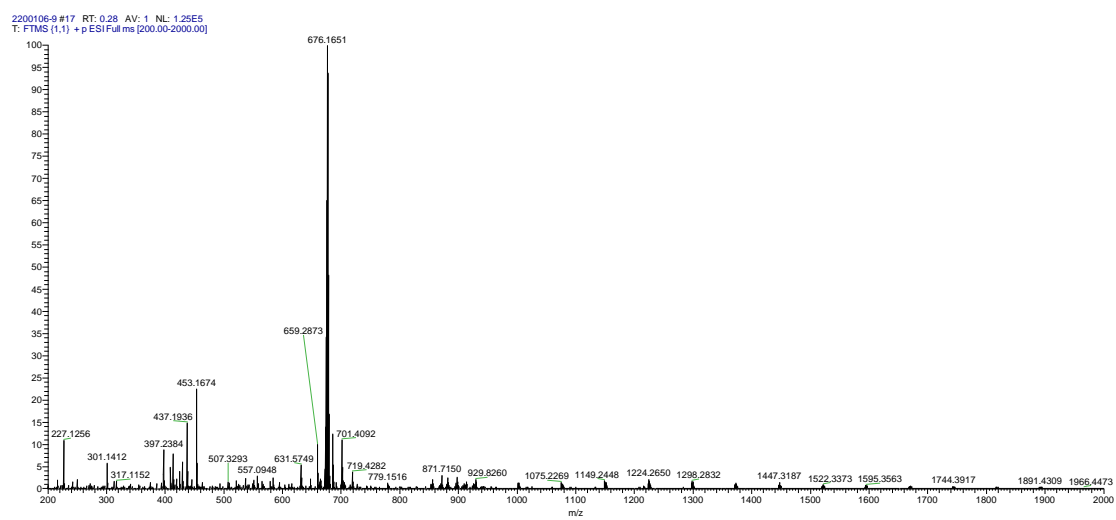


Figure S14. HRMS spectrum of **9**

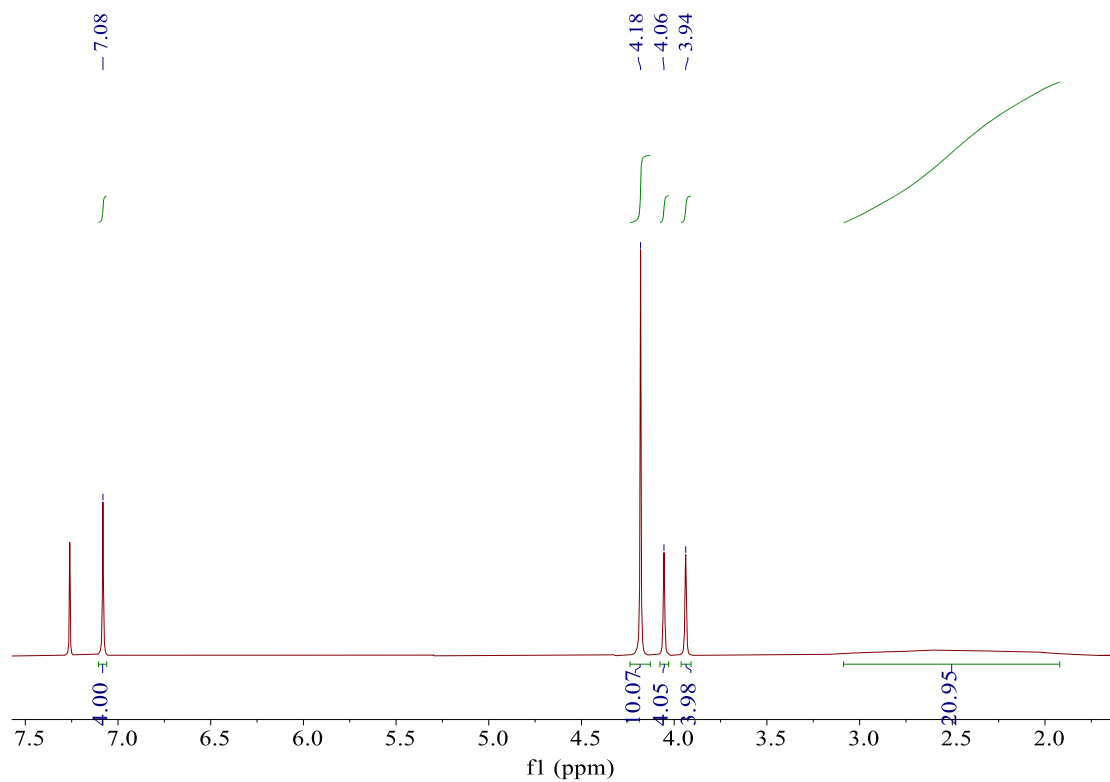


Figure S15. ^1H NMR spectrum of **10** (CDCl_3)

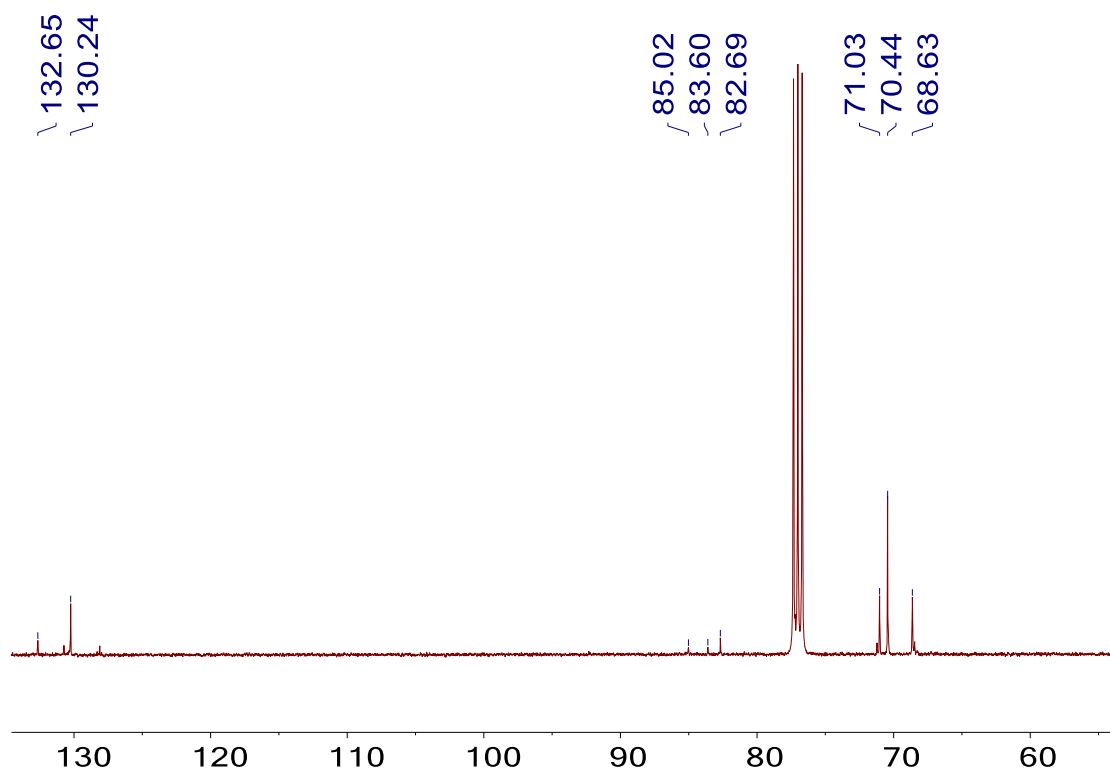


Figure S16. ^{13}C NMR spectrum of **10** (CDCl_3)

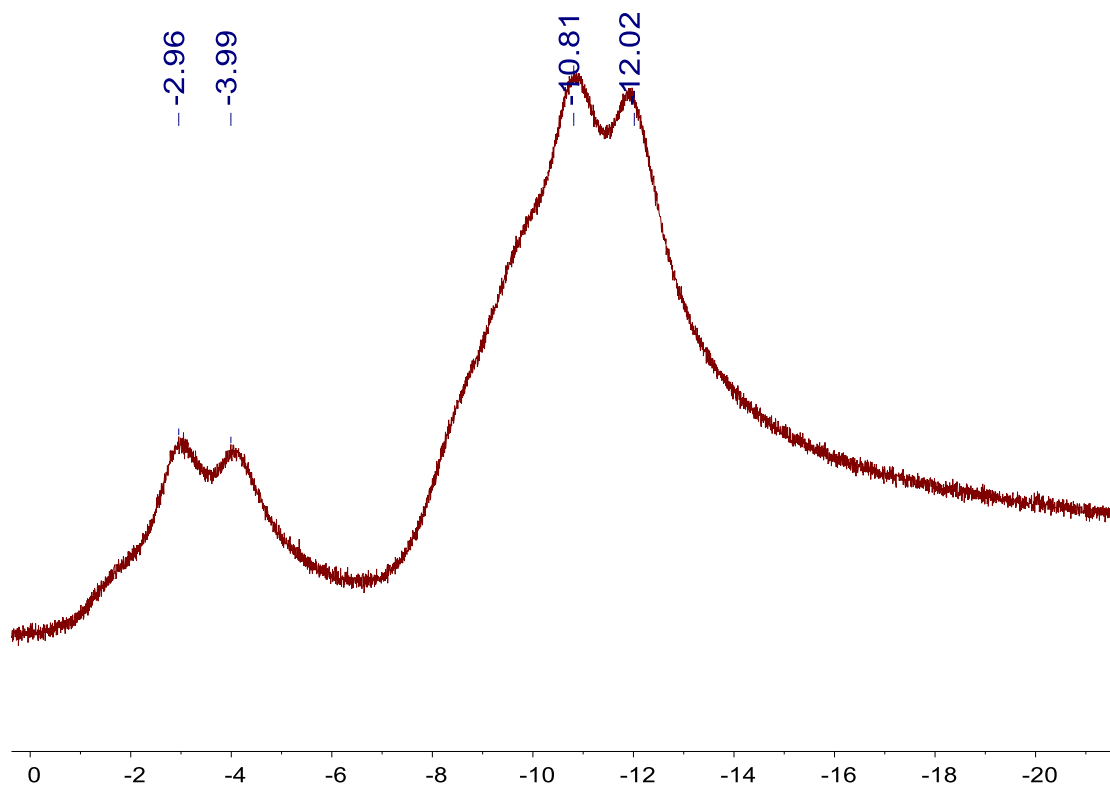


Figure S17. ^{11}B NMR spectrum of **10** (CDCl_3)

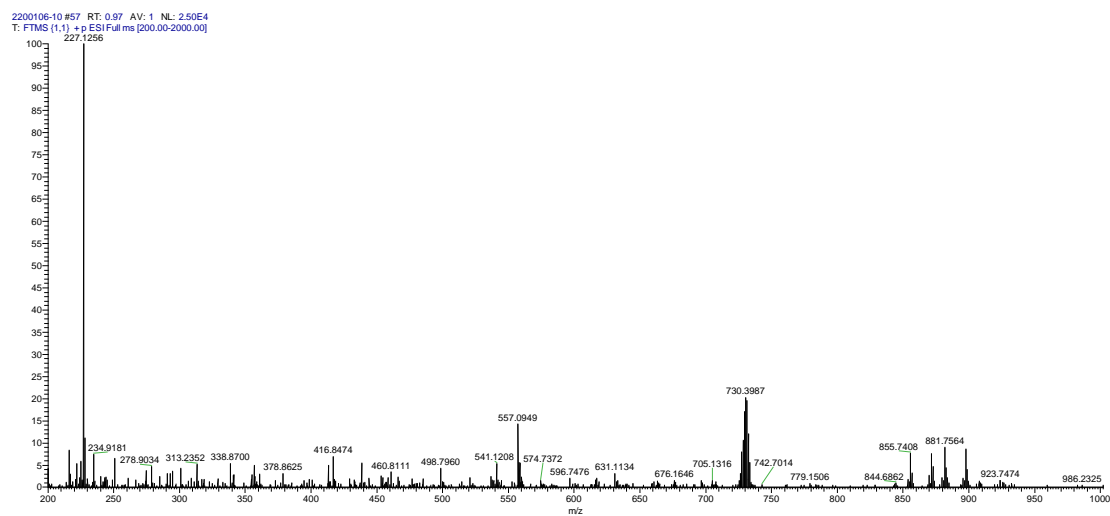


Figure S18. HRMS spectrum of **10**

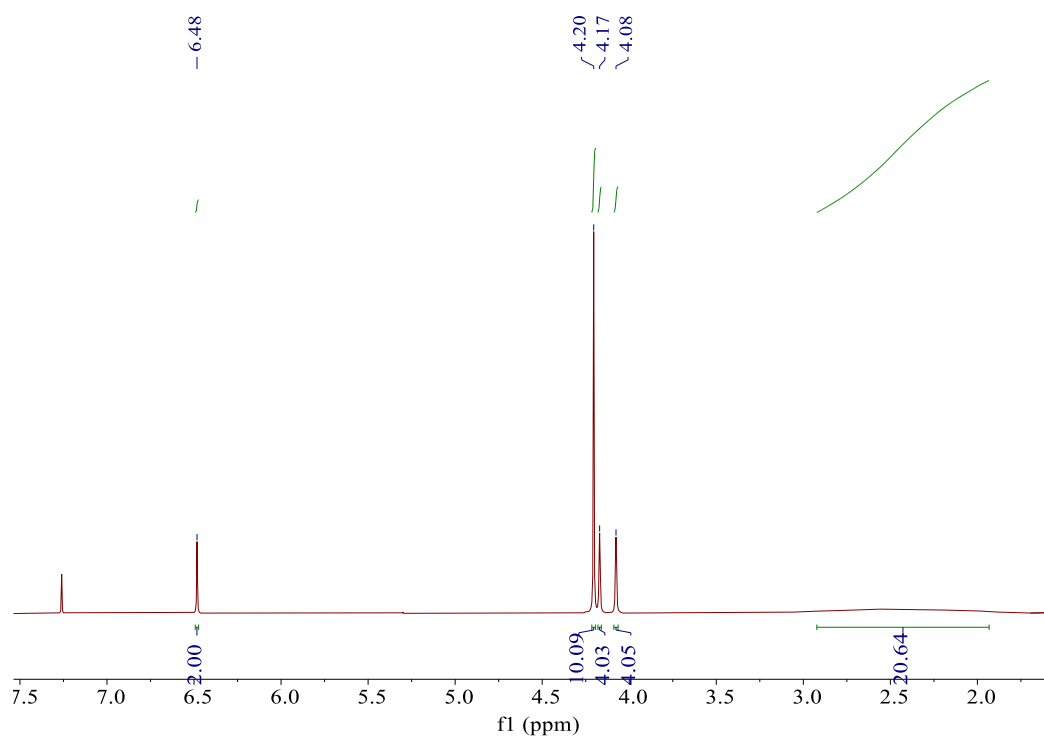


Figure S19. ^1H NMR spectrum of **11** (CDCl_3)

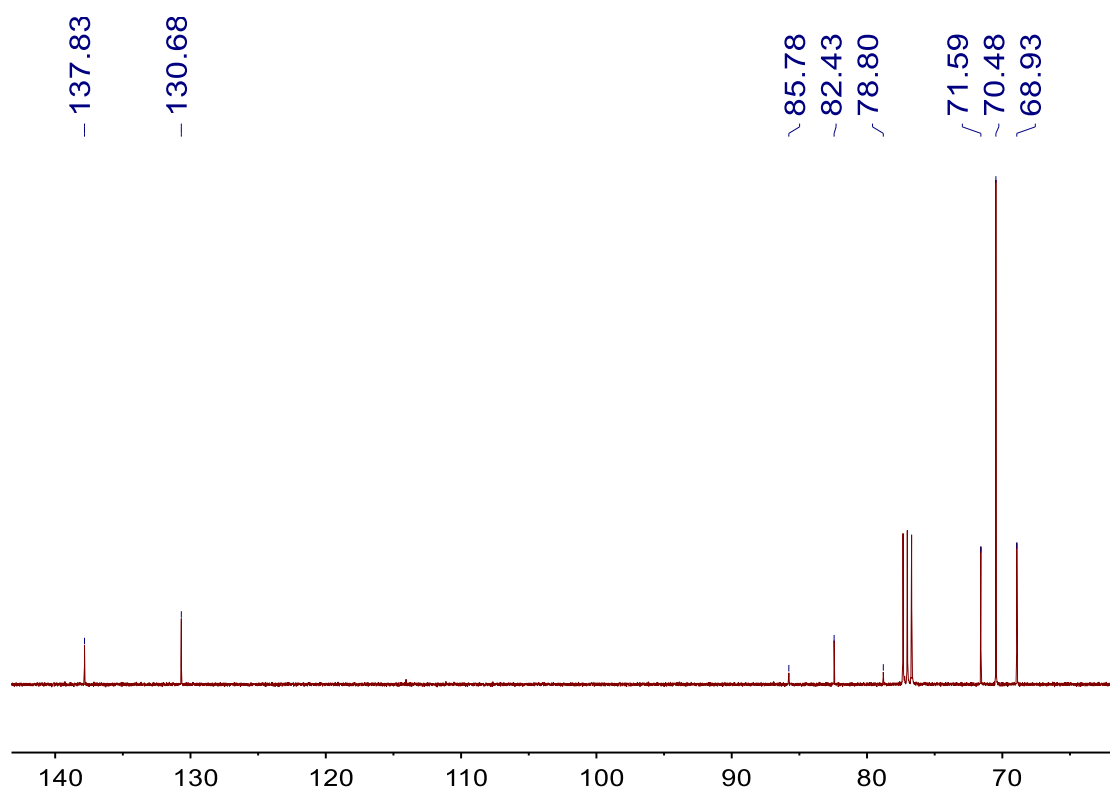


Figure S20. ^{13}C NMR spectrum of **11** (CDCl_3)

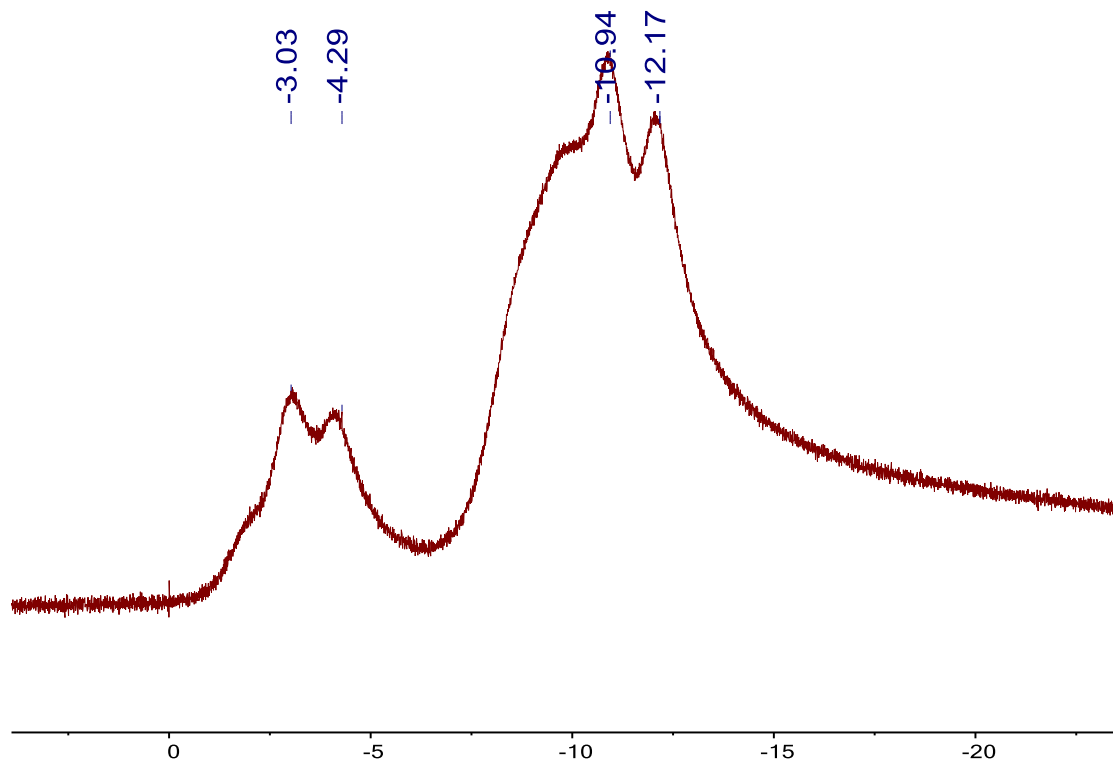


Figure S21. ^{11}B NMR spectrum of **11** (CDCl_3)

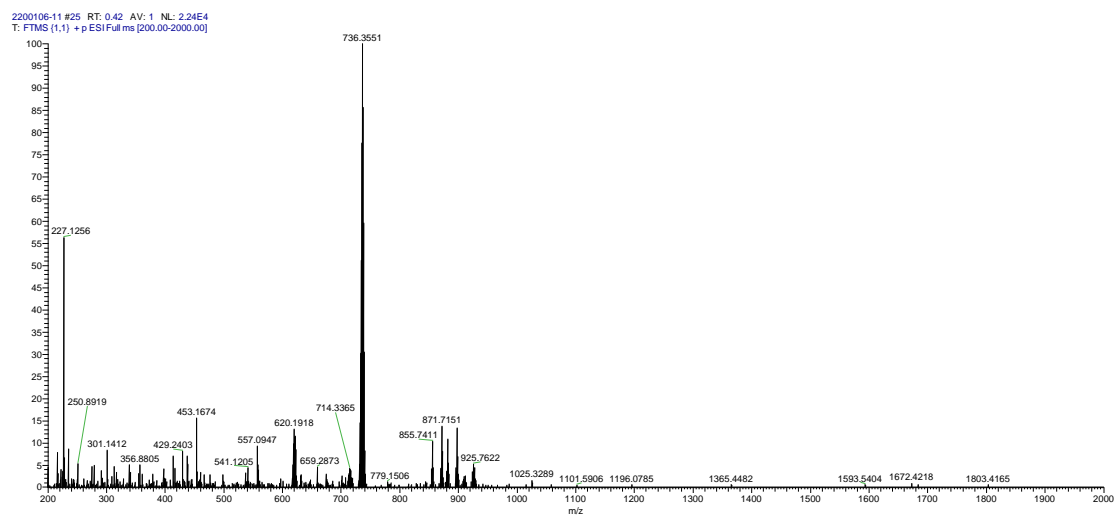
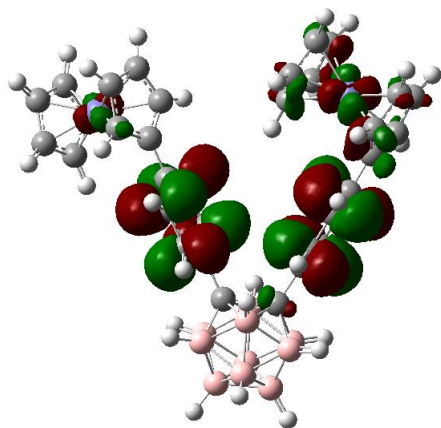
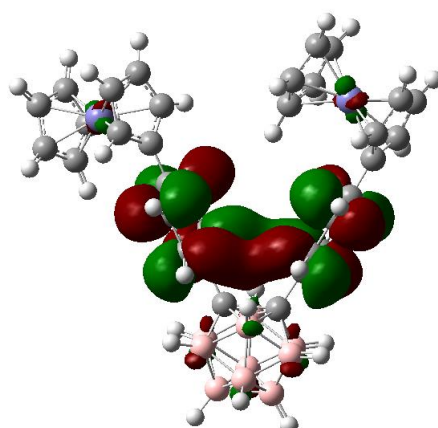


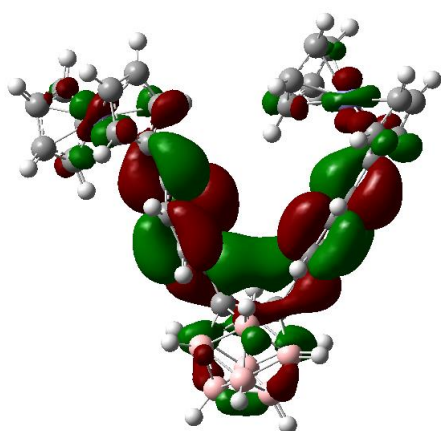
Figure S22. HRMS spectrum of **11**



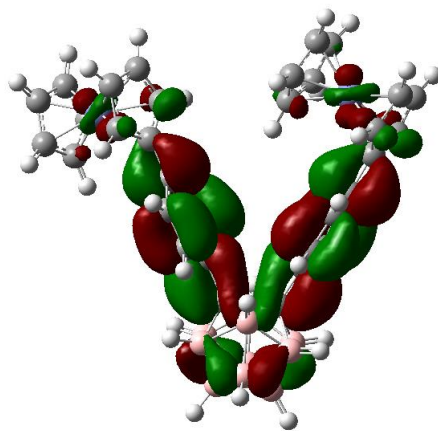
LUMO+4



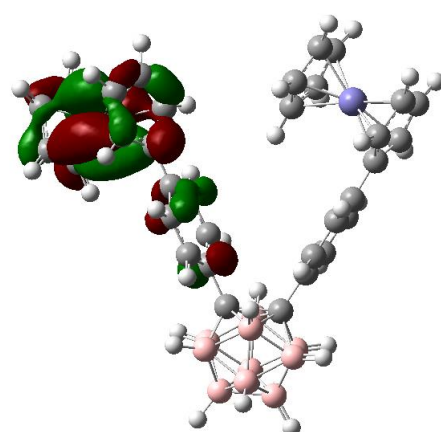
LUMO+2



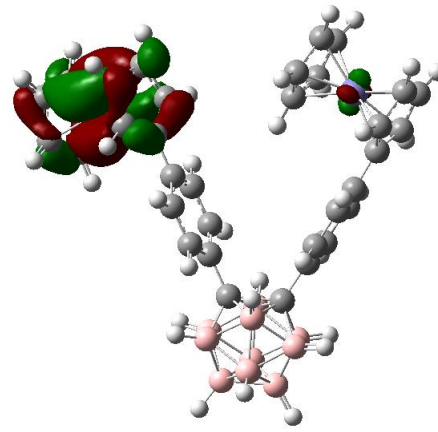
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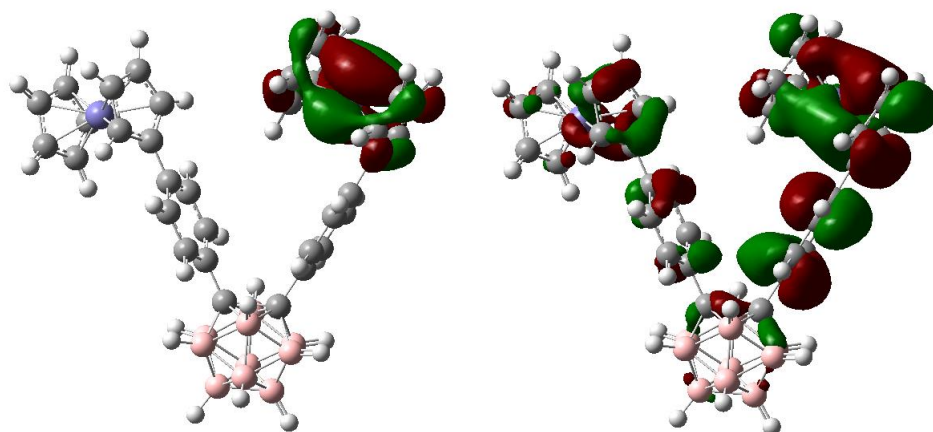
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HOMO

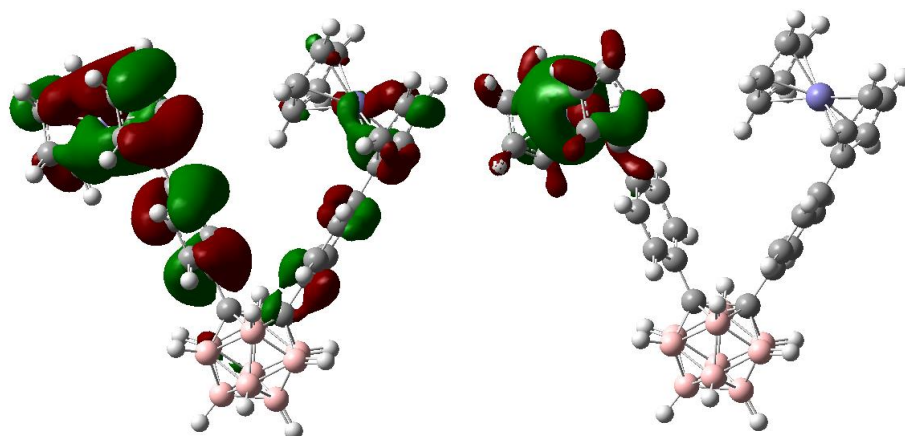


HOMO-2



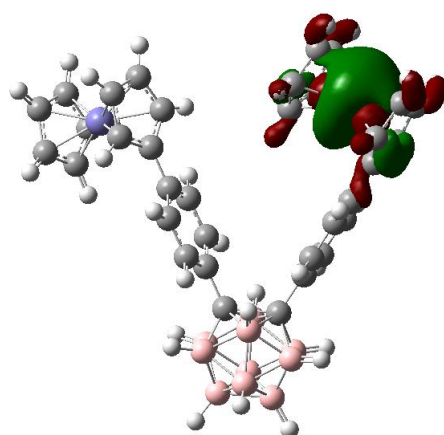
HOMO-3

HOMO-4



HOMO-5

HOMO-6



HOMO-7

Figure S23. Frontier molecular orbital distributions related to electron transitions in the absorption spectra for **8**.

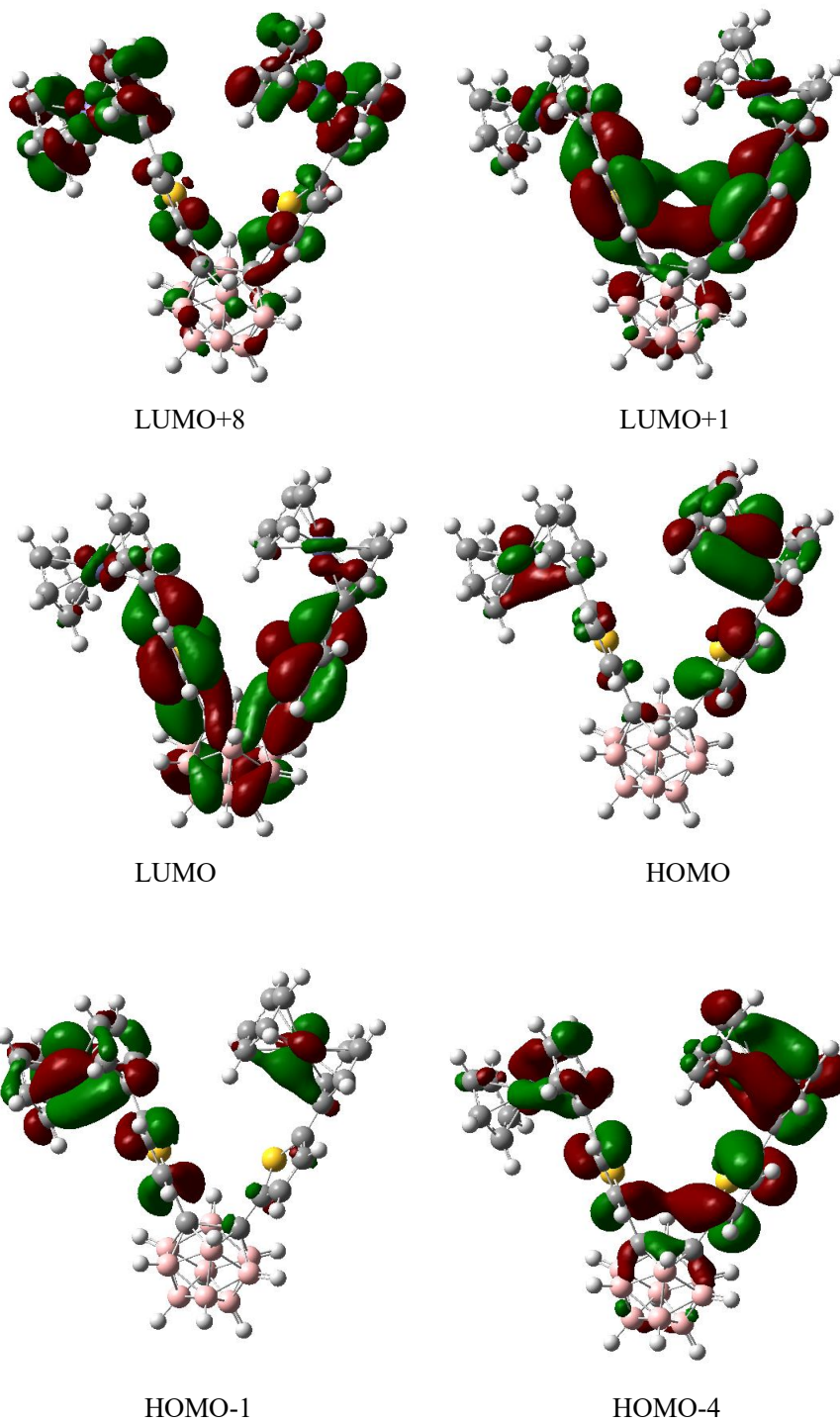


Figure S24. Frontier molecular orbital distributions related to electron transitions in the absorption spectra for **9**

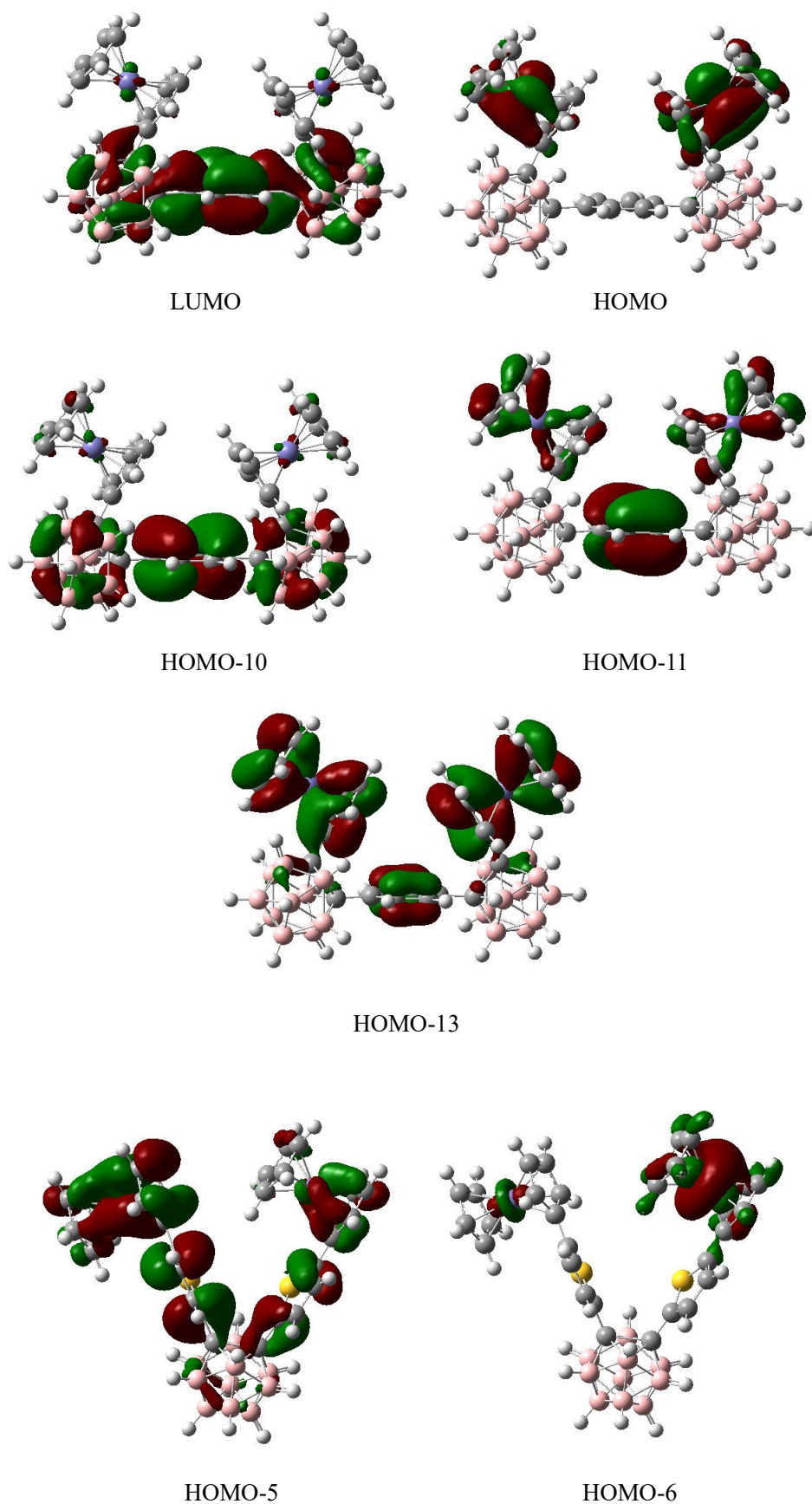
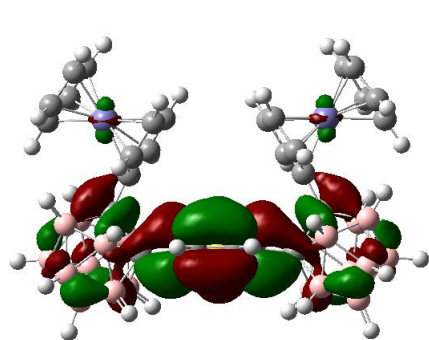
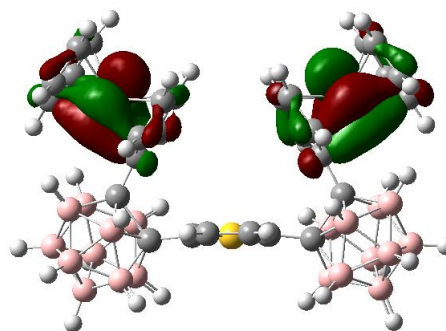


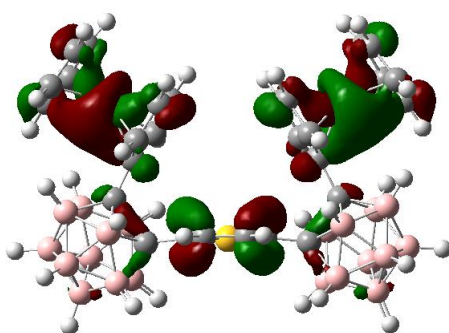
Figure S25. Frontier molecular orbital distributions related to electron transitions in the absorption spectra for **10**.



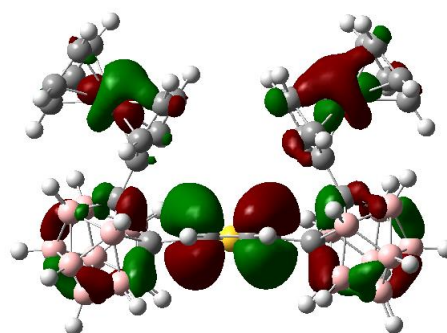
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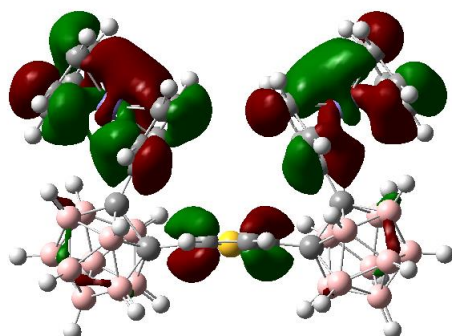
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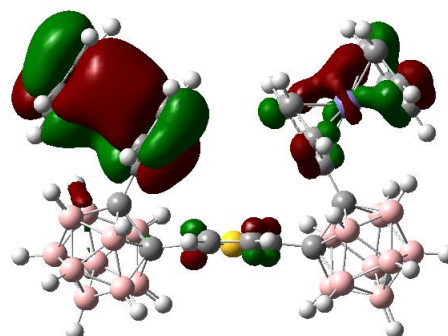
HOMO-4



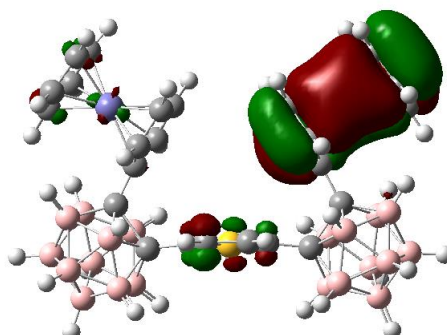
HOMO-6



HOMO-7



HOMO-8



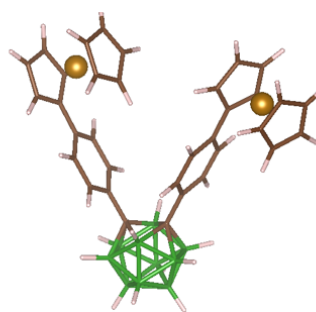
HOMO-9

Figure S26. Frontier molecular orbital distributions related to electron transitions in the absorption spectra for **11**

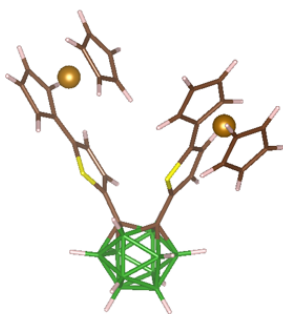
Table S1. Cartesian coordinates and energies for optimized structures of **8**

Energy: -1813.86004343 a.u.

Fe	2.08692	4.16156	-0.1181
C	3.61205	2.77775	0.22819
C	3.96218	3.66408	-0.84857
C	3.62653	4.95993	1.03025
C	3.97697	4.99888	-0.35227
C	3.39703	3.60066	1.38749
C	0.14344	3.94641	0.59063
C	0.72116	5.31329	-1.18036
C	0.37755	5.30114	0.20533
C	0.34238	3.12061	-0.55691
C	0.69935	3.96528	-1.65173
C	3.47924	1.31215	0.15779
H	4.18131	3.37351	-1.8664
H	3.52012	5.81396	1.6851
H	4.19122	5.88717	-0.93085
H	3.08307	3.25478	2.36225
H	-0.11473	3.6017	1.58265
H	0.98035	6.18691	-1.7632
H	0.3323	6.16419	0.8558
H	0.27473	2.04108	-0.57949
H	0.93866	3.64015	-2.65523
C	3.46122	0.63257	-1.07298
C	3.37617	0.53438	1.32297
H	3.55962	1.18897	-1.99939
C	3.29721	-0.74576	-1.13551
C	3.20718	-0.84504	1.26286
H	3.43224	1.01125	2.2959
C	3.14106	-1.5118	0.03106
H	3.29043	-1.23017	-2.10464
H	3.13152	-1.40368	2.1874
C	2.93773	-2.9994	-0.05133
B	2.37787	-3.84848	1.33741
B	4.00161	-4.12184	0.67436
B	2.16813	-3.62629	-1.46785
B	3.86823	-3.9777	-1.08959
C	1.29074	-3.62962	0.0109
B	3.00051	-5.49307	1.19213
B	1.30787	-5.15207	0.77729
H	2.16937	-3.24994	2.3298
C	-4.48163	1.95701	0.70945
C	-5.37033	-0.40823	-1.96665
C	-6.99666	-0.45813	-0.32697
H	-2.77369	1.66488	-0.70073
H	-4.23601	-0.80197	2.59586
H	-6.86386	1.25194	-1.76904
H	-5.81553	1.36737	2.41154
H	-4.40657	-2.3331	-1.34267
H	-6.31107	-2.39664	0.56651
H	-4.91775	2.8846	0.36451
H	-4.75481	-0.08383	-2.79483
H	-7.82624	-0.17684	0.30759



B	3.92457	-5.58508	-0.33359
H	4.92762	-3.67306	1.25805
B	2.79191	-5.2634	-1.67739
B	1.17645	-5.01551	-0.98481
H	1.85728	-2.88022	-2.32339
H	4.7059	-3.43556	-1.72522
C	0.15479	-2.66303	0.2115
B	2.26766	-6.22113	-0.26539
H	3.27328	-6.11259	2.16552
H	0.36942	-5.43235	1.44016
H	4.87915	-6.27686	-0.46148
H	2.92378	-5.71239	-2.76676
H	0.14537	-5.18377	-1.53992
C	-0.48427	-2.57643	1.45781
C	-0.3177	-1.84161	-0.82414
H	2.01452	-7.37742	-0.33669
H	-0.15259	-3.20071	2.27904
C	-1.54204	-1.69665	1.66414
C	-1.37394	-0.96141	-0.6151
H	0.13443	-1.89174	-1.80642
C	-2.0112	-0.86508	0.63437
H	-1.99697	-1.64119	2.64804
H	-1.7244	-0.35268	-1.44271
C	-3.10792	0.09027	0.86951
Fe	-5.01765	0.06866	0.02483
C	-3.35521	1.30138	0.13517
C	-4.11303	0.0107	1.89294
C	-6.4875	0.29788	-1.42556
C	-4.95238	1.15809	1.79438
C	-5.18984	-1.60032	-1.20198
C	-6.19475	-1.63143	-0.18906

Table S2. Cartesian coordinates and energies for optimized structures of **9**

Energy: -2455.36440695 a.u.

Fe	3.09261	3.28098	-0.14052	B	1.24552	-5.94122	0.91232
C	4.13686	1.47456	-0.25106	B	-0.28225	-5.04899	0.80333
C	4.01321	2.07236	-1.55253	H	1.33408	-3.74928	2.41448
C	5.15131	3.56198	-0.20685	B	1.92754	-6.06897	-0.73696
C	4.64302	3.34921	-1.52342	H	3.65846	-4.86819	0.91834
C	4.83393	2.41846	0.58052	B	0.83829	-5.18217	-1.84554
C	1.90787	3.81898	1.4799	B	-0.53164	-4.57731	-0.8924
C	1.73349	4.78026	-0.61335	H	0.67529	-2.52952	-1.99765
C	2.23814	4.97437	0.70786	H	3.2329	-4.07395	-1.96676
C	1.19783	2.91241	0.63677	C	-0.61252	-2.28571	0.7039
C	1.09131	3.50558	-0.65705	B	0.17422	-6.16253	-0.50437
C	3.66537	0.15772	0.16113	H	1.40363	-6.76682	1.74836
H	3.52532	1.62626	-2.40883	H	-1.18386	-5.12869	1.56464
H	5.65949	4.44986	0.14356	H	2.58032	-6.99465	-1.08749
H	4.70079	4.04514	-2.3491	H	0.69784	-5.46286	-2.98861
H	5.06763	2.28602	1.6277	H	-1.6066	-4.33121	-1.31987
H	2.17226	3.64947	2.51492	C	-0.84379	-1.88815	2.00126
H	1.84364	5.46663	-1.44215	S	-1.36101	-1.16485	-0.41826
H	2.79916	5.83211	1.05358	H	-0.44727	-7.15567	-0.68712
H	0.83299	1.93385	0.91846	H	-0.48022	-2.44118	2.85797
H	0.62792	3.05601	-1.52458	C	-1.59811	-0.69227	2.10283
C	3.89084	-0.49772	1.3544	C	-1.96236	-0.16542	0.88112
S	2.69679	-0.82935	-0.90372	C	-2.70852	1.06072	0.62153
C	3.28321	-1.77566	1.42035	Fe	-4.65375	1.25043	-0.11302
C	2.59402	-2.11819	0.27865	C	-2.7229	1.82823	-0.59395
C	1.91392	-3.39457	-0.00376	C	-3.54375	1.75085	1.56619
B	1.2086	-4.22233	1.34191	C	-6.21018	1.25917	-1.48832
B	2.58655	-4.89037	0.41907	C	-4.04027	2.93294	0.94581
B	0.81872	-3.48846	-1.32463	C	-5.42719	-0.64923	-0.44837
B	2.3383	-4.42682	-1.27853	C	-6.24627	0.05615	0.4837
C	0.09933	-3.49326	0.24484	C	-3.53483	2.9801	-0.38803
C	-5.40449	0.09369	-1.66713	H	-4.71253	3.64981	1.39703
C	-6.73073	1.23578	-0.1592	H	-4.88446	-1.56447	-0.2537
H	-2.19809	1.57435	-1.50514	H	-6.44327	-0.23774	1.50579
H	-3.77037	1.41568	2.56888				
H	-6.37358	2.03784	-2.22108				
H	-3.7482	3.74345	-1.12359				
H	-4.8513	-0.1669	-2.5593				
H	-7.35796	1.99338	0.29096				
H	-1.85138	-0.22102	3.04513				
H	4.48442	-0.07565	2.15654				
H	3.36434	-2.43606	2.27497				

Table S3. Cartesian coordinates and energies for optimized structures of **10**

Energy: -1813.86004343 a.u.

Fe	2.08692	4.16156	-0.1181				
C	3.61205	2.77775	0.22819				
C	3.96218	3.66408	-0.84857				
C	3.62653	4.95993	1.03025				
C	3.97697	4.99888	-0.35227				
C	3.39703	3.60066	1.38749				
C	0.14344	3.94641	0.59063				
C	0.72116	5.31329	-1.18036				
C	0.37755	5.30114	0.20533				
C	0.34238	3.12061	-0.55691				
C	0.69935	3.96528	-1.65173				
C	3.47924	1.31215	0.15779				
H	4.18131	3.37351	-1.8664				
H	3.52012	5.81396	1.6851				
H	4.19122	5.88717	-0.93085				
H	3.08307	3.25478	2.36225				
H	-0.11473	3.6017	1.58265				
H	0.98035	6.18691	-1.7632				
H	0.3323	6.16419	0.8558				
H	0.27473	2.04108	-0.57949				
H	0.93866	3.64015	-2.65523				
C	3.46122	0.63257	-1.07298				
C	3.37617	0.53438	1.32297				
H	3.55962	1.18897	-1.99939				
C	3.29721	-0.74576	-1.13551				
C	3.20718	-0.84504	1.26286				
H	3.43224	1.01125	2.2959				
C	3.14106	-1.5118	0.03106				
H	3.29043	-1.23017	-2.10464				
H	3.13152	-1.40368	2.1874				
C	2.93773	-2.9994	-0.05133				
B	2.37787	-3.84848	1.33741				
B	4.00161	-4.12184	0.67436				
B	2.16813	-3.62629	-1.46785				
B	3.86823	-3.9777	-1.08959				
C	1.29074	-3.62962	0.0109				
B	3.00051	-5.49307	1.19213				
B	1.30787	-5.15207	0.77729				
H	2.16937	-3.24994	2.3298				
C	-4.48163	1.95701	0.70945				
C	-5.37033	-0.40823	-1.96665				
C	-6.99666	-0.45813	-0.32697				
H	-2.77369	1.66488	-0.70073				
H	-4.23601	-0.80197	2.59586				
H	-6.86386	1.25194	-1.76904				
H	-5.81553	1.36737	2.41154				
H	-4.40657	-2.3331	-1.34267				
H	-6.31107	-2.39664	0.56651				
H	-4.91775	2.8846	0.36451				
H	-4.75481	-0.08383	-2.79483				
H	-7.82624	-0.17684	0.30759				
B	3.92457	-5.58508	-0.33359				
H	4.92762	-3.67306	1.25805				
B	2.79191	-5.2634	-1.67739				
B	1.17645	-5.01551	-0.98481				
H	1.85728	-2.88022	-2.32339				
H	4.7059	-3.43556	-1.72522				
C	0.15479	-2.66303	0.2115				
B	2.26766	-6.22113	-0.26539				
H	3.27328	-6.11259	2.16552				
H	0.36942	-5.43235	1.44016				
H	4.87915	-6.27686	-0.46148				
H	2.92378	-5.71239	-2.76676				
H	0.14537	-5.18377	-1.53992				
C	-0.48427	-2.57643	1.45781				
C	-0.3177	-1.84161	-0.82414				
H	2.01452	-7.37742	-0.33669				
H	-0.15259	-3.20071	2.27904				
C	-1.54204	-1.69665	1.66414				
C	-1.37394	-0.96141	-0.6151				
H	0.13443	-1.89174	-1.80642				
C	-2.0112	-0.86508	0.63437				
H	-1.99697	-1.64119	2.64804				
H	-1.7244	-0.35268	-1.44271				
C	-3.10792	0.09027	0.86951				
Fe	-5.01765	0.06866	0.02483				
C	-3.35521	1.30138	0.13517				
C	-4.11303	0.0107	1.89294				
C	-6.4875	0.29788	-1.42556				
C	-4.95238	1.15809	1.79438				
C	-5.18984	-1.60032	-1.20198				
C	-6.19475	-1.63143	-0.18906				

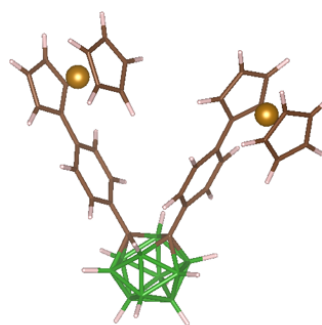
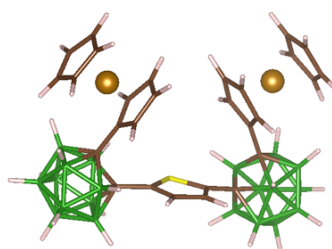


Table S4. Cartesian coordinates and energies for optimized structures of **11**

Energy: -2234.44786275 a.u.

Fe	3.8135	2.33612	-0.14422
C	3.02739	0.40677	0.05877
C	2.43737	1.08137	-1.06471
C	2.74539	1.19493	1.22676
C	1.78964	2.25437	-0.5876
C	1.97865	2.32407	0.82588
C	5.8662	2.29485	-0.51337
C	4.76217	4.08831	0.43053
C	4.51008	4.10419	-0.97473
C	5.19244	2.99375	-1.5579
C	5.5998	2.96792	0.71611
C	3.72054	-0.91114	0.02456
H	2.48808	0.75475	-2.09302
H	3.07164	0.97172	2.23179
H	1.27823	2.98431	-1.19952
H	1.6318	3.11393	1.4777
H	6.44991	1.39359	-0.63004
H	4.36112	4.78407	1.1552
H	3.88484	4.81395	-1.49945
H	5.1795	2.71492	-2.60276
H	5.94845	2.66544	1.6941
B	3.30356	-1.99088	-1.26305
B	3.83004	-1.8065	1.50034
B	5.27112	-1.19717	0.65624
B	4.93839	-1.31046	-1.08807
C	2.71994	-2.35822	0.30923
B	3.31771	-3.65581	-0.6233
B	4.72013	-3.02263	-1.50097
H	2.52666	-1.62138	-2.06967
B	3.64878	-3.54024	1.11727
B	5.25988	-2.83611	1.33201
H	3.40301	-1.31709	2.4836
B	5.94699	-2.53976	-0.29322
H	5.83751	-0.27294	1.1259
H	5.2724	-0.46384	-1.84199
C	1.27138	-2.21245	0.59966
B	4.95108	-3.97916	-0.00691
H	2.51649	-4.41606	-1.04418
H	4.99118	-3.42235	-2.58328
H	-5.14844	-5.13781	-0.87678
Fe	-3.90192	2.27179	0.1722
C	-2.95926	0.97505	1.49259
C	-2.36832	1.20022	-0.73428
H	-6.93762	-2.66365	-1.16728
C	-2.19934	2.16956	1.35453
C	-1.83669	2.30907	-0.01898
C	-5.16116	3.04507	-1.29407
C	-5.90708	2.2193	-0.40203
C	-4.57875	4.10196	-0.53072
C	-5.78469	2.76026	0.91229
C	-4.9636	3.92561	0.83266
H	-3.39643	0.60086	2.40652
H	-2.27861	1.02396	-1.7961
H	-1.97019	2.86717	2.14833
H	-1.28552	3.13226	-0.45042
H	-5.03826	2.88353	-2.35635
H	-6.44252	1.32001	-0.66951
H	-3.93311	4.88164	-0.91202
H	-6.21523	2.34423	1.81295
H	-4.65868	4.54711	1.66379



H	3.07632	-4.22307	1.89431
H	5.91754	-3.10058	2.28204
H	7.11128	-2.59257	-0.51113
S	0.07122	-2.25906	-0.6647
C	0.67333	-2.16799	1.83886
H	5.38722	-5.08131	-0.01717
C	-1.23265	-2.24247	0.49466
C	-0.7422	-2.18623	1.77956
H	1.23387	-2.15579	2.7648
C	-2.64633	-2.40154	0.06942
H	-1.37806	-2.18769	2.65519
B	-3.11318	-1.83014	-1.48355
B	-3.8773	-2.06694	1.22052
B	-3.5841	-3.71899	0.6177
B	-3.10307	-3.57045	-1.08461
C	-3.68561	-0.96235	-0.09903
B	-4.78583	-1.23886	-1.36282
B	-4.45422	-2.86556	-1.9887
H	-2.28783	-1.32325	-2.15613
B	-5.26794	-1.38891	0.34335
B	-5.23917	-3.1071	0.78073
H	-3.56267	-1.71115	2.29873
B	-4.76584	-4.03491	-0.67114
H	-3.04673	-4.48463	1.34078
H	-2.23689	-4.23613	-1.53587
C	-3.06092	0.35597	0.19934
B	-5.79937	-2.60337	-0.84073
H	-5.09524	-0.30551	-2.01868
H	-4.61411	-3.11511	-3.13627
H	-5.91412	-0.56103	0.88496
H	-5.96205	-3.52677	1.62121