β–*disubstituted* Phosphorous Corroles

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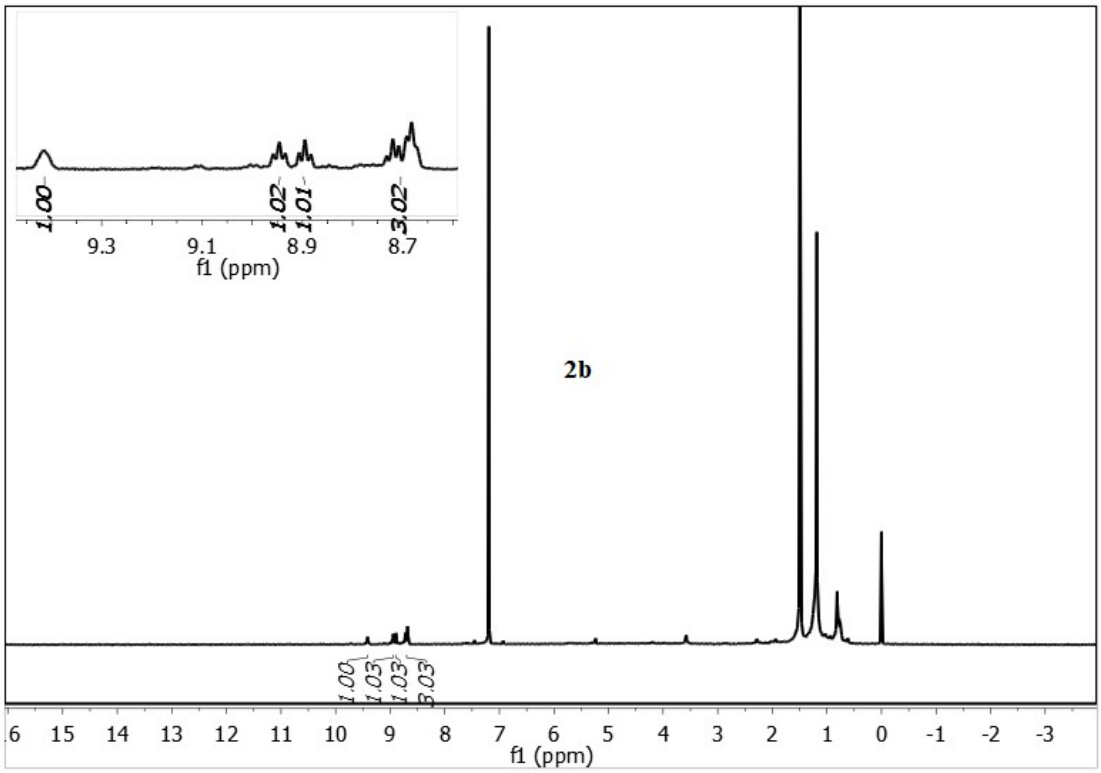


Fig S1. The ^{1}H-NMR spectrum of **2b**.

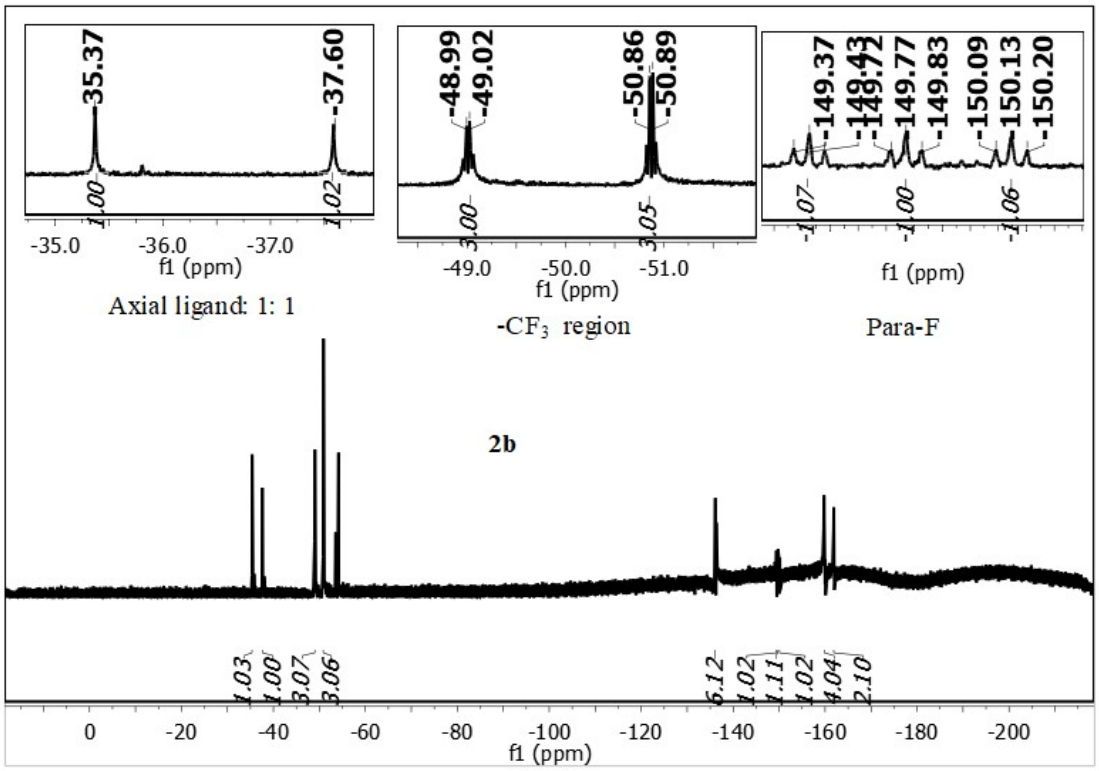


Fig S2. The ^{19}F-NMR spectrum of **2b**

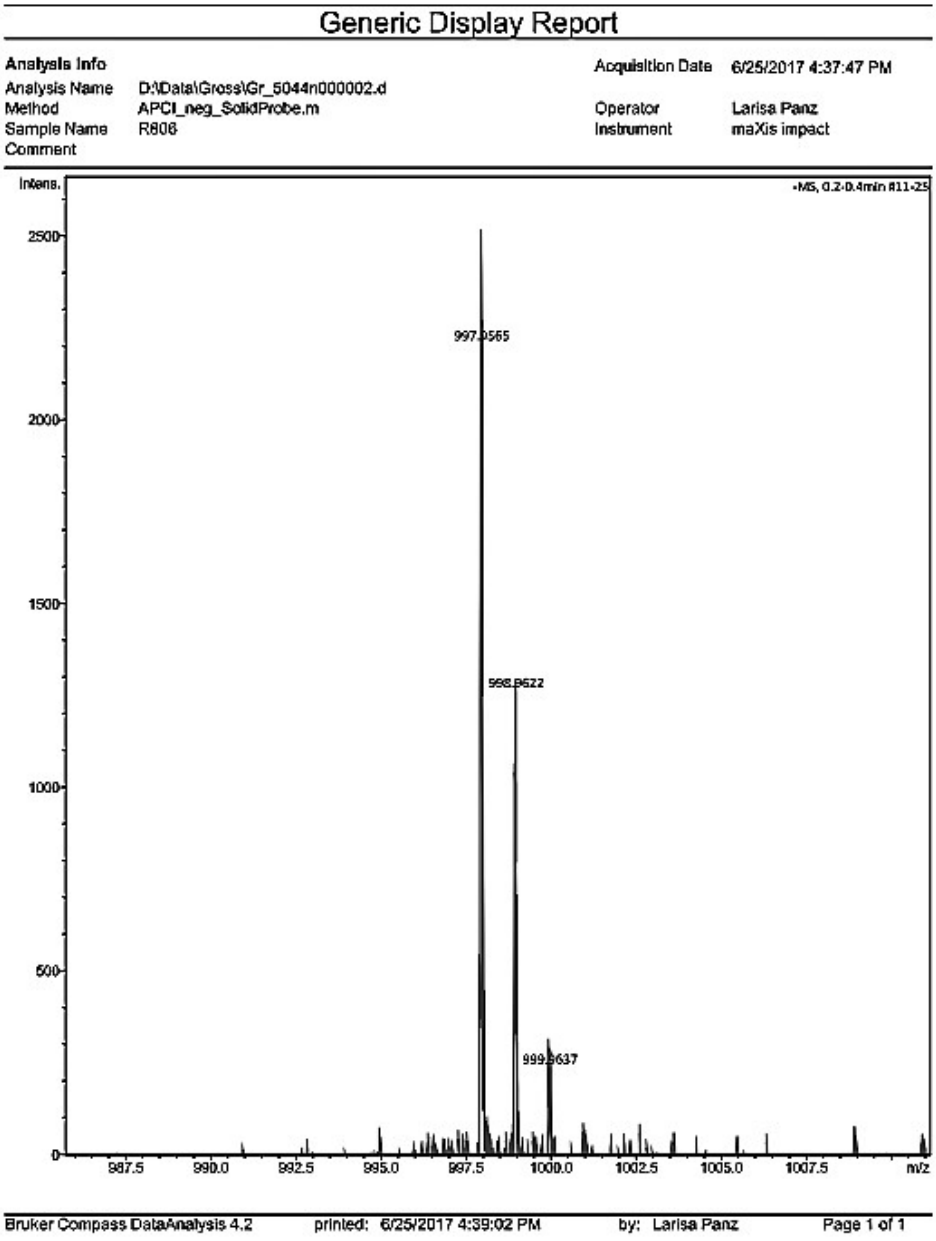


Fig S3. The APCI mass spectrum of **2b**.

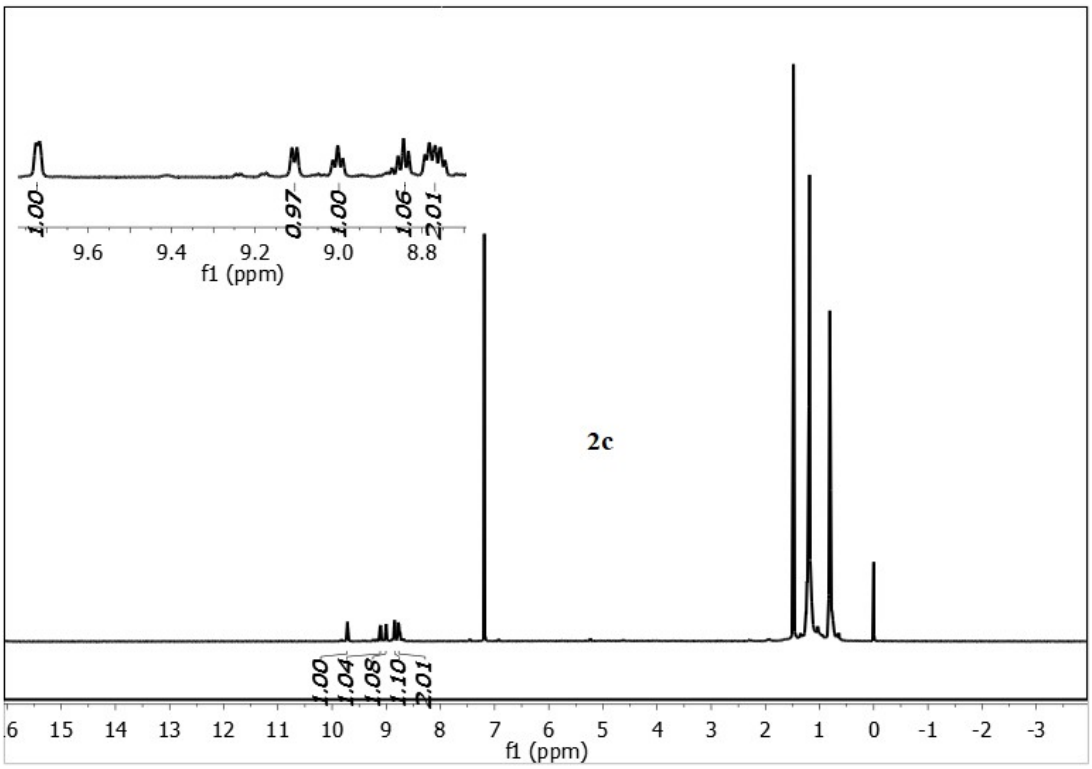


Fig S4. The ^{1}H-NMR spectrum of **2c**.

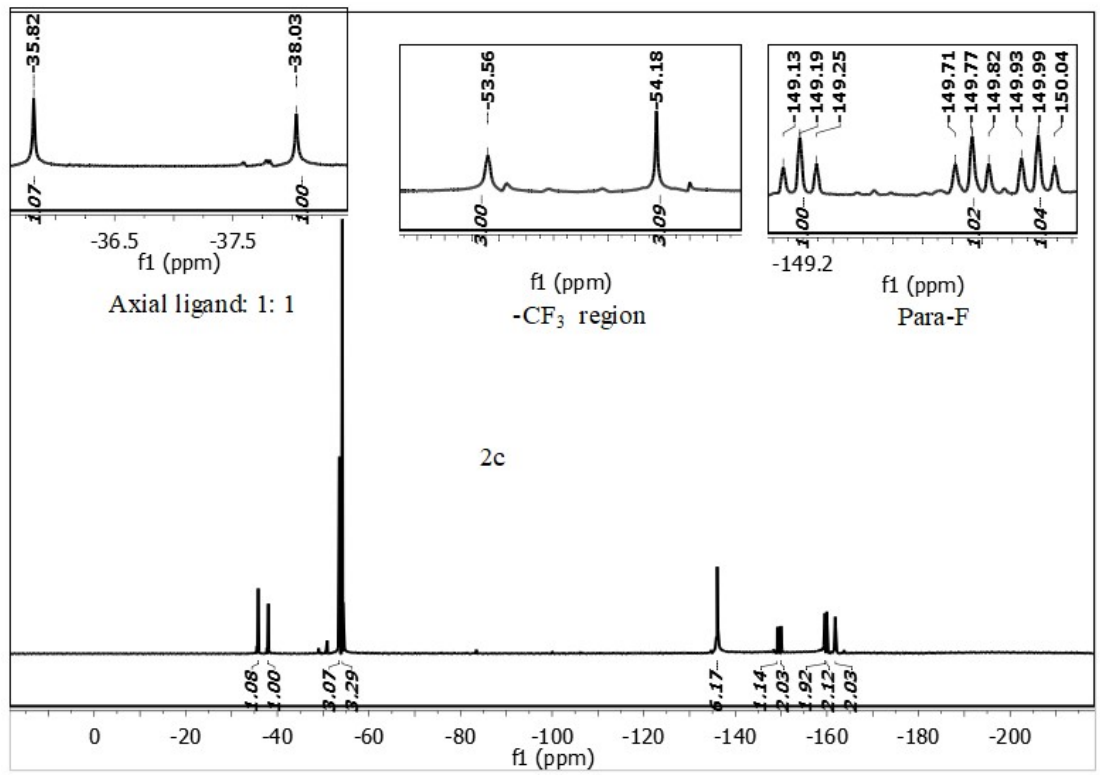


Fig S5. The ^{19}F-NMR spectrum of **2c**.

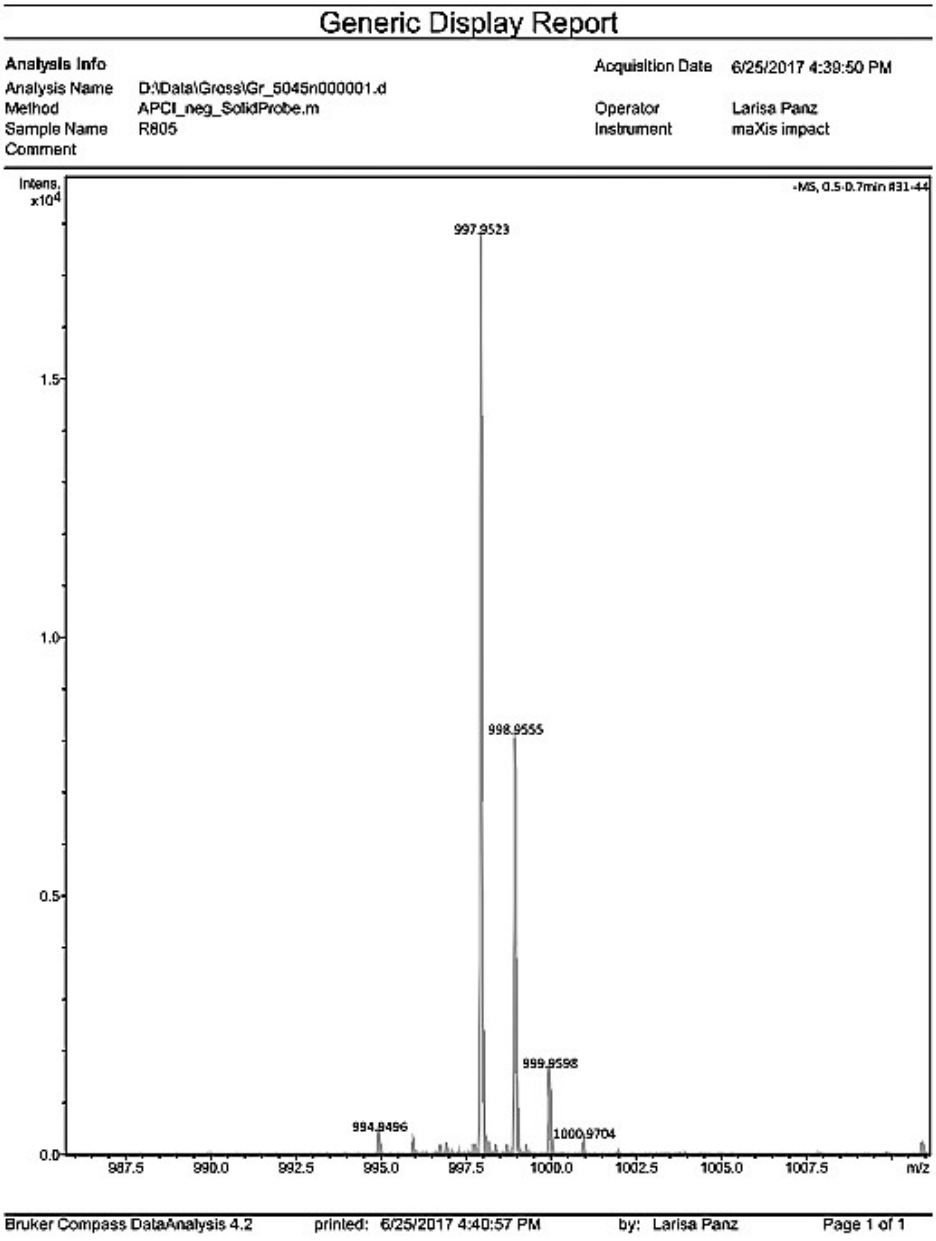


Fig S6. The APCI mass spectrum of **2c**.

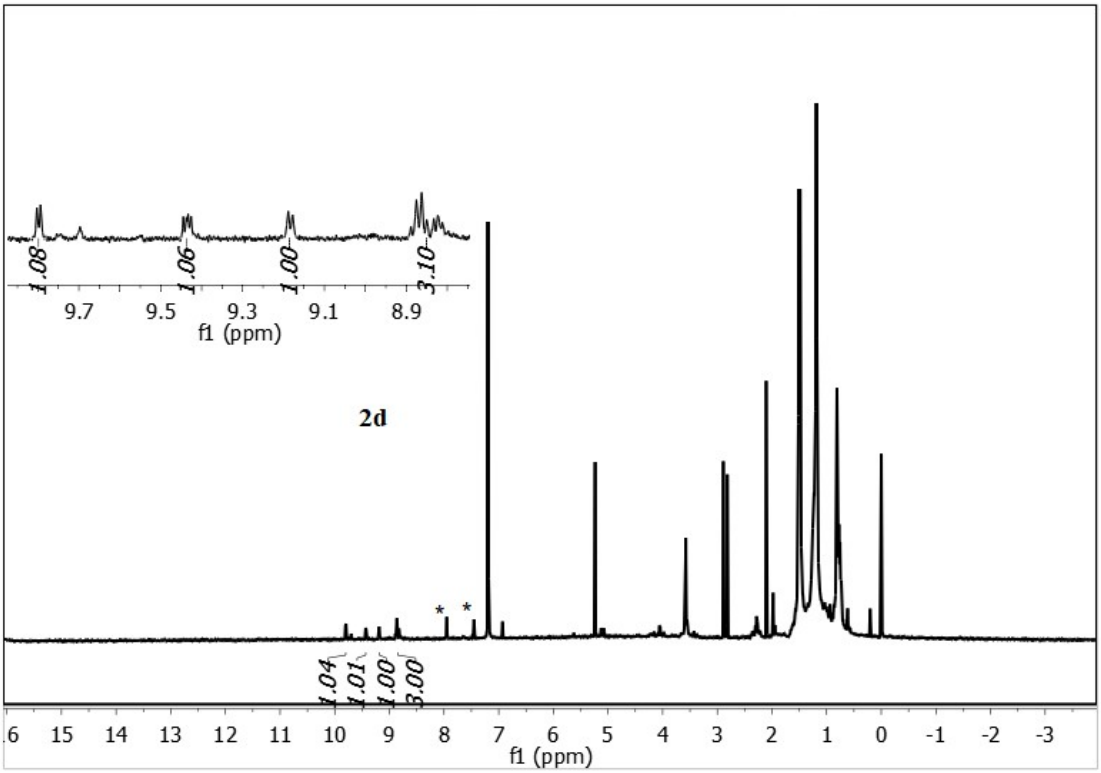


Fig S7. The ^{1}H-NMR spectrum of **2d**.

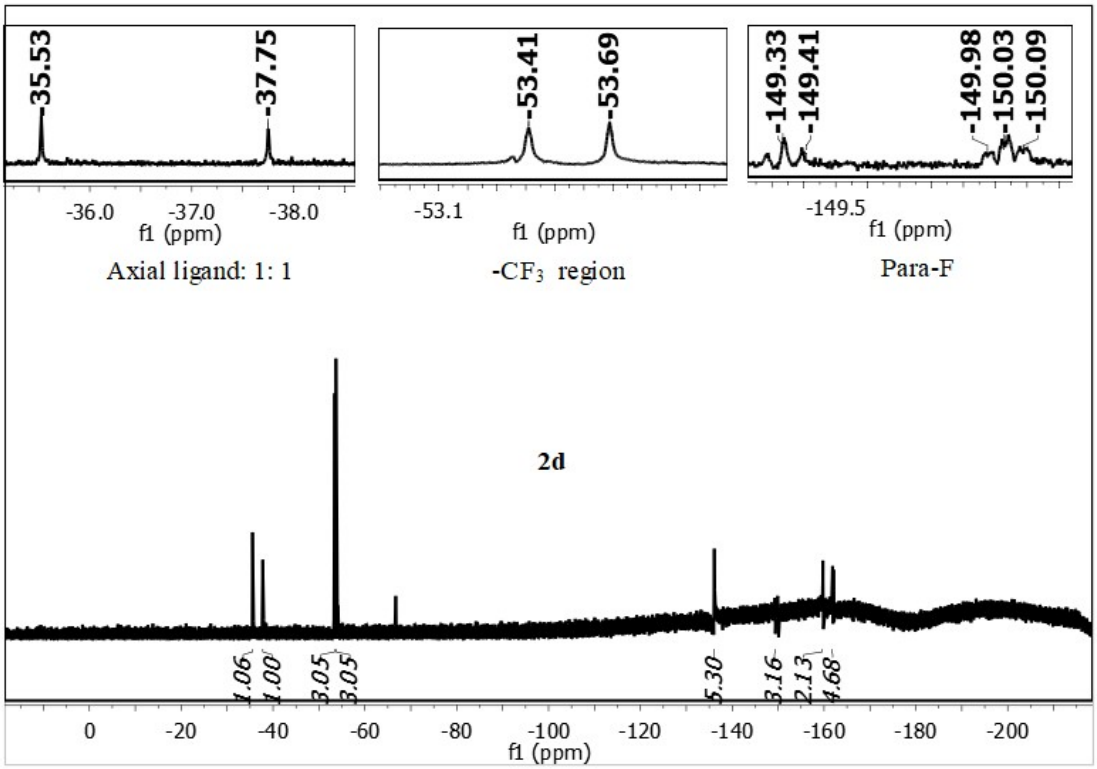


Fig S8. The ^{19}F-NMR spectrum of **2d**.

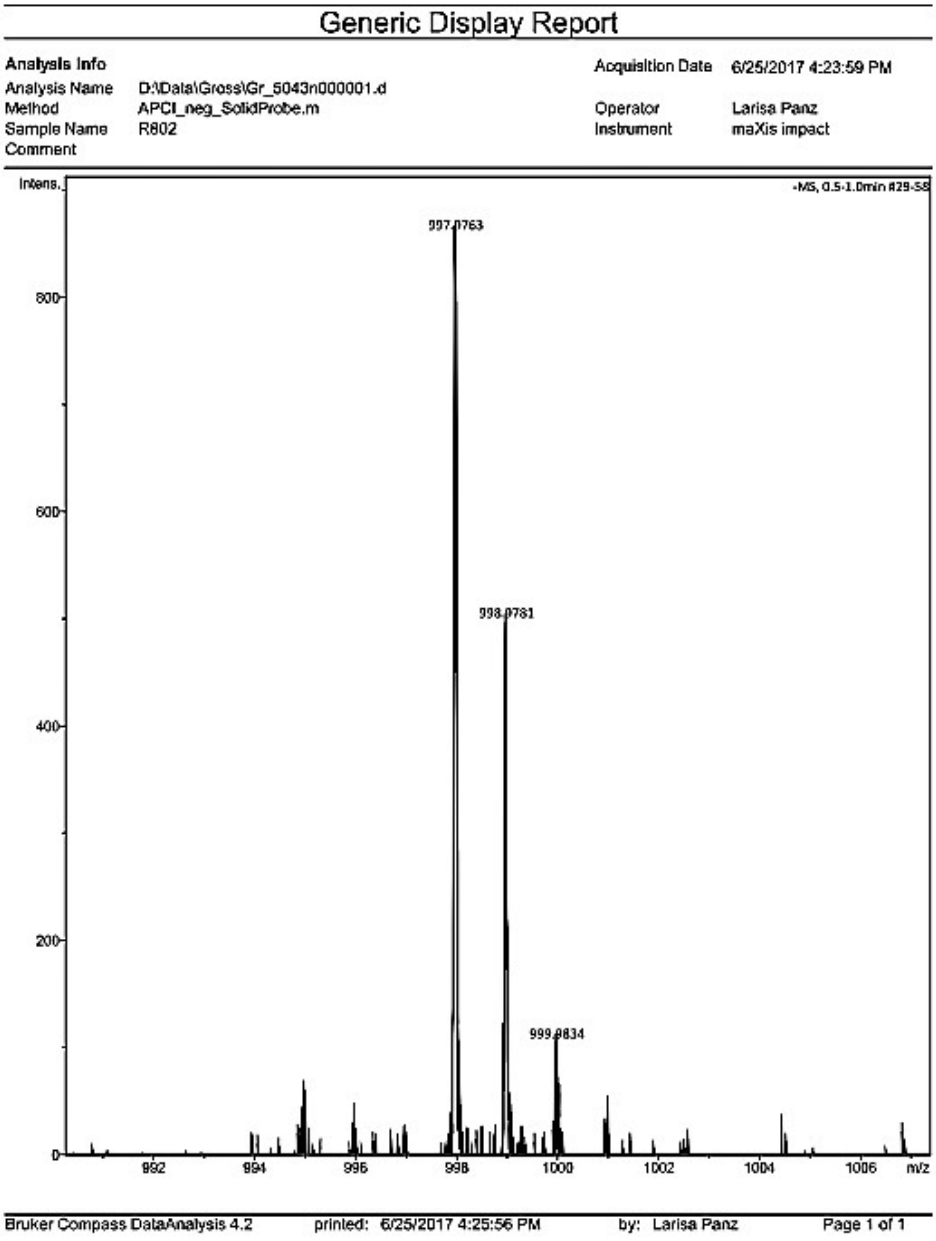


Fig S9. The APCI mass spectrum of **2d**.

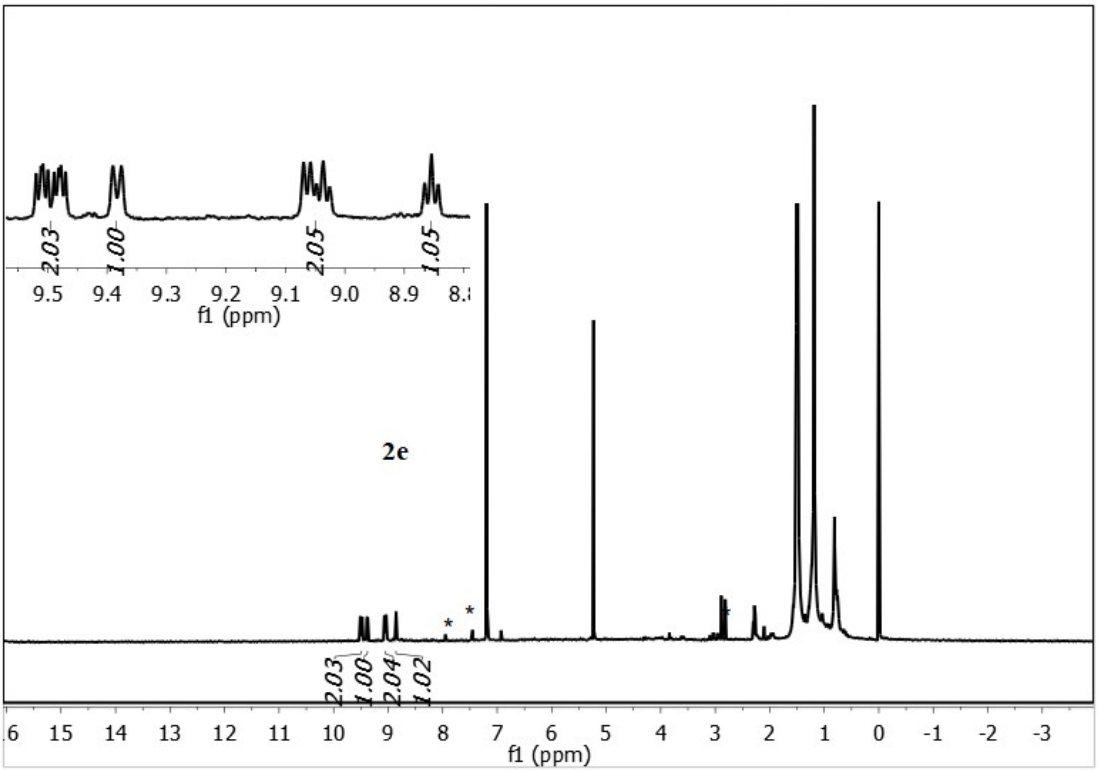


Fig S10. The [1]H-NMR spectrum of **2e**.

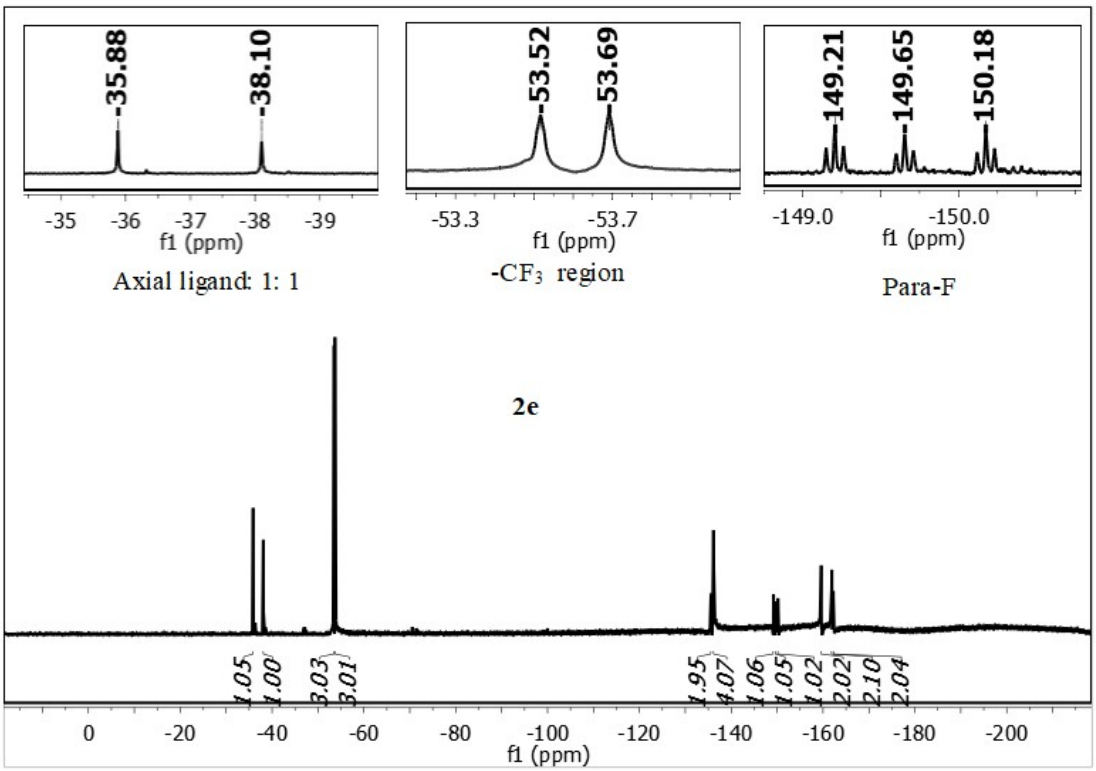


Fig S11. The [19]F-NMR spectrum of **2e**.

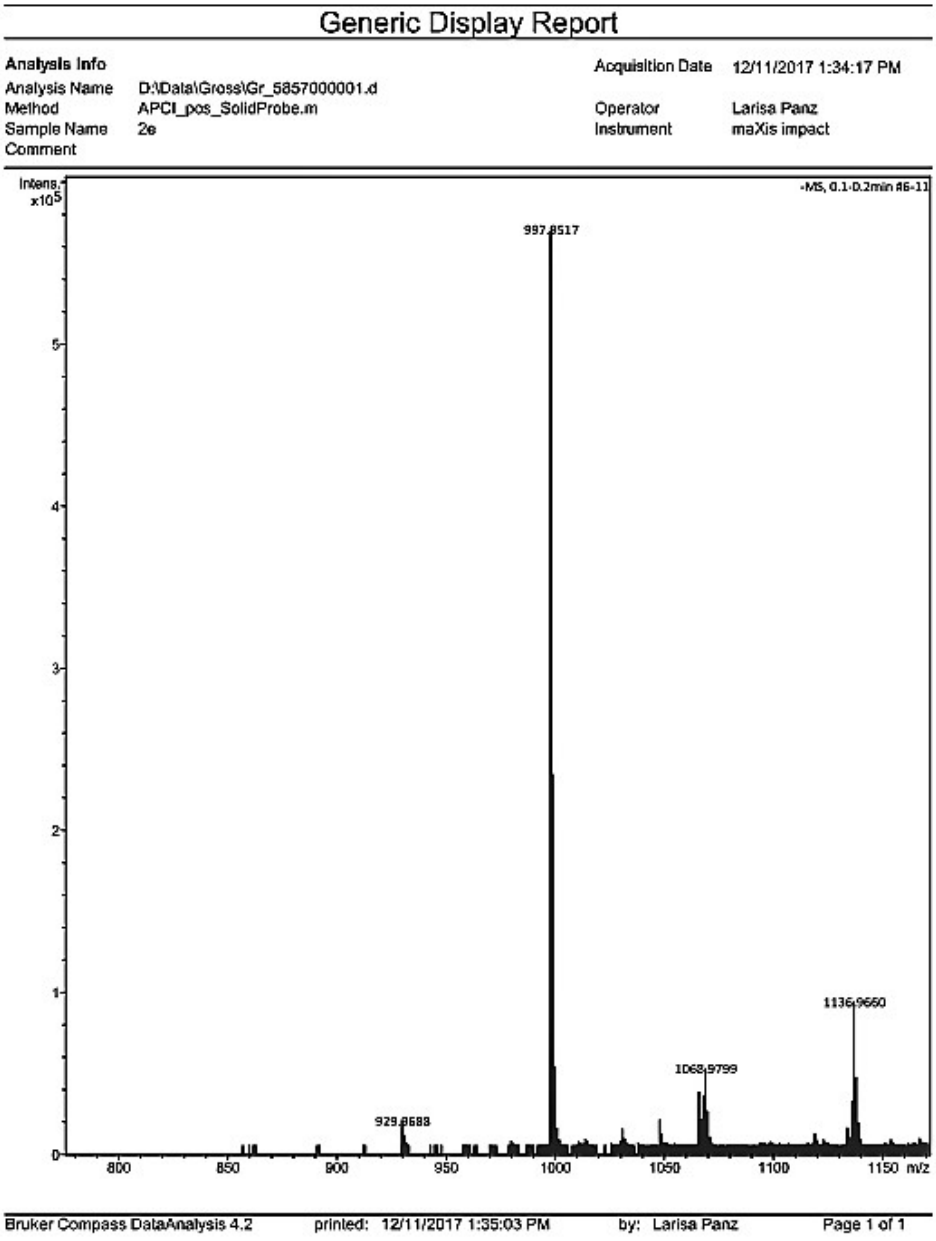


Fig S12. The APCI mass spectrum of **2e**.

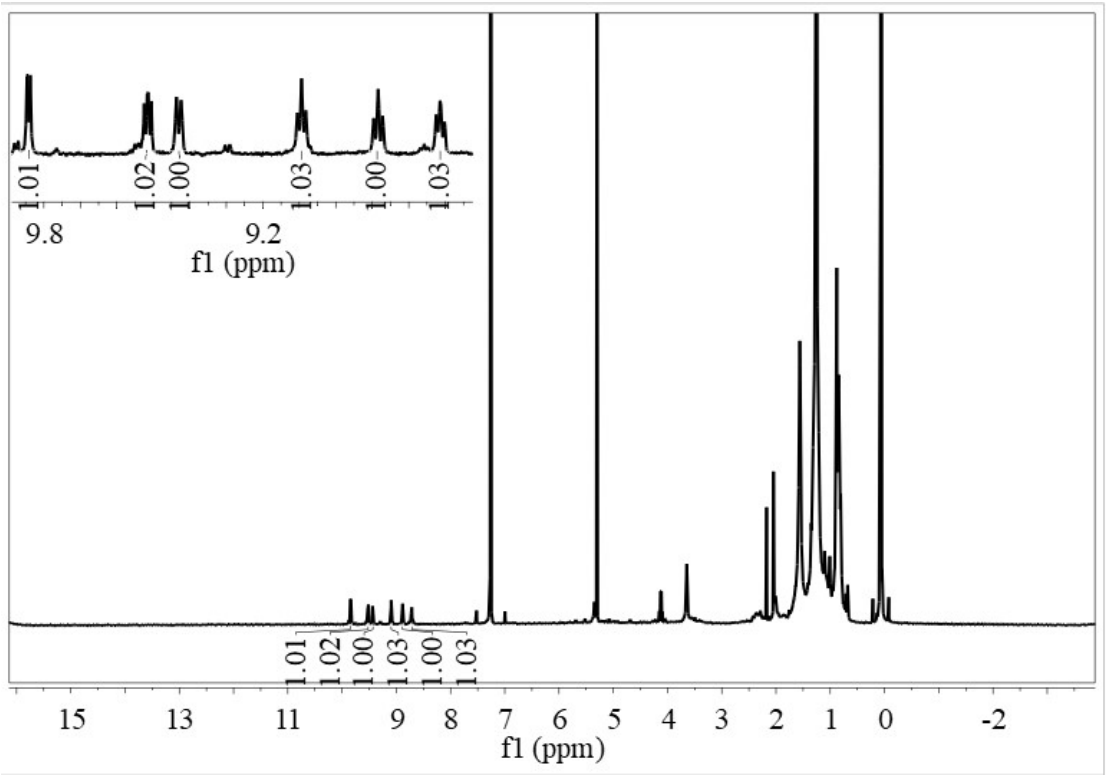


Fig S13. The ^{1}H-NMR spectrum of **2f**.

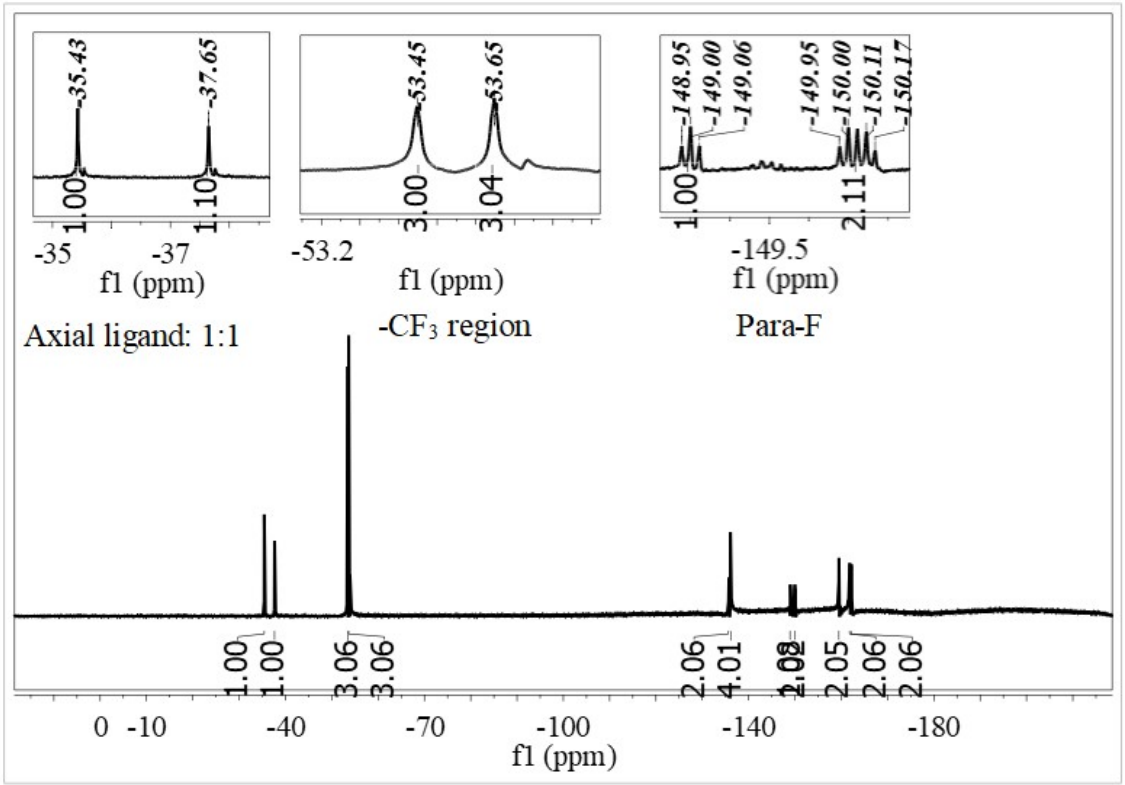


Fig S14. The ^{19}F-NMR spectrum of **2f**.

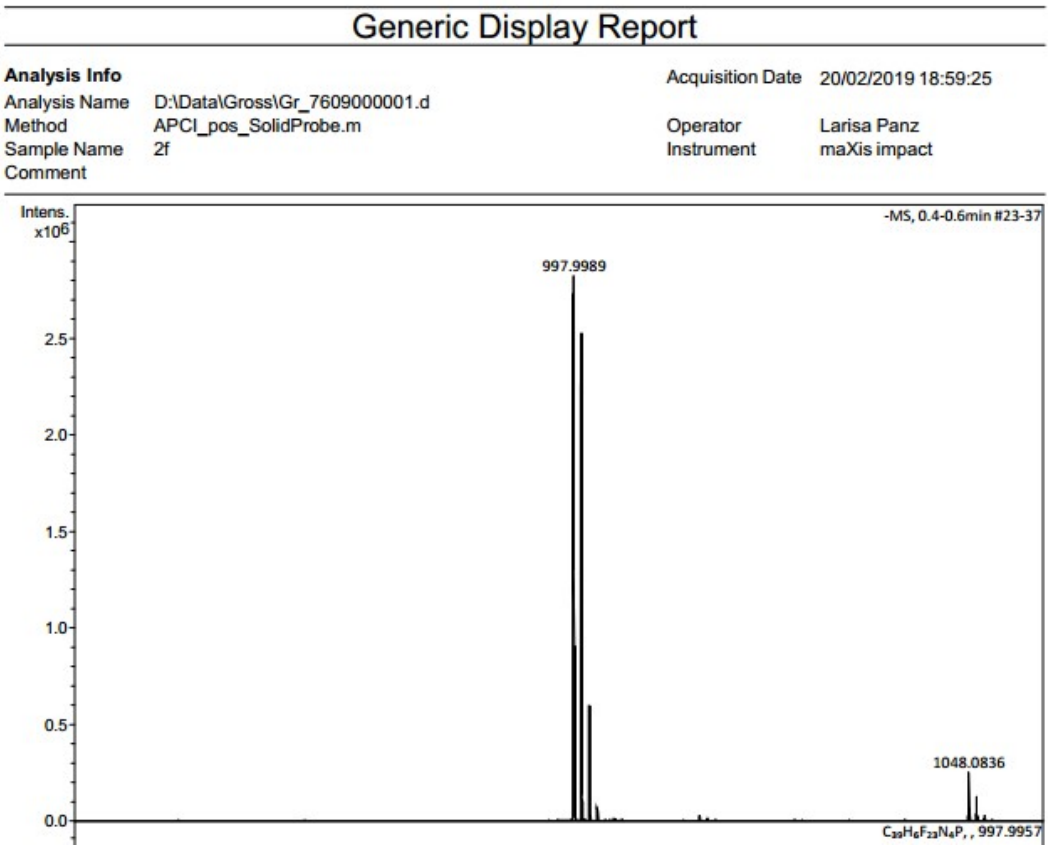


Fig S15. The APCI mass spectrum of **2f**.

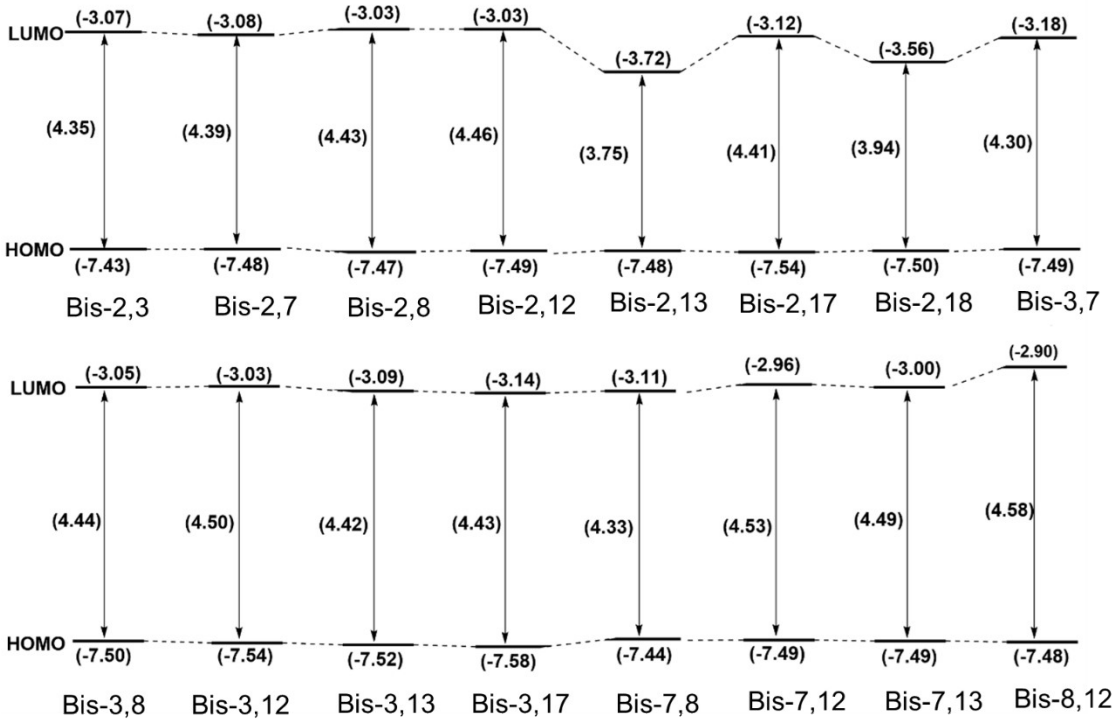


Fig S16. Calculated HOMO, LUMO and HOMO – LUMO band gap energies (eV).

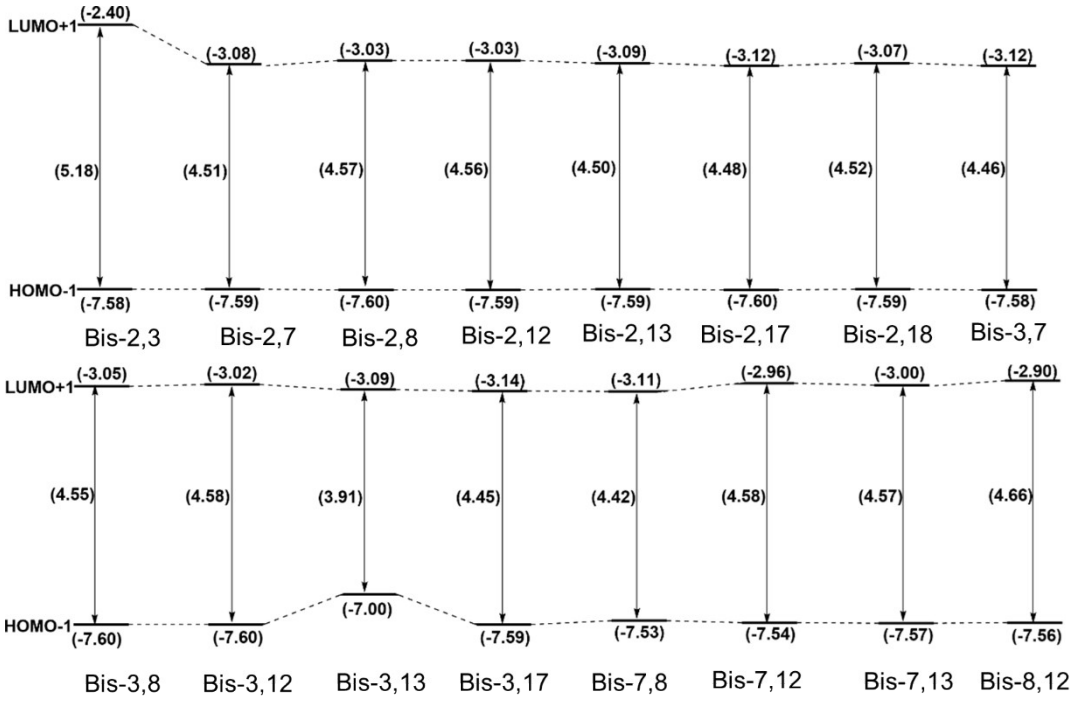


Fig S17. Calculated HOMO-1, LUMO+1 and their band gap energies (eV).

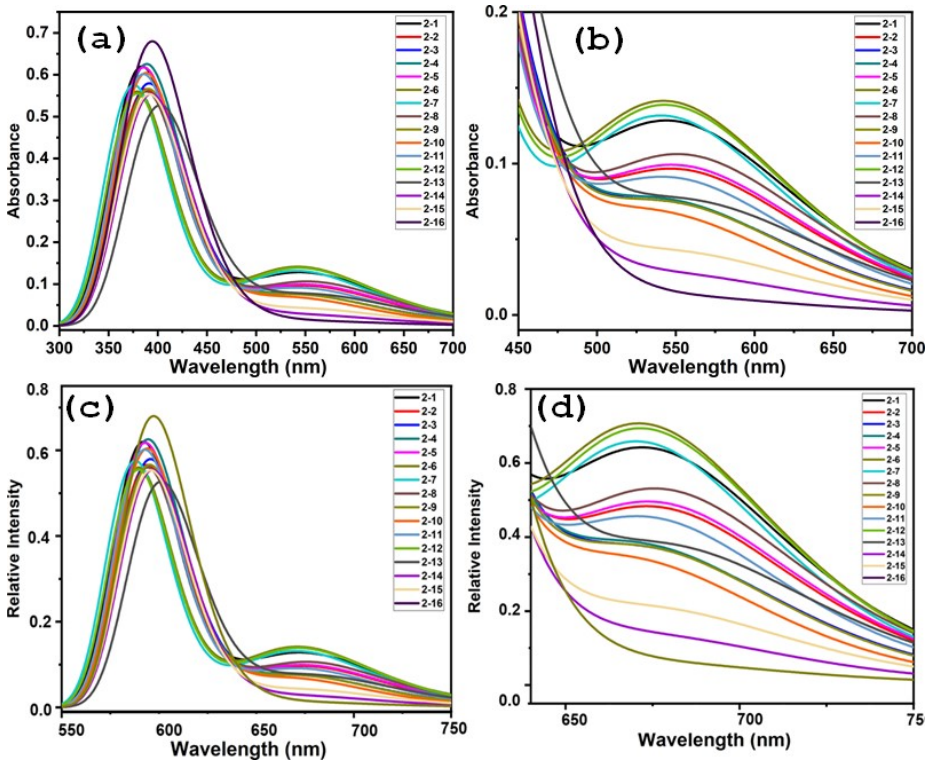


Fig S18. Calculated UV-vis and fluorescence emission spectra of all 16 bi-CF_3 isomers. Compounds **2-X** here can be corresponded into the compounds **Bis-XX** in **Fig S20**.

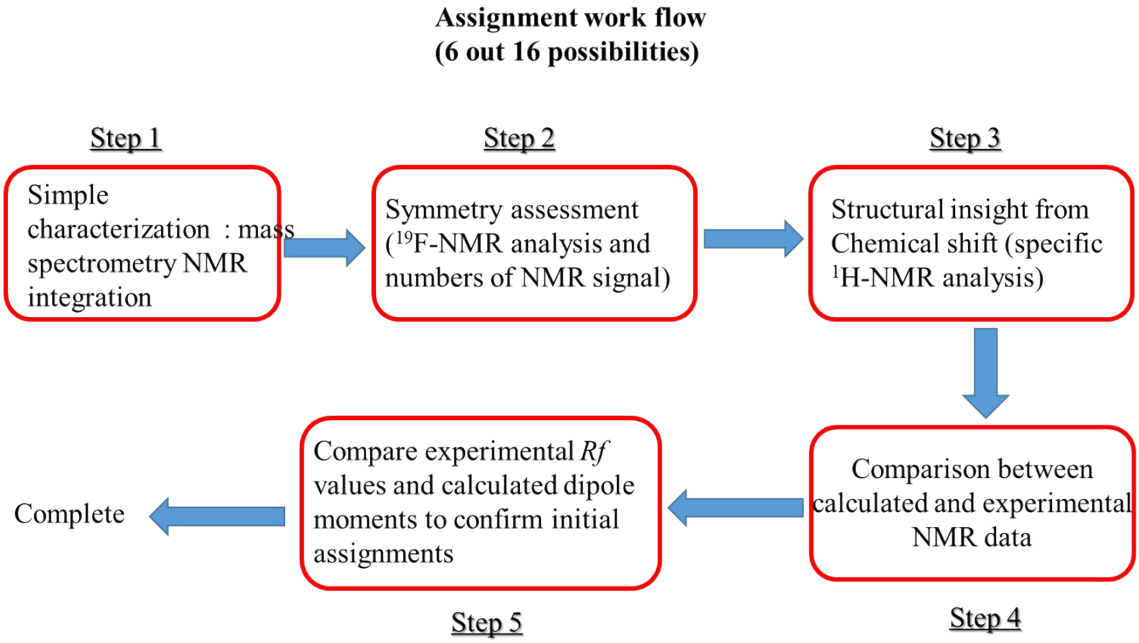


Fig S19. Assignment work flow of 6 bis-CF_3 isomers from 16 possible species.

substitution	name	2a (REF)	2b	2c	2d	2e	2f
2,3	2-1	N/A	Assigned from NMR data – no doublets in ^{1}H NMRS; one C_3H atom is available; Starting material was **1b** bearing a CF_3 group at C_3H	N/A: symmetrical condition is not compliant; already assign to **2b**	N/A: already assigned to compound **2b**; symmetrical condition is not compliant	N/A: already assigned to compound **2b**; presence of at least one doublet in ^{1}H NMR	N/A: no doublets are predicted in ^{1}H-NMRS; symmetrical condition is not compliant
2,7	2-2	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17}H but it did not.	N/A: symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: No signal of C_{18}H in the ^{1}H-NMR	N/A: no CF_3 group at C_7H; no CF_3 group at C_8H or C_{12}H
2,8	2-3	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17}Hbut it did not	N/A: symmetrical condition is not compliant; no CF_3 group at C_7H; C_8H is occupied	N/A: No signal of C_{18}H in the ^{1}H-NMR	N/A: no CF_3 group at C_7H
2,12	2-4	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17} H but it did not	N/A: no CF_3 group at C_7H; C_{12}H is occupied	N/A: No signal of C_{18}H in the ^{1}H-NMR	N/A: no CF_3 group at C_7H
2,13	2-5	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17}H but it did not	N/A: symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: No signal of C_{18}H in the ^{1}H-NMR	N/A: no CF_3 group at C_7H; no CF_3 group at C_8H or C_{12}H
2,17	2-6	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	Assigned from NMR data: matched symmetrical condition; broad C_2H doublet signal and also one CF_3 occupy at C_{17}H	N/A: no CF_3 group at C_7H	N/A: No signal of C_{18}H in the ^{1}H-NMR; symmetrical condition is not compliant	N/A: no CF_3 group at C_7H; no CF_3 group at C_8H or C_{12}H
2,18	2-7	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant	N/A: symmetrical condition is not compliant; no CF_3 group at C_7H; no available C_2H or C_{18}H	N/A: symmetrical condition is not compliant	N/A: no CF_3 group at C_7H; symmetrical condition is not compliant; no CF_3 group at C_8H or C_{12}H
3,7	2-8	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_2H or C_{18}H but it did not	N/A: symmetrical condition is not compliant	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H	N/A: no CF_3 group at C_8H or C_{12}H
3,8	2-9	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_2H or C_{18} H but it did not	N/A: symmetrical condition is not compliant; C_8H is occupied	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H	Assigned from NMR data: not C2v symmetry; should have C2H or C18H (showed chemical shift at 9.85 ppm); should have available C8H or C12H; the shape of ^{1}H-NMR looks like the superimposition of 1b and 1d; Starting material was **1b** bearing a CF_3 group at C_7H
3,12	2-10	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_2H or C_{18}H but it did not	N/A: symmetrical condition is not compliant; C_{12}H is occupied	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H	N/A: symmetrical condition is not compliant
3,13	2-11	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_2H or C_{18}H but it did not	Assigned from NMR data- should have available C_2H or C_{18}H (showed chemical shift at 9.80 ppm) ; should contain C_8H and C_{12}H (showed chemical shift from 8.89-8.84 ppm); Starting material was 1b bearing a CF_3 group at C_7H; near C2v symmetry from ^{19}F-NMR	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H	N/A: already assigned to compound **2d**; no CF_3 group at C_8H or C_{12}H; symmetrical condition is not compliant
3,17	2-12	Structurally characterized, symmetrical NMR spectrum	N/A: already structurally characterized as compound **2a**	N/A: already structurally characterized as compound **2a**	N/A: already structurally characterized as compound **2a**	N/A: already structurally characterized as compound **2a**	N/A: already structurally characterized as compound **2a**
7,8	2-13	N/A	N/A: no CF_3 group at C_7H	N/A: presence of at least one doublet in ^{1}H NMR	N/A: symmetrical condition is not compliant; C_8H is occupied; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H; presence of at least one doublet in ^{1}H NMR	N/A: no CF_3 group at C_7H; symmetrical condition is not compliant
7,12	2-14	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17}H and another CF_3 should at C_2H or C_{18}H but it did not	N/A: C_{12}H is occupied; no CF_3 group at C_7H	Assigned from NMR data showing NMR that has C_2H or C_8H signal and C_{12}H or C_{13}H signal and not C2v symmetry	N/A: no CF_3 group at C_7H; symmetrical condition is not compliant
7,13	2-15	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17}H and another CF_3 should at C_2H or C_{18}H but it did not	N/A: symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H	N/A: no CF_3 group at C_7H; symmetrical condition is not compliant
8,12	2-16	N/A	N/A: doublets are predicted in ^{1}H NMRS; symmetrical condition is not compliant; no CF_3 group at C_7H	N/A: symmetrical condition is not compliant; one CF_3 should occupy at C_7H or C_{17}H and another CF_3 should at C_2H or C_{18}H but it did not	N/A: symmetrical condition is not compliant; no CF_3 group at C_7H; no available C_8H and C_{12}H	N/A: symmetrical condition is not compliant; has C_2H and C_{18}H	N/A: no CF_3 group at C_7H; symmetrical condition is not compliant

Fig S20. NMR assignments of all 6 isomers in table form with individual reasons for assignments clarified.

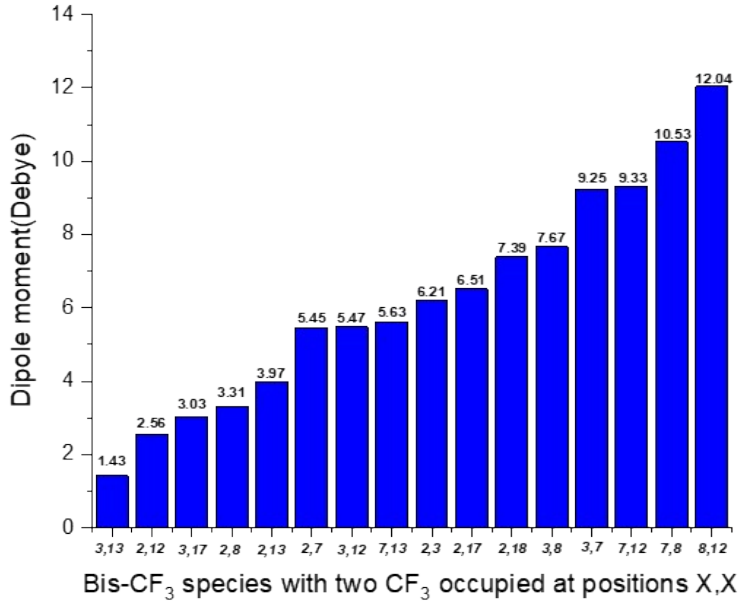
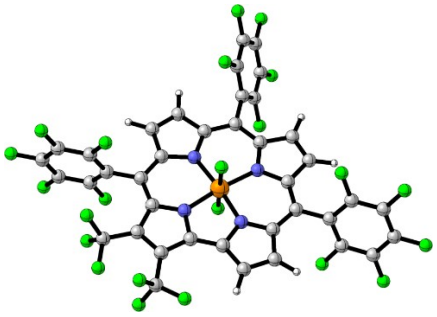


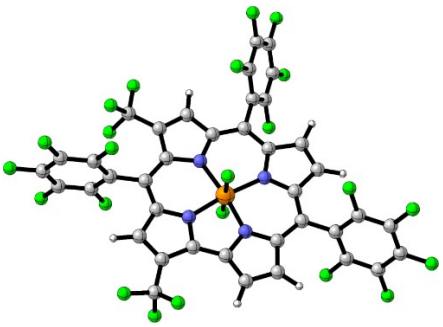
Figure 21. DFT calculated dipole moments of all 16 bis–isomers with incrementally increased dipole moment from left to right.

Cartesian Coordinates of Optimized Geometries:



P	-0.32521	-0.40038	0.00352
F	-0.32848	-0.40200	1.74701
F	-0.32366	-0.37507	-1.73980
F	-5.30347	-0.96520	-2.24851
F	-8.91877	-3.30227	-0.19627
F	-7.89085	-1.84823	-2.31194
F	-4.74275	-2.96799	2.08285
F	-7.32710	-3.85839	1.99574
F	4.53983	0.45533	-2.38501
F	-2.34332	4.07467	2.31756
F	-0.60945	4.59793	-2.12944
F	4.53726	0.45266	2.40686
F	7.21952	1.05489	-2.38151
F	7.21695	1.05248	2.40686
F	-2.99262	6.73357	2.36948
F	8.56600	1.35314	0.01351
F	-1.25282	7.25780	-2.05948
F	-2.44956	8.34073	0.18576
N	0.71924	1.13956	0.02007
N	1.20486	-1.47235	-0.00411
N	-1.18171	-2.04149	-0.01101
N	-1.97056	0.49003	0.00777
C	-0.38061	-3.16439	-0.02340
C	2.56181	-1.21038	-0.00330
C	0.23916	2.45166	0.05142
C	-2.50940	-2.42446	-0.03704
C	0.98318	-2.83741	-0.01633
C	-3.25294	-0.10608	-0.01508
C	-3.53560	-1.47508	-0.04217
C	-2.14354	1.87511	0.03681
C	-1.21425	-4.30958	-0.05527
C	-2.52744	-3.85519	-0.06588

C	2.13012	1.18977	0.02441
C	-4.94891	-1.93781	-0.07904
C	-7.10383	-2.12306	-1.22055
C	-1.10717	2.81363	0.05971
C	-1.45789	4.26172	0.09249
C	-5.78537	-1.67923	-1.17340
C	-3.54752	2.14953	0.03180
C	3.20885	-2.49733	-0.01429
C	3.02213	0.11642	0.00952
C	-4.21479	0.95371	0.00462
C	2.22859	-3.48930	-0.02253
C	4.48001	0.43285	0.01079
C	-6.81901	-3.13781	0.94289
C	-7.62257	-2.85743	-0.15819
C	-5.50525	-2.67845	0.97266
C	1.36707	3.33551	0.07918
C	2.50366	2.57588	0.05912
C	-2.06265	4.84740	1.21226
C	5.19117	0.59679	-1.18171
C	5.19012	0.59505	1.20414
C	-1.20123	5.10714	-0.99472
C	6.54746	0.89888	1.21700
C	6.54870	0.90028	-1.19267
C	7.22820	1.05056	0.01256
C	-2.39952	6.19756	1.25261
C	-1.52181	6.46180	-0.97310
C	-2.12570	7.00874	0.15527
H	-0.88065	-5.33510	-0.07069
H	1.30418	4.41045	0.11519
H	-3.98171	3.13542	0.04398
H	-5.28265	0.80907	0.00318
H	-3.41750	-4.46333	-0.09246
H	3.52160	2.92915	0.07084
C	4.65184	-2.81191	-0.01708
F	5.32969	-2.30362	-1.13093
F	4.86249	-4.18550	-0.02295
F	5.33184	-2.31240	1.09937
C	2.47344	-5.00966	-0.03480
F	1.28839	-5.65625	-0.04286
F	3.17572	-5.34347	-1.13838
F	3.17086	-5.36204	1.06608



P	0.41911	-0.67267	-0.01260
F	0.41957	-0.64531	-1.75389
F	0.40182	-0.63520	1.72877
F	5.39339	-0.26324	2.26972
F	9.40674	-1.88339	0.26616
F	8.10138	-0.63795	2.36167
F	5.26442	-2.36470	-2.04834
F	7.97102	-2.74601	-1.93394
F	-4.46818	-0.83908	2.43399
F	1.54596	4.08566	-2.34505
F	-0.24190	4.29051	2.10505
F	-4.56310	-1.15079	-2.34510
F	-7.18055	-1.26347	2.51483
F	-7.27585	-1.57467	-2.26250
F	1.68789	6.81969	-2.40689
F	-8.59182	-1.62983	0.16699
F	-0.10172	7.02525	2.02818
F	0.86400	8.30412	-0.22485
N	-0.93587	0.64532	-0.02817
N	-0.85680	-2.00822	-0.01390
N	1.57577	-2.11817	-0.00051
N	1.86479	0.51339	-0.00978
C	1.00220	-3.37697	0.01080
C	-2.23490	-1.99241	0.00402
C	-0.68059	2.01518	-0.07140
C	2.94941	-2.24429	0.04076
C	-0.39663	-3.30816	-0.00781
C	3.23603	0.17161	0.02272
C	3.77683	-1.11705	0.05489
C	1.77129	1.90569	-0.04511
C	2.03815	-4.34335	0.05837
C	3.23880	-3.64685	0.07658
C	-2.34434	0.44387	-0.02711
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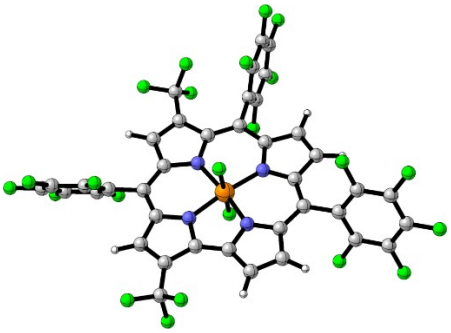

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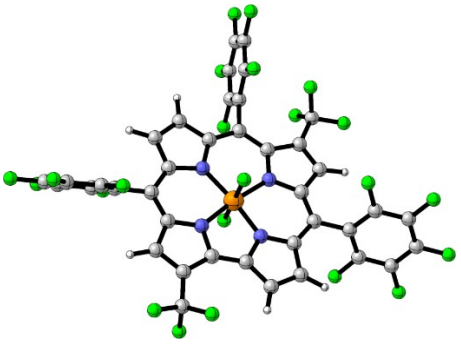

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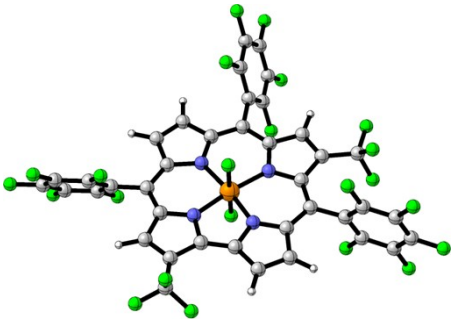

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F	-1.22831	4.14496	2.10856
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C	2.93455	0.72437	0.02351
C	-4.42506	-1.79128	0.03532
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H	-3.17212	-4.32581	0.05190
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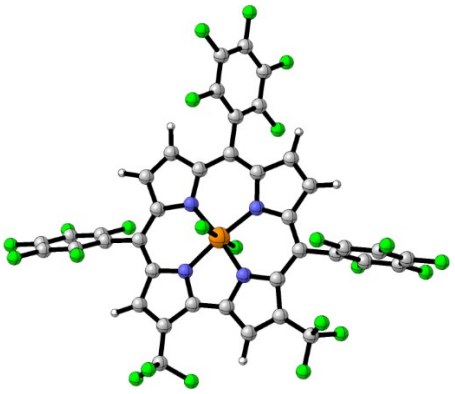

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C	2.90783	-3.03969	-0.03069
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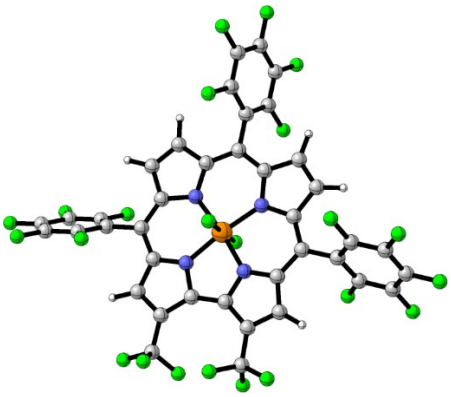

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C	-1.82972	3.75230	0.04999
C	-4.85187	0.55987	0.02416
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C	7.66660	0.82342	-0.06361
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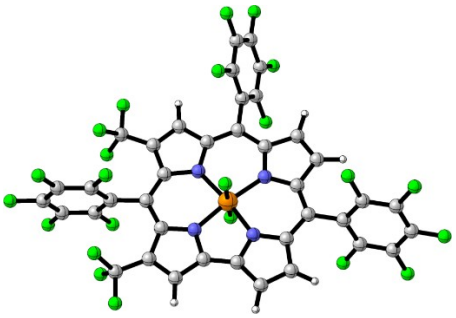

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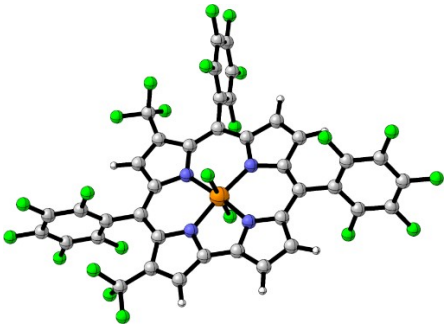

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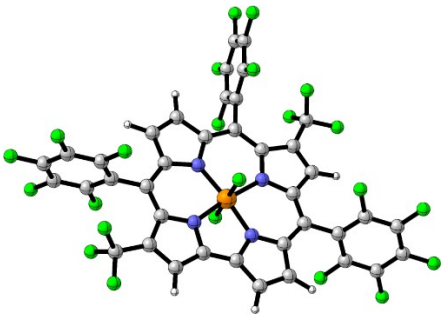

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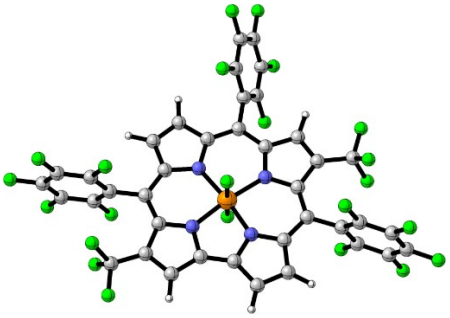

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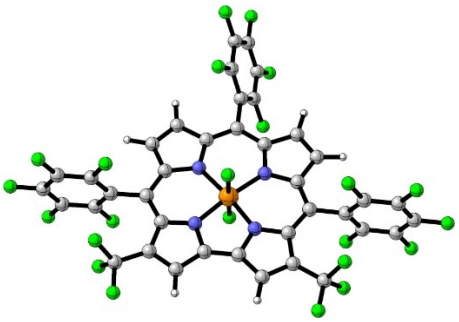

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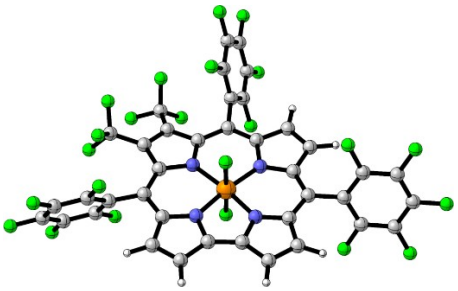

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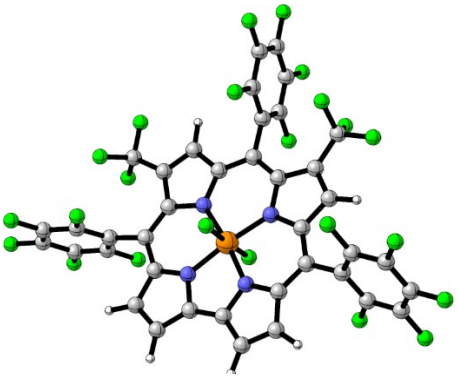

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F	7.66363	-3.37906	-2.02550
F	-4.76909	-1.68958	2.44541
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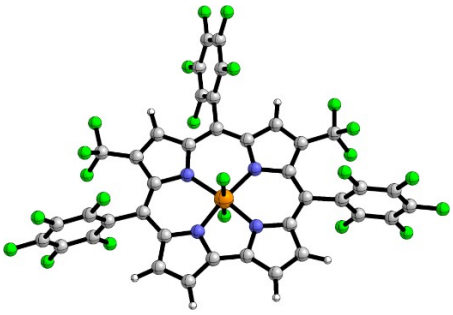

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C	-6.92517	-2.15890	-1.22799

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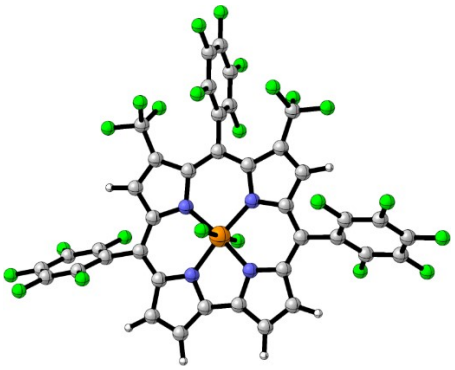

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