

**Fine-tuning The Acceptor-Donor Ability of Star Shaped Triarylborane-Triphenylamine
Conjugates: Synthesis, Characterization and Anion Binding Studies**

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1. Optical properties

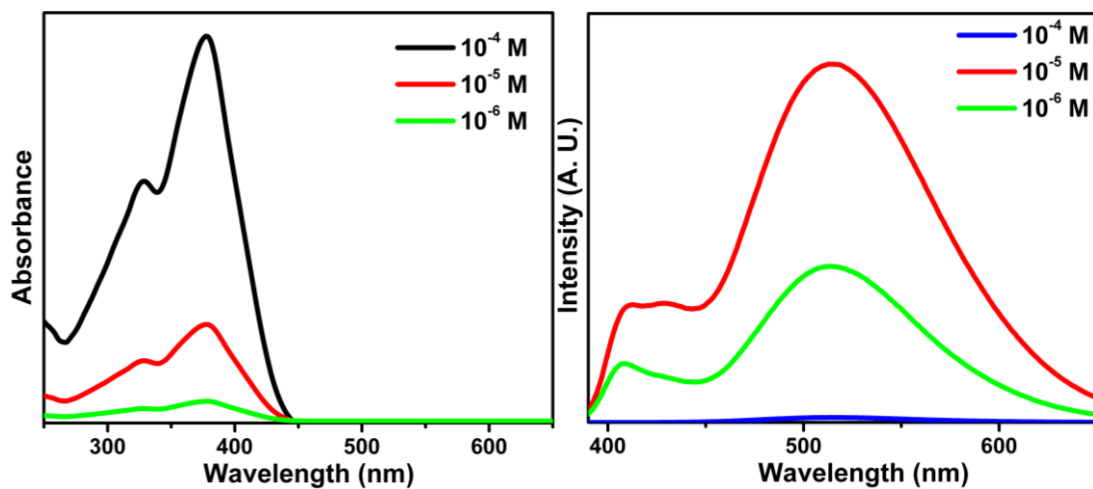


Figure S1: UV-Visible (left) and fluorescence (right) spectra of **1** in dichloromethane at various concentrations (λ_{ex} at 375 nm).

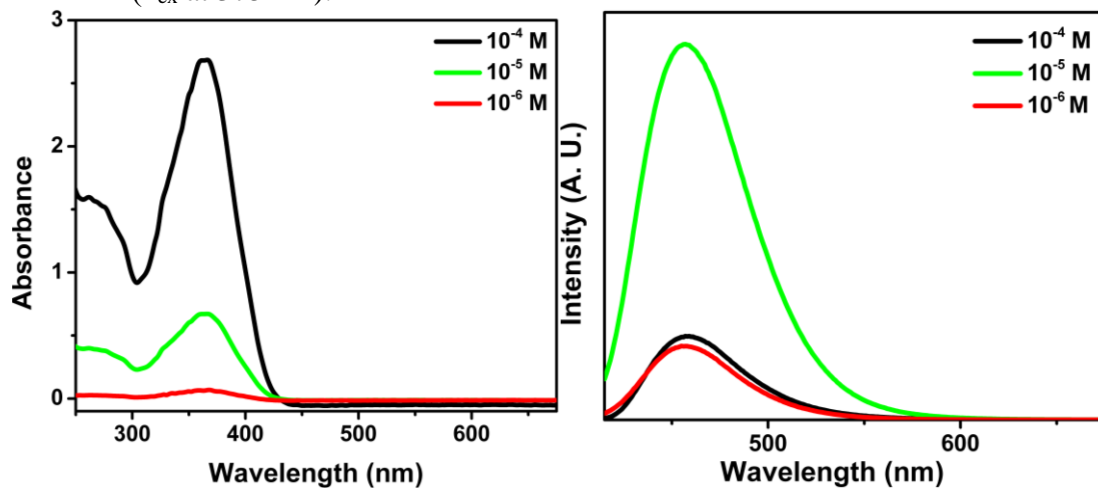


Figure S2: UV-Visible (left) and fluorescence (right) spectra of **2** in dichloromethane at various concentrations (λ_{ex} at 375 nm).

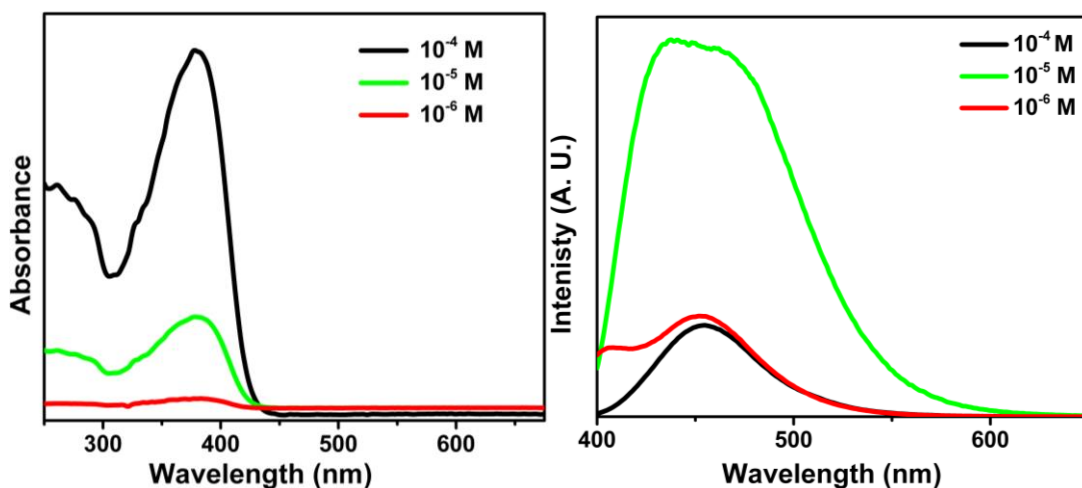


Figure S3: UV-Visible (left) and fluorescence (right) spectra of **3** in dichloromethane at various concentrations (λ_{ex} at 375 nm).

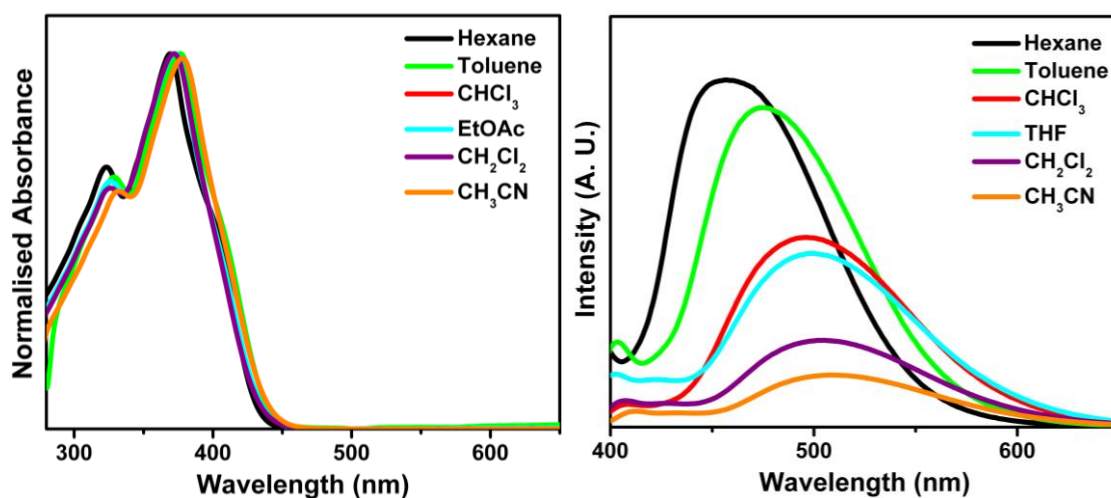


Figure S4: UV-Visible (right) and Fluorescence (left) spectra of **1** in solvents with different polarity (10 μM ; λ_{ex} at 375 nm).

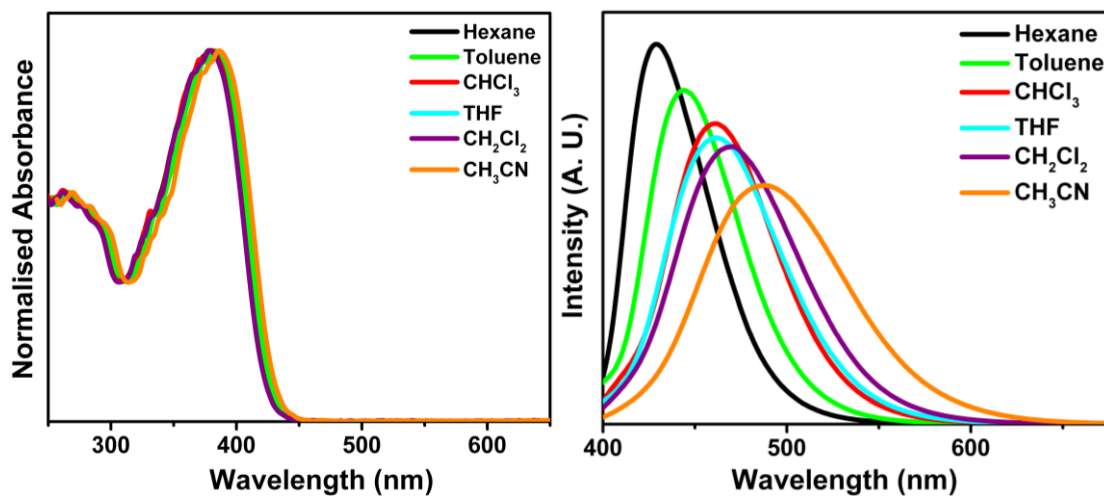


Figure S5: UV-Visible (right) and Fluorescence (left) spectra of **2** in solvents with different polarity (10 μM ; λ_{ex} at 375 nm).

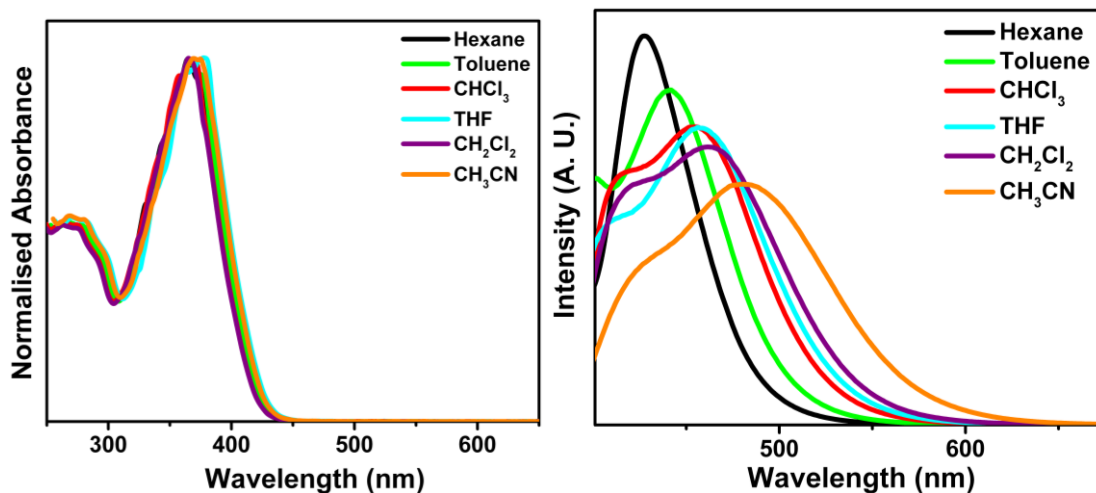


Figure S6: UV-Visible (right) and Fluorescence (left) spectra of **3** in solvents with different polarity (10 μM ; λ_{ex} at 375 nm).

Table S1: Optical data of **1** in different solvents.

S. No	Solvent	λ_{abs} (nm)	λ_{em} (nm)	$\lambda_{\text{em}} - \lambda_{\text{abs}}$ (cm^{-1})	Quantum yields (%)
1	Hexane	369	458	5266.27	40.4
2	Toluene	376	475	5543.11	37.8
3	CHCl_3	373	492	6484.45	22.5
4	THF	372	499	6841.64	21.8
5	CH_2Cl_2	391	515	6157.97	11.3
6	CH_3CN	378	520	7224.26	9.2

Table S2: Optical data of **2** in different solvents.

S. No	Solvent	λ_{abs} (nm)	λ_{em} (nm)	$\lambda_{\text{em}} - \lambda_{\text{abs}}$ (cm^{-1})	Quantum yields (%)
1	Hexane	378	429	3145.01	76.2
2	Toluene	383	443	3536.3	74.5
3	CHCl_3	379	461	4693.25	72.2
4	THF	372	461	5189.75	71.4
5	CH_2Cl_2	378	470	5178.43	70.5
6	CH_3CN	386	486	5330.61	68.8

Table S3: Optical data of **3** in different solvents.

S. No	Solvent	λ_{abs} (nm)	λ_{em} (nm)	$\lambda_{\text{em}} - \lambda_{\text{abs}}$ (cm^{-1})	Quantum yields (%)
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1	Hexane	364	407	2902.51	78.9
2	Toluene	366	420	3512.88	77.1
3	CHCl ₃	369	432	3952.12	75.4
4	THF	378	436	3519.25	73.6
5	CH ₂ Cl ₂	365	440	4670.26	74.5
6	CH ₃ CN	369	461	5408.30	72.1

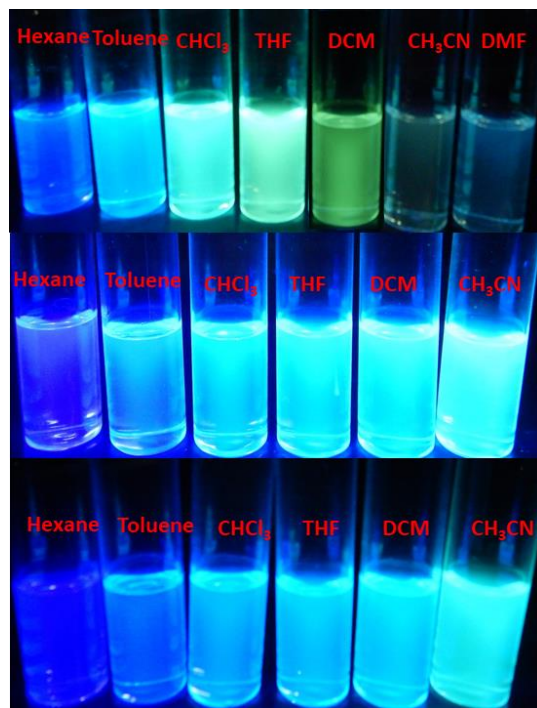


Figure S7: Digital photos of compounds **1**, **2** and **3** with different solvents.

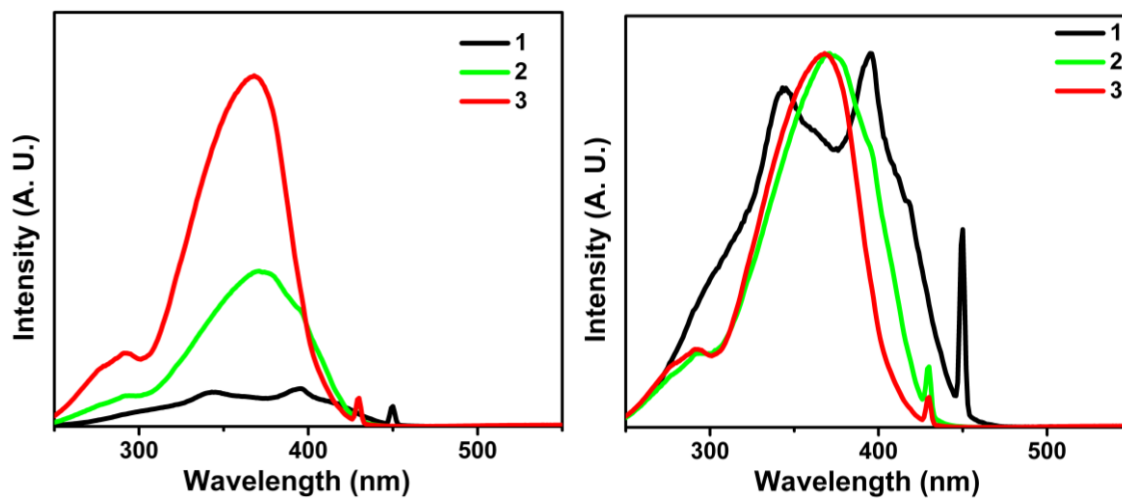


Figure S8: The excitation spectra (left) and normalised (right) of **1**, **2** and **3**.

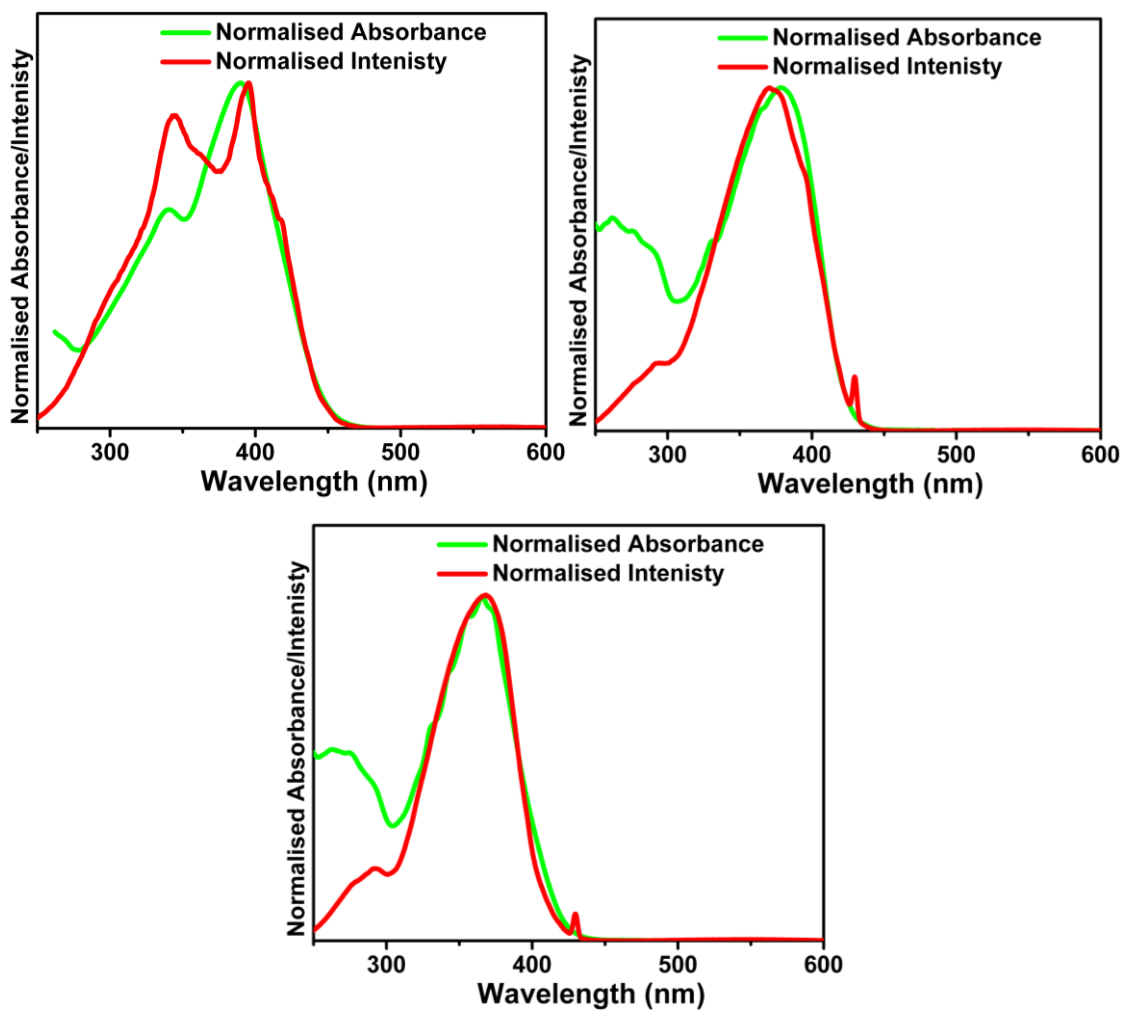


Figure S9: The compared normalised absorption and excitation spectra of **1** (top left), **2** (top left) and **3** (bottom).

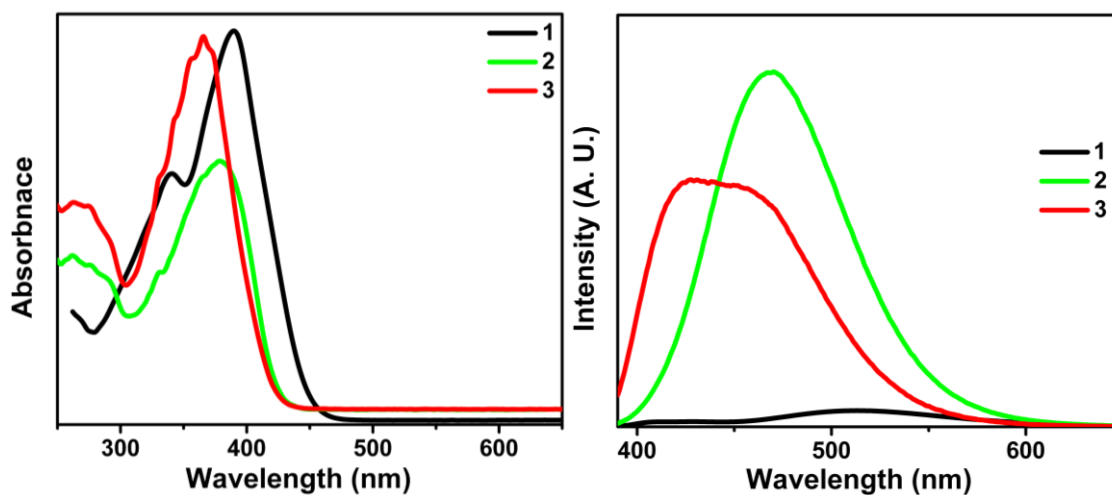


Figure S10: Compared UV-Visible (left) and Fluorescence (right) spectra of **1**, **2** and **3** in dichloromethane (10 μ M; λ_{ex} at 375 nm).

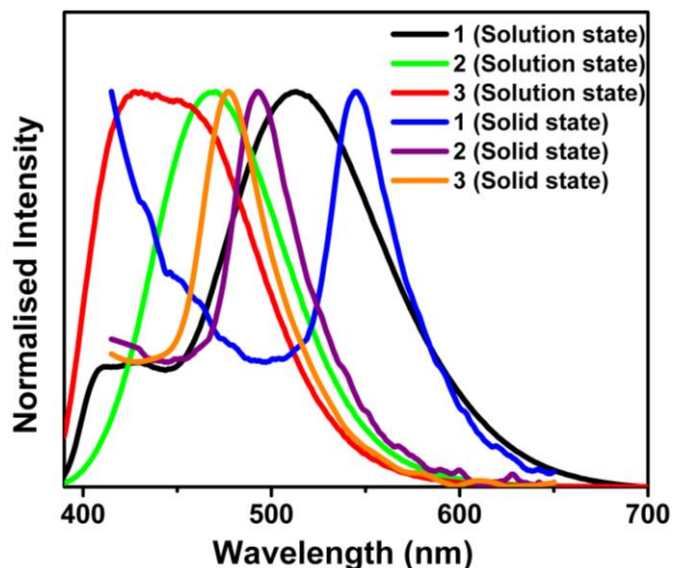


Figure S11: Compared fluorescence spectra of **1**, **2** and **3** in solution and solid state.

2. Sensing studies

Absorbance and Fluorescence titrations studies in Dichloromethane medium

The titration studies were carried out by placing 2 mL of compounds **1**, **2** and **3** were in 1×10^{-5} M stock solution in dichloromethane. A septum screw capped quartz cuvette of 1 cm width and followed by gradual incremental addition of 1×10^{-3} M DCM solution of anions. The experiment was repeated for at least three times at 298 K to obtain concordant value. Compounds **1**, **2** or **3** were excited at 375 nm and the emissions were monitored in the range of 400-700 nm (2 nm slit width kept constant for both source and detector).

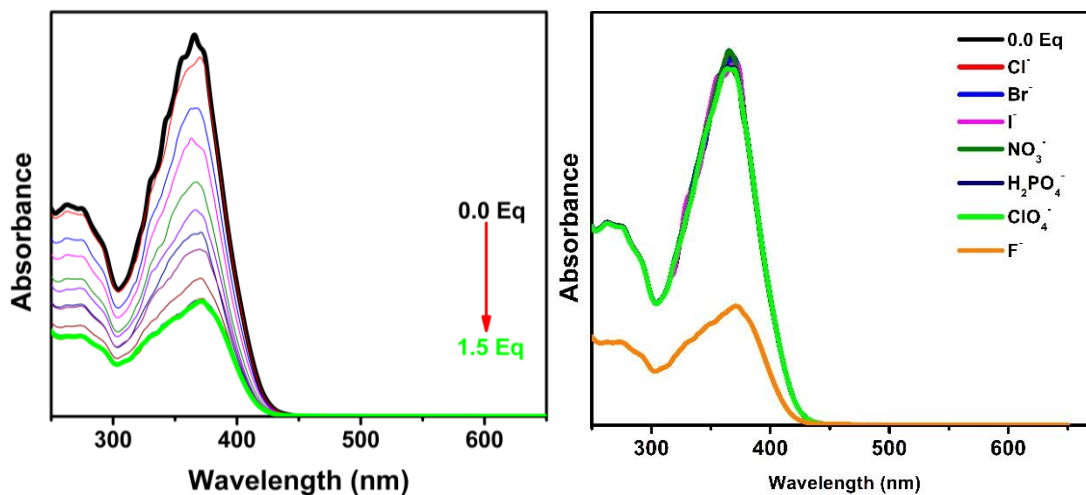


Figure S12: Changes associated with UV-Visible spectra of **3** with fluoride ions (left) and in presence of various anions (right) (DCM, 10 μ M).

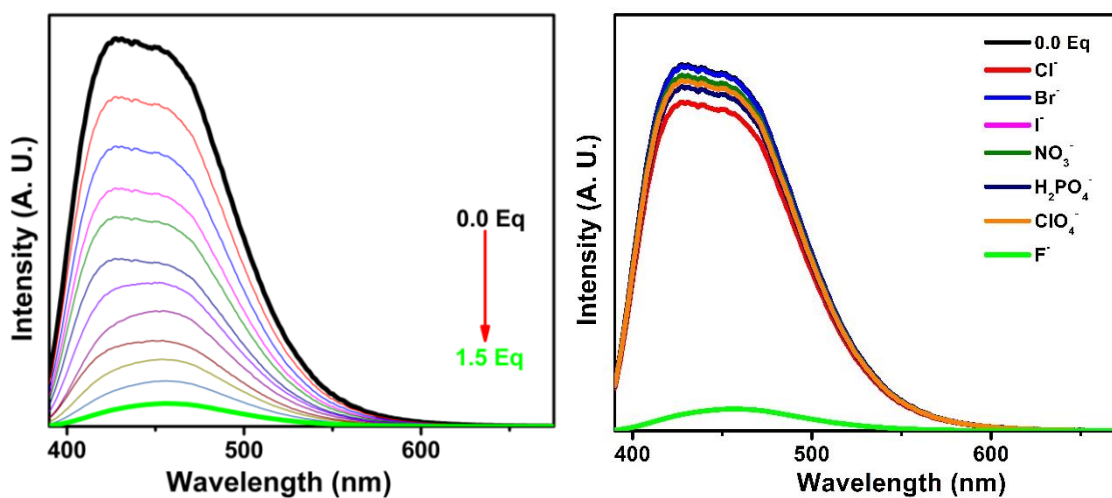


Figure S13: Changes associated with PL spectra of **3** with fluoride ions (left) and in presence of various anions (right) (DCM, 10 μ M).

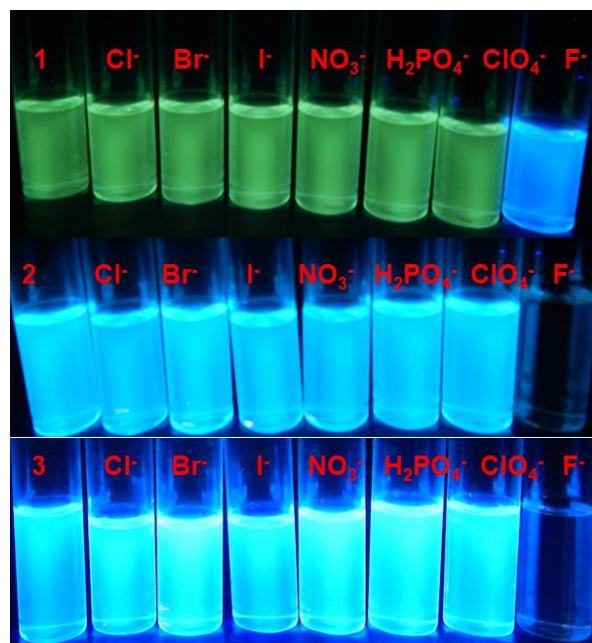


Figure S14: Digital photograph of compounds **1**, **2** and **3** with different anions.

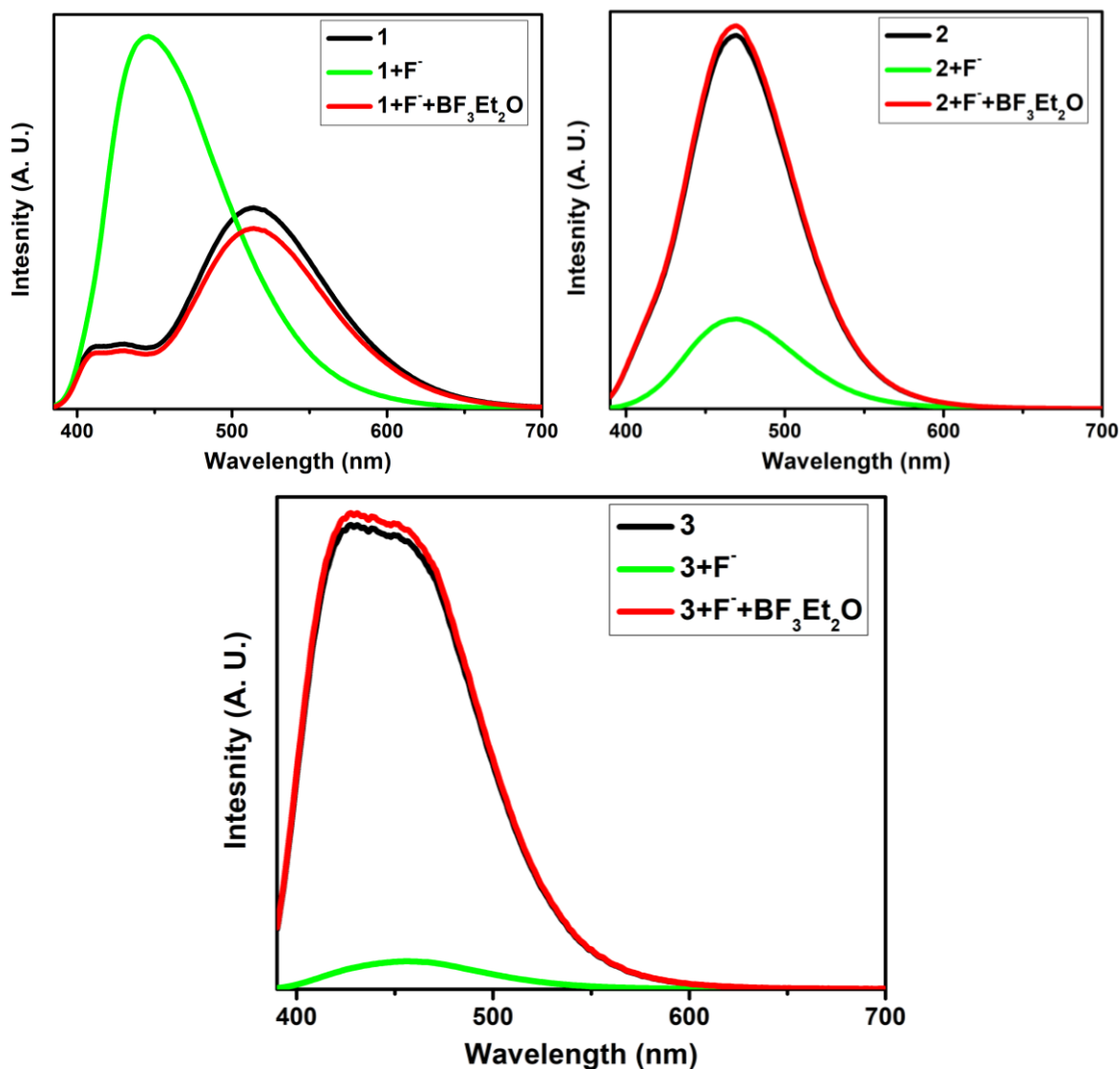


Figure S15: Reversible studies of **1**, **2** and **3**

3. Determination of Binding Constant²

Solution of compounds **1** or **2** or **3** (2 mL, 1×10^{-5} M) were placed in a septa screw capped quartz cuvette and was titrated against incremental amount of fluoride ions. The change in absorbance of the band around 375 nm with respect to fluoride concentration was used for calculations.

Sensor + F⁻ ↔ F⁻• **sensor**; here sensor is compound **1** or **2** or **3**

$$I = K_s[\text{sensor}] + K_p[\text{F} \cdot \text{sensor}]$$

$$I_0 = K_s[\text{sensor}]_0$$

$$[\text{sensor}]_0 = [\text{sensor}] + [\text{F} \cdot \text{sensor}]$$

$$K = [\text{F} \cdot \text{sensor}] / [\text{sensor}][\text{F}]$$

$$I/I_0 = (1 + (K_p/K_s)K[\text{F}]) / (1 + K[\text{F}]) (1 - I/I_0) / [\text{F}] \rightarrow K(I/I_0) - K(K_p/K_s)I/I_0 = 1 + K(1 - I/I_0) / [\text{F}]$$

Here, I_0 is initial absorbance of respective band (375 nm), I is absorbance of respective band upon addition of 1.0 equiv of Fluoride. The association constant was obtained from the slope of $(1 - I/I_0)/[F^-]$ Vs I/I_0 .

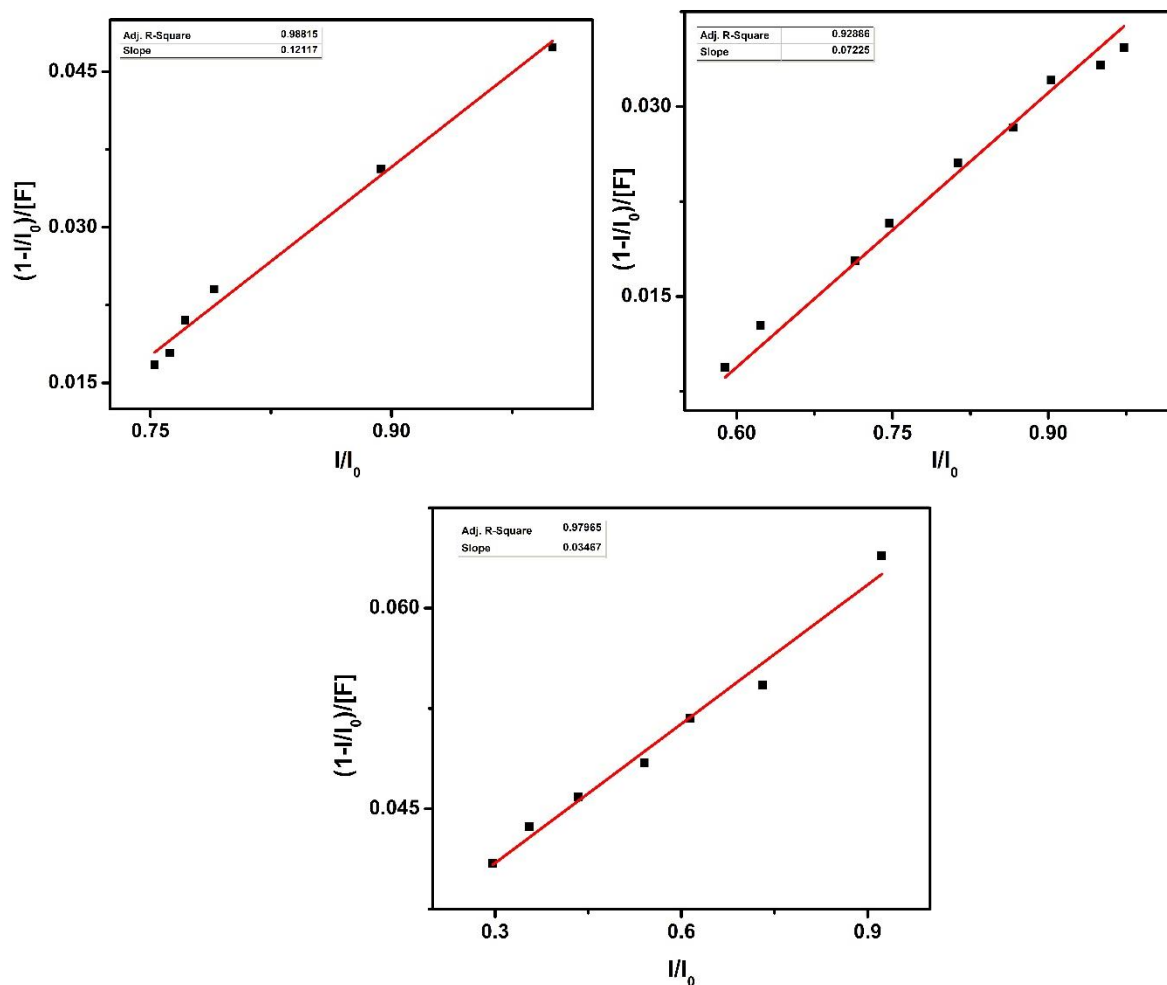


Figure S16: The association constant of **1**, **2** and **3** obtained via plot of I/I_0 Vs $(1 - I/I_0)/[F^-]$ (λ_{abs} at 375 nm) in dichloromethane

4. Determination of quenching efficiency

Solution of compounds **1** or **2** or **3** (2 mL, 1×10^{-5} M) were placed in a septa screw capped quartz cuvette and was titrated against incremental amount of fluoride ions and monitored change in fluorescence band around ~ 470 nm. Fluorescence quenching efficiency for **1** and **2** were calculated by the following equation.

$$\eta = (I_0 - I)/I_0 \times 100 (\%)$$

Where, I_0 is the initial PL intensity of the sensors (**1** or **2** or **3**) and I is the intensity after addition of 1 equivalent of fluoride.

5. Calculation of Limit of Detection (LoD)

The limit of detection of compound **1**, **2** and **3** were calculated from the fluorescence quenching titration experiment. The intercept to X-axis ($\log[F^-]$) was obtained by linear fitting of the $(I_{\max}-I)/(I_{\max}-I_{\min})$ vs $\log[F^-]$, where I_{\max} , I and I_{\min} are the initial fluorescence intensity, PL intensity at particular concentration and PL intensity at saturation point respectively. Limit of detection were calculated using the formula, $([F^-] \times \text{MWPA})/1000$ (multiplied by 10^9 to get the values in ppb), where MWPA is the molecular weight of F^- source.

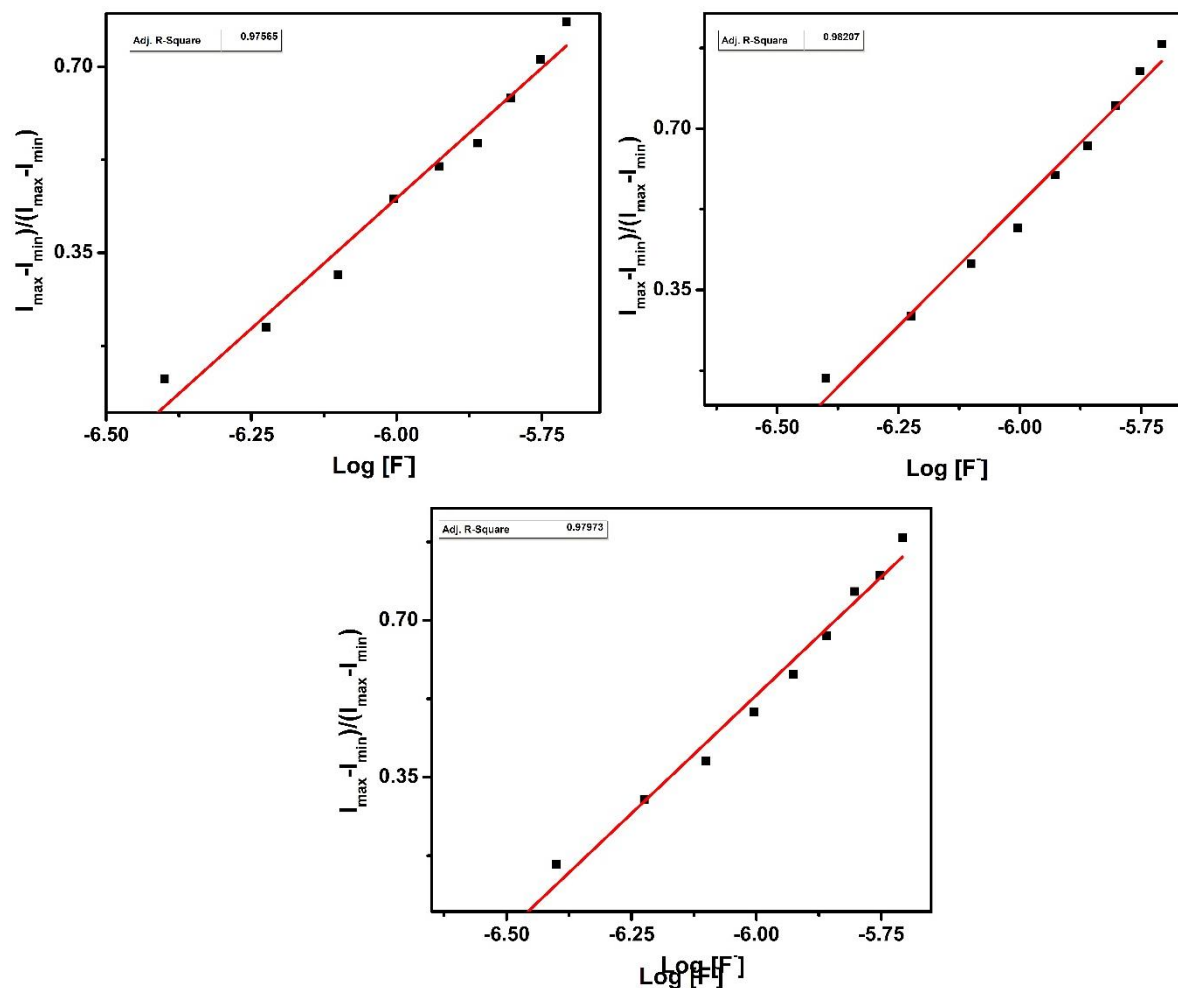


Figure S17: $(I_{\max}-I)/(I_{\max}-I_{\min})$ vs $\log[F^-]$ plots for PL data obtained for **1** (top left) **2** (top right) and **3** (bottom) in Dichloromethane.

6. Structural Characterization

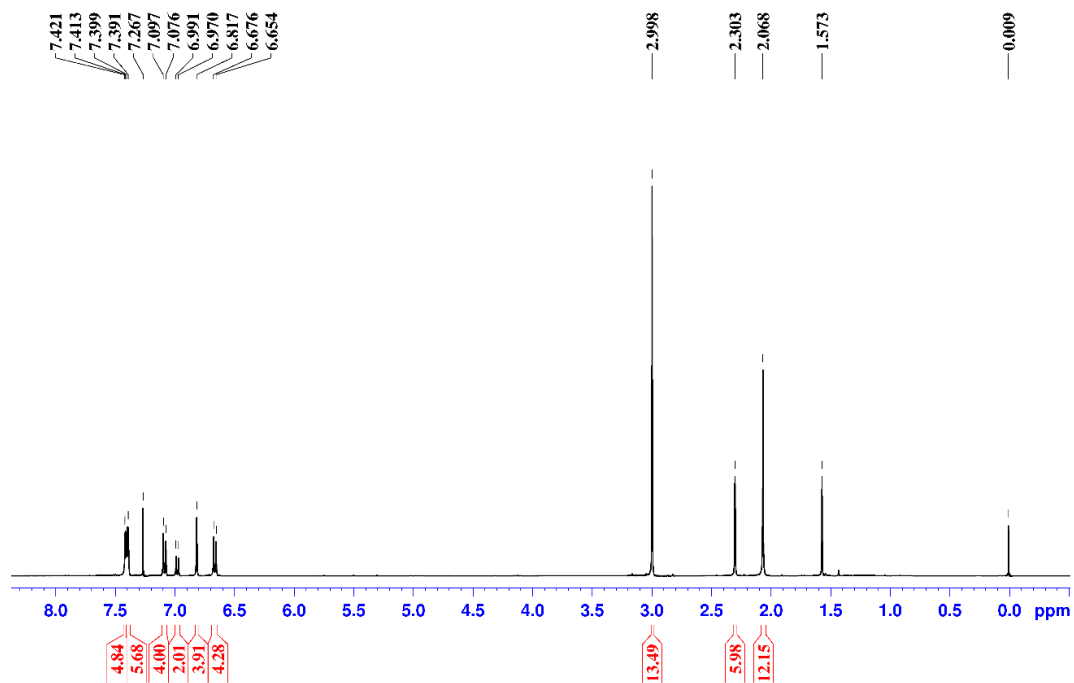


Figure S18: ^1H NMR (CDCl_3 , 400 MHz) of compound **1**

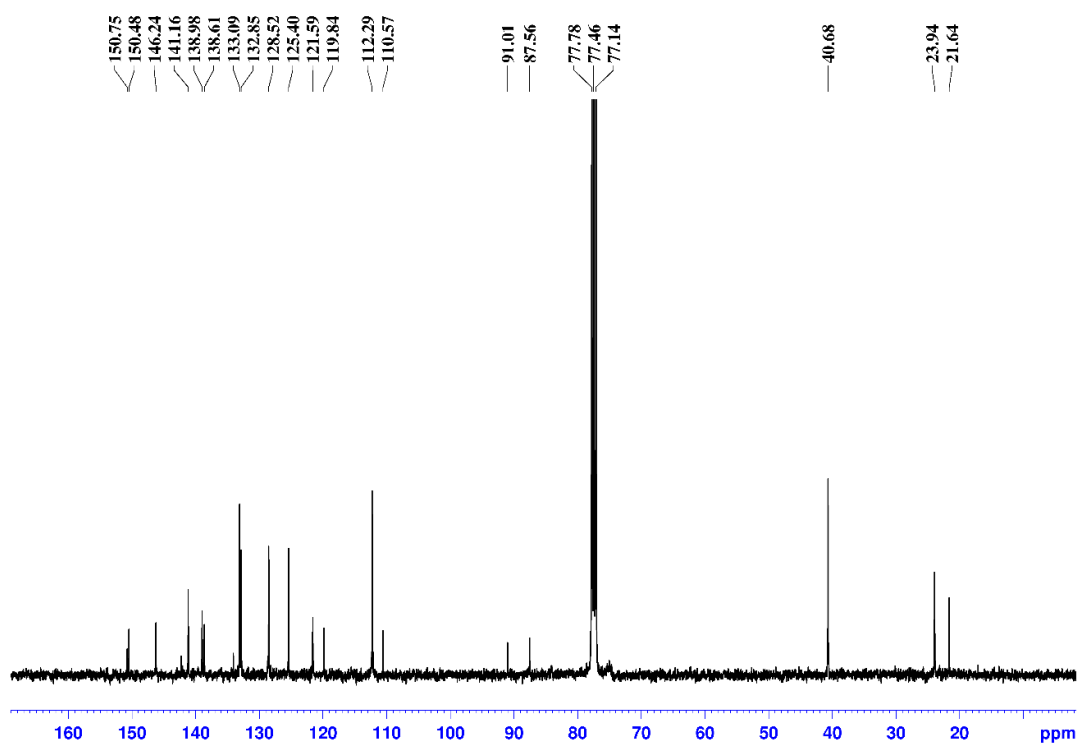


Figure S19: ^{13}C NMR (CDCl_3 , 400 MHz) of compound **1**

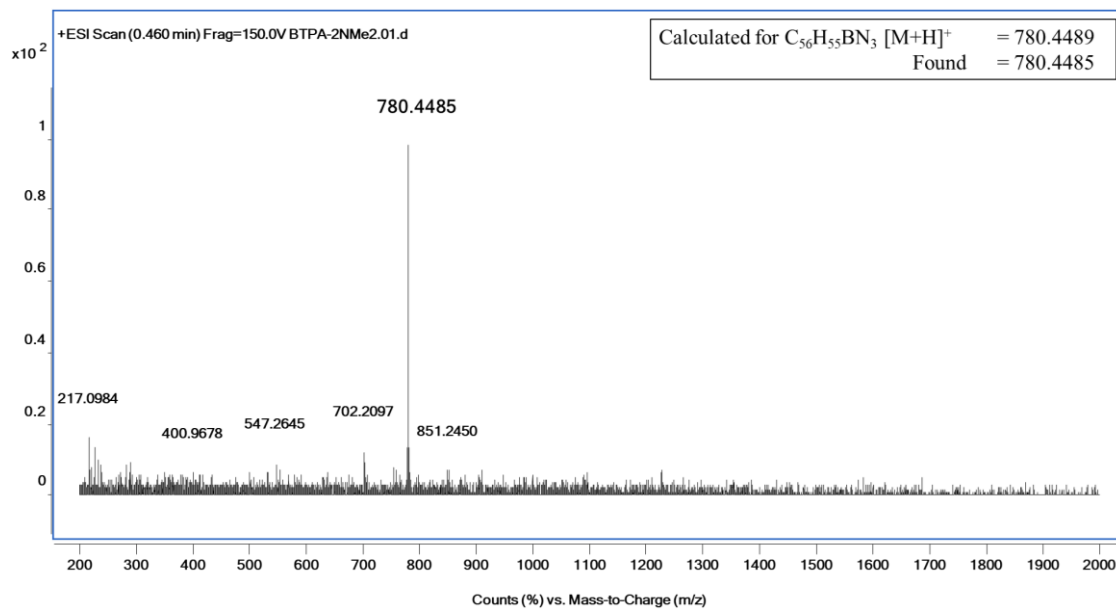


Figure S20: HRMS of compound 1

PT-TFA-BMes2-2Ph

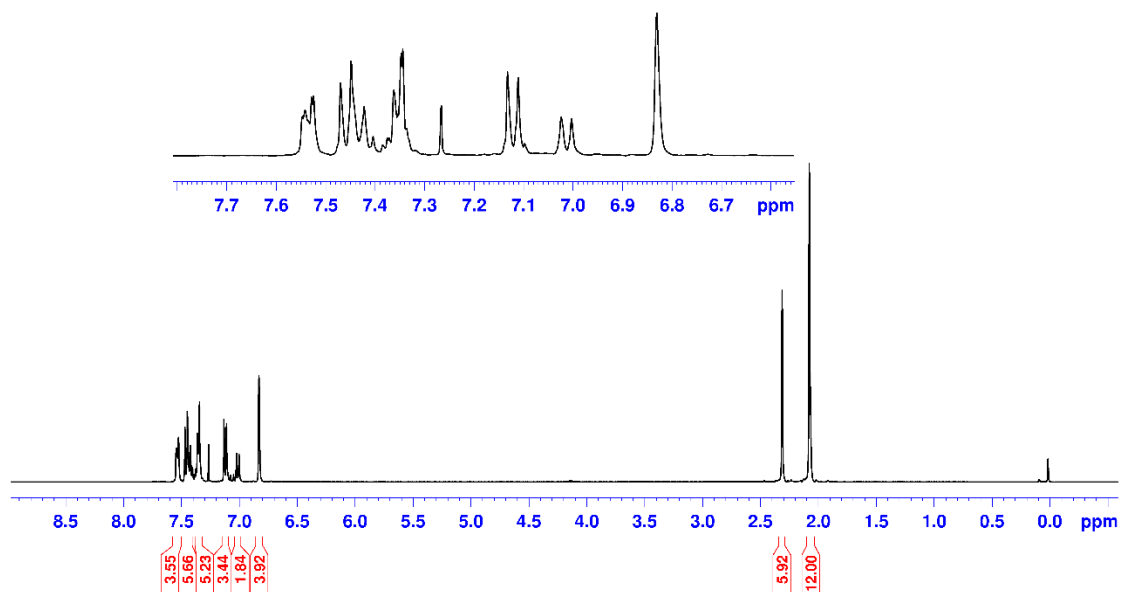


Figure S21: ^1H NMR (CDCl_3 , 400 MHz) of compound **2**

PT-TPH-BMes-2PH

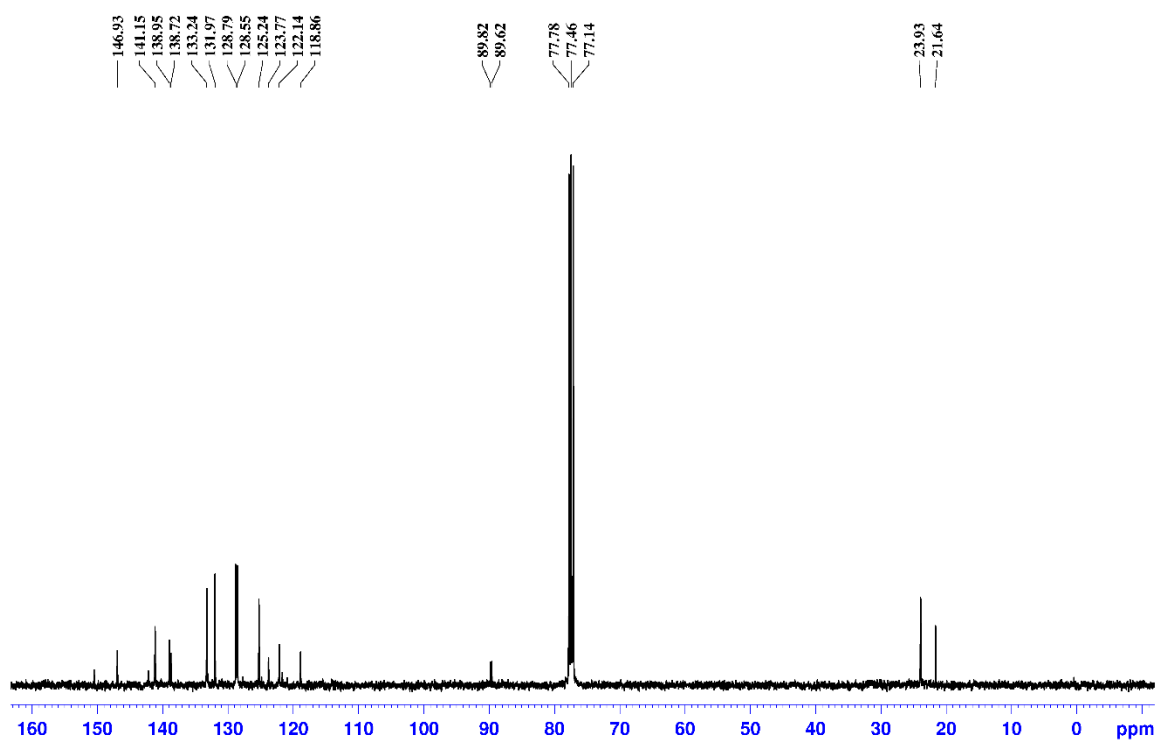


Figure S22: ^{13}C NMR (CDCl_3 , 400 MHz) of compound **2**

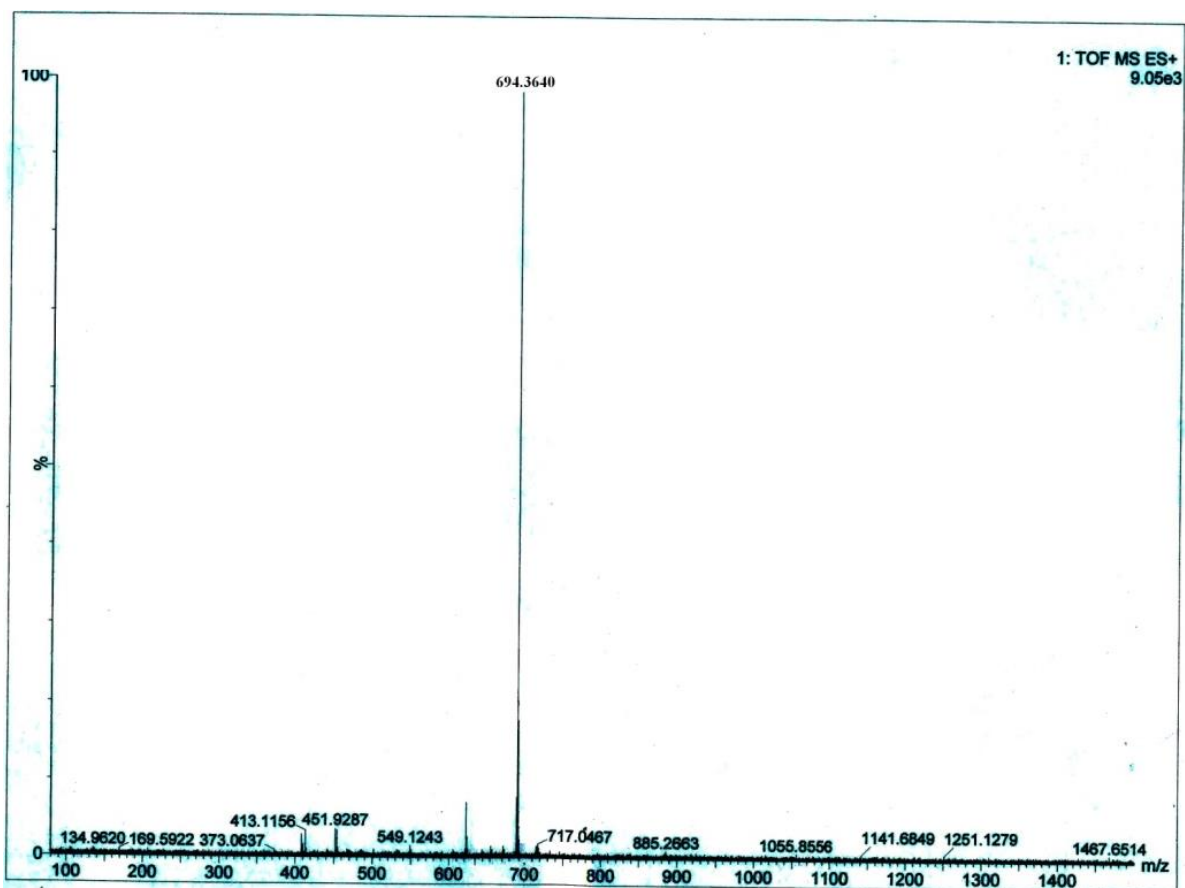


Figure S23: HRMS of compound 2

PT-TFA-BMES2-2CN

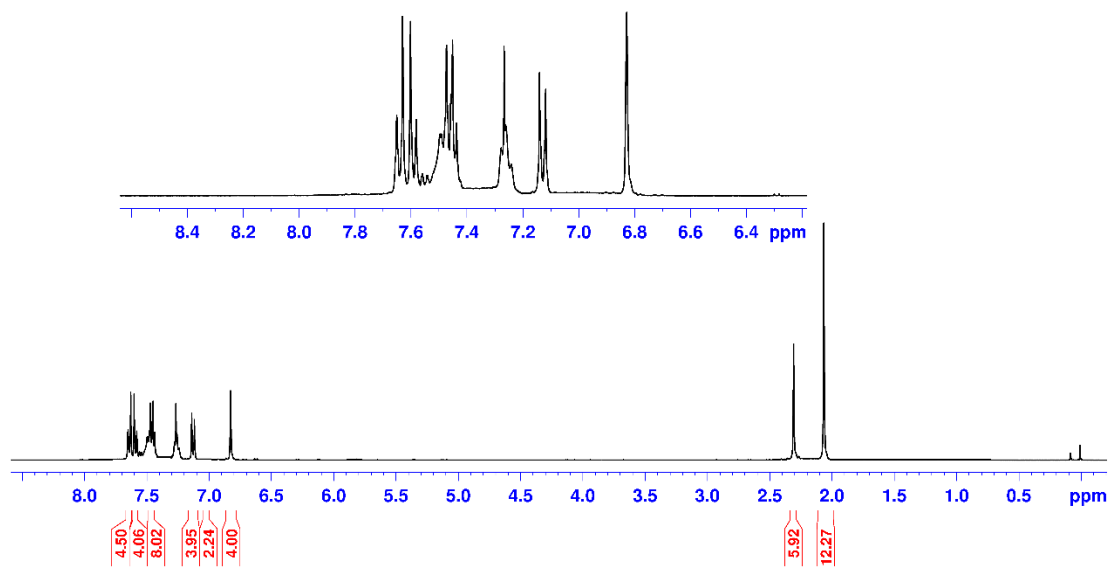


Figure S24: ^1H NMR (CDCl_3 , 400 MHz) of compound 3

PT-TPA-BMes2-2CN

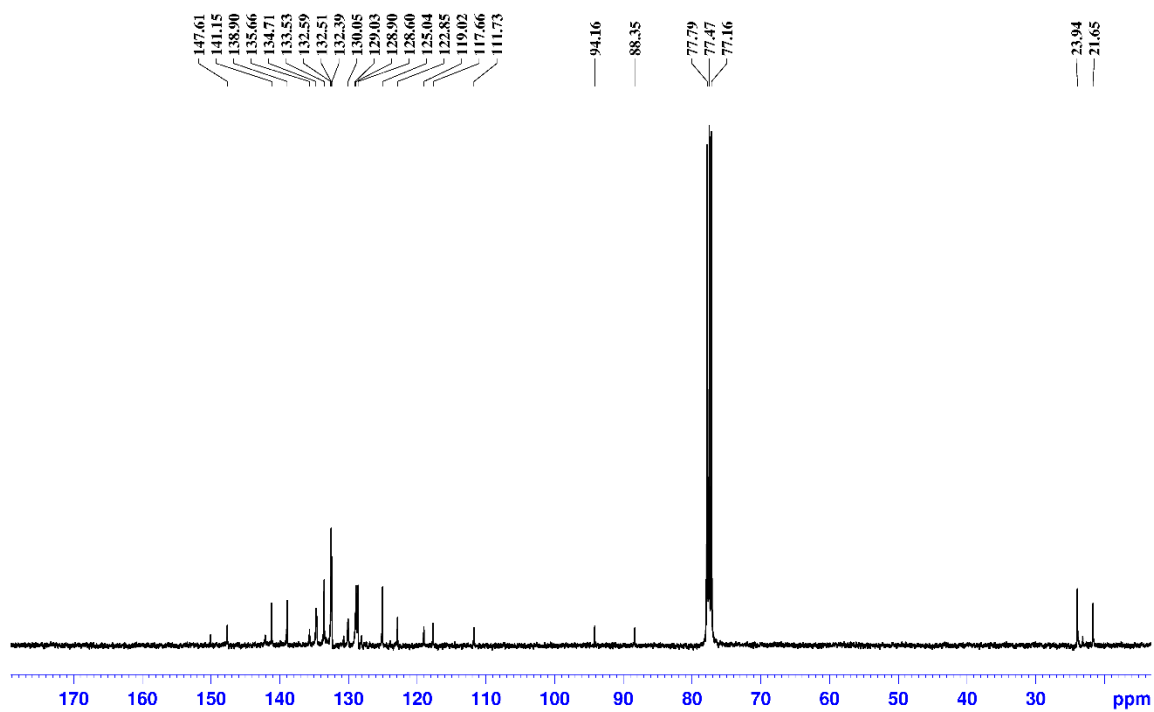


Figure S25: ^{13}C NMR (CDCl_3 , 400 MHz) of compound **3**

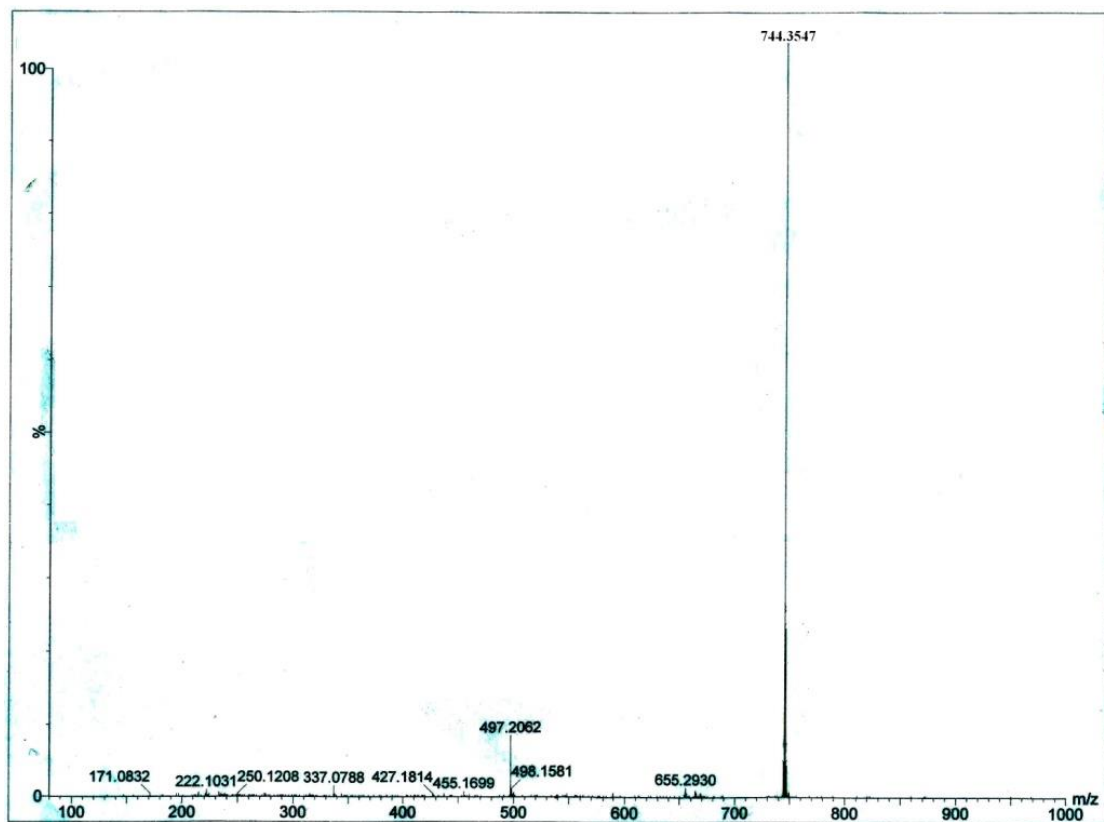


Figure S26: HRMS of compound 3

8. DFT Computational data

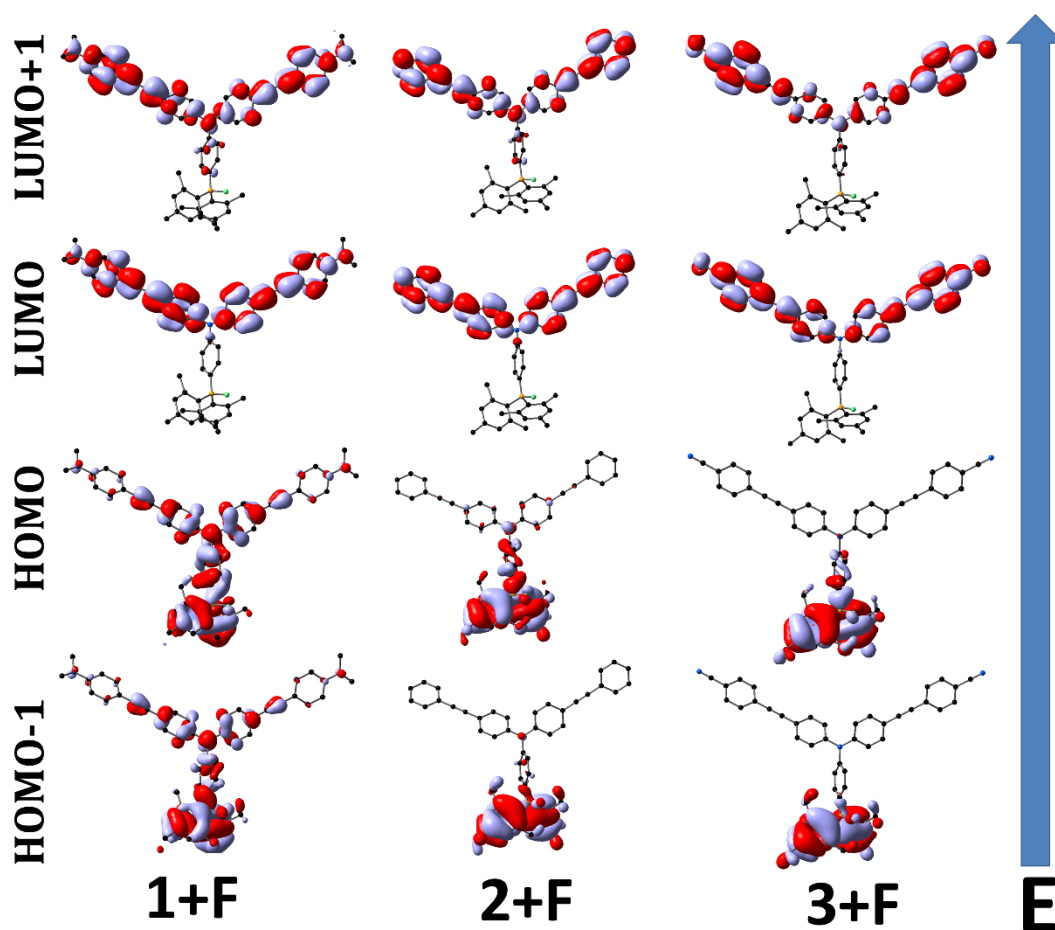
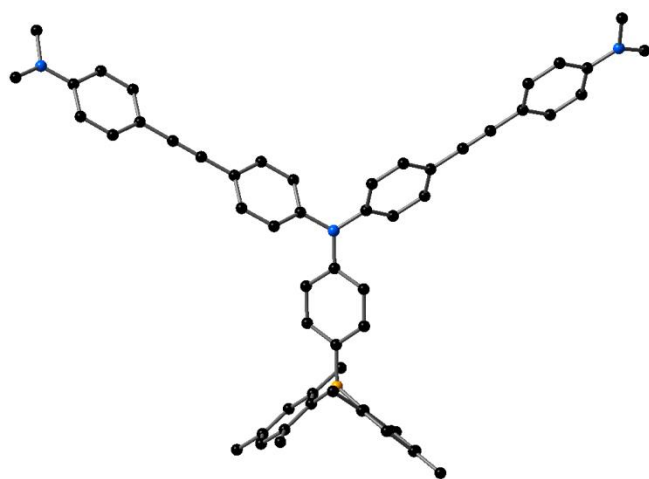


Figure S27: Optimized geometries and selected molecular orbital of $1+F^-$, $2+F^-$ and $3+F^-$.

Table S4: Spatial coordinate for optimized **1**



Atom	X	Y	Z
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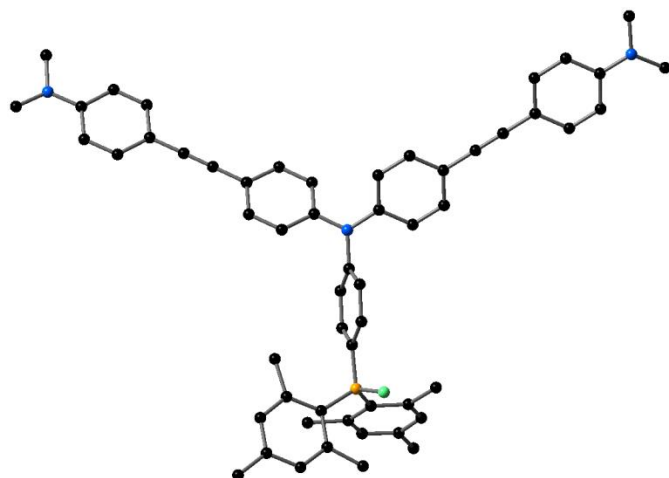
C	1.22414469	-1.08805176	0.04218180
C	1.42331572	-2.19428504	-0.79948107
C	2.24591947	-0.72380689	0.93435160
C	2.60838496	-2.91607189	-0.74973704
H	0.64106528	-2.48318282	-1.49428758
C	3.43709642	-1.43658634	0.97349316
H	2.09880762	0.12337276	1.59667644
C	3.64540936	-2.55143937	0.13445049
H	2.75070046	-3.76724289	-1.40836394
H	4.21822294	-1.14501498	1.66878184
C	-1.22415962	-1.08800347	-0.04349504
C	-1.42340009	-2.19408185	0.79835659
C	-2.24591628	-0.72382278	-0.93570472
C	-2.60853777	-2.91576395	0.74876965
H	-0.64115239	-2.48293121	1.49318695
C	-3.43716461	-1.43649644	-0.97469424
H	-2.09873877	0.12323366	-1.59817390
C	-3.64556047	-2.55117356	-0.13544612
H	-2.75092276	-3.76680915	1.40754347
H	-4.21828176	-1.14496912	-1.67001201
C	0.00001547	1.04892605	-0.00064619
C	-1.04423228	1.77036071	0.61117674
C	1.04427779	1.77041721	-0.61239052
C	-1.03124560	3.15813218	0.61054336
H	-1.85384019	1.23351084	1.09433632
C	1.03136054	3.15818607	-0.61153215
H	1.85384842	1.23359753	-1.09564802
C	0.00008397	3.90850565	-0.00041077
H	-1.84252618	3.68533285	1.10528660
H	1.84264898	3.68542980	-1.10621525
N	0.00001362	-0.36199291	-0.00073003

B	0.00019339	5.47153268	-0.00008335
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C	-0.80764831	6.06374896	2.43282822
C	-1.95379734	7.12062182	0.56934200
C	-1.67316352	6.73132400	3.31254142
C	-2.80407409	7.75347648	1.47607430
C	-2.68133554	7.57649897	2.85933778
H	-1.54827478	6.58065919	4.38416252
H	-3.58871000	8.40467348	1.09355483
C	0.93104632	6.24380750	-1.03197136
C	0.80815524	6.06514271	-2.43267902
C	1.95460301	7.12040993	-0.56845460
C	1.67397007	6.73294937	-3.31191409
C	2.80511705	7.75358284	-1.47475236
C	2.68239339	7.57751943	-2.85812495
H	1.54913026	6.58295857	-4.38363254
H	3.58996290	8.40425823	-1.09177665
C	-0.28011249	5.22042755	-3.06939788
H	-1.01627418	5.85872892	-3.57605336
H	0.13856358	4.55173121	-3.83118003
H	-0.81823476	4.60385783	-2.34841434
C	2.18448203	7.36871424	0.90857221
H	2.43960568	6.44588405	1.44380074
H	3.01076914	8.07099087	1.05930616
H	1.29544264	7.78435873	1.39335744
C	3.61271518	8.28535909	-3.81485177
H	3.51849249	9.37577834	-3.73211359
H	4.66211496	8.03959600	-3.60891289
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H	0.82062585	4.60457863	2.34711661

H	1.01420686	5.85516978	3.57988380
H	-0.13966842	4.54580992	3.82726236
C	-2.18363228	7.36993918	-0.90751437
H	-1.29444676	7.78552551	-1.39208138
H	-2.43915253	6.44752809	-1.44328169
H	-3.00964765	8.07263566	-1.05778054
C	-3.61139150	8.28403541	3.81654688
H	-3.51735040	9.37448117	3.73398794
H	-4.66083547	8.03816812	3.61094226
H	-3.40113489	8.00945433	4.85524695
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C	-5.90154407	-3.91978674	-0.20652736
C	4.86136992	-3.28665944	0.17668612
C	5.90121810	-3.92031538	0.20601330
C	-7.11256435	-4.66299225	-0.23233580
C	-8.16159782	-4.33083318	-1.11233242
C	-7.31005309	-5.76740446	0.62021444
C	-9.34377037	-5.05548125	-1.13910733
H	-8.03746458	-3.48931264	-1.78756504
C	-8.48838599	-6.49791143	0.60118019
H	-6.51711088	-6.05375376	1.30483610
C	-9.54795119	-6.15730009	-0.27383789
H	-10.11470468	-4.76046840	-1.84071410
H	-8.58332393	-7.34221564	1.27326058
C	7.11212434	-4.66369720	0.23212693
C	8.16100328	-4.33165067	1.11235605
C	7.30964075	-5.76819209	-0.62030148
C	9.34305471	-5.05648154	1.13945017
H	8.03683518	-3.49007742	1.78751625
C	8.48785898	-6.49888131	-0.60094448
H	6.51681047	-6.05447645	-1.30507992

C	9.54727845	-6.15837199	0.27428102
H	10.11386742	-4.76154997	1.84122528
H	8.58279327	-7.34326780	-1.27292173
C	-10.84295275	-8.09458281	0.49493693
H	-11.85222283	-8.49706105	0.39019298
H	-10.12861384	-8.86685715	0.16814436
H	-10.67180074	-7.90491457	1.56160447
C	-11.72583530	-6.60996699	-1.31059776
H	-12.06566928	-5.56756157	-1.27995528
H	-11.34551947	-6.81400556	-2.32404100
H	-12.59688005	-7.24509939	-1.13868711
C	10.84212929	-8.09597740	-0.49394326
H	10.67099935	-7.90648395	-1.56063793
H	11.85138699	-8.49847465	-0.38913715
H	10.12775091	-8.86816576	-0.16701726
C	11.72470064	-6.61149980	1.31179511
H	12.06470046	-5.56914418	1.28144112
H	11.34394189	-6.81563818	2.32505311
H	12.59572512	-7.24672777	1.14013129
N	10.73671999	-6.86973412	0.27817384
N	-10.73746719	-6.86851251	-0.27743464

Table S5: Spatial coordinate for optimized 1+F⁻ adduct



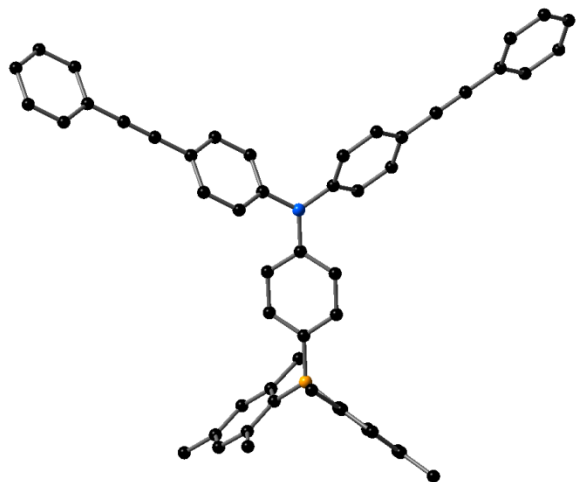
Atom	X	Y	Z
C	1.22414469	-1.08805176	0.04218180
C	1.42331572	-2.19428504	-0.79948107
C	2.24591947	-0.72380689	0.93435160
C	2.60838496	-2.91607189	-0.74973704
H	0.64106528	-2.48318282	-1.49428758
C	3.43709642	-1.43658634	0.97349316
H	2.09880762	0.12337276	1.59667644
C	3.64540936	-2.55143937	0.13445049
H	2.75070046	-3.76724289	-1.40836394
H	4.21822294	-1.14501498	1.66878184
C	-1.22415962	-1.08800347	-0.04349504
C	-1.42340009	-2.19408185	0.79835659
C	-2.24591628	-0.72382278	-0.93570472
C	-2.60853777	-2.91576395	0.74876965
H	-0.64115239	-2.48293121	1.49318695
C	-3.43716461	-1.43649644	-0.97469424
H	-2.09873877	0.12323366	-1.59817390
C	-3.64556047	-2.55117356	-0.13544612
H	-2.75092276	-3.76680915	1.40754347
H	-4.21828176	-1.14496912	-1.67001201
C	0.00001547	1.04892605	-0.00064619

C	-1.04423228	1.77036071	0.61117674
C	1.04427779	1.77041721	-0.61239052
C	-1.03124560	3.15813218	0.61054336
H	-1.85384019	1.23351084	1.09433632
C	1.03136054	3.15818607	-0.61153215
H	1.85384842	1.23359753	-1.09564802
C	0.00008397	3.90850565	-0.00041077
H	-1.84252618	3.68533285	1.10528660
H	1.84264898	3.68542980	-1.10621525
N	0.00001362	-0.36199291	-0.00073003
B	0.00019339	5.47153268	-0.00008335
C	-0.93051071	6.24337961	1.03226582
C	-0.80764831	6.06374896	2.43282822
C	-1.95379734	7.12062182	0.56934200
C	-1.67316352	6.73132400	3.31254142
C	-2.80407409	7.75347648	1.47607430
C	-2.68133554	7.57649897	2.85933778
H	-1.54827478	6.58065919	4.38416252
H	-3.58871000	8.40467348	1.09355483
C	0.93104632	6.24380750	-1.03197136
C	0.80815524	6.06514271	-2.43267902
C	1.95460301	7.12040993	-0.56845460
C	1.67397007	6.73294937	-3.31191409
C	2.80511705	7.75358284	-1.47475236
C	2.68239339	7.57751943	-2.85812495
H	1.54913026	6.58295857	-4.38363254
H	3.58996290	8.40425823	-1.09177665
C	-0.28011249	5.22042755	-3.06939788
H	-1.01627418	5.85872892	-3.57605336
H	0.13856358	4.55173121	-3.83118003
H	-0.81823476	4.60385783	-2.34841434

C	2.18448203	7.36871424	0.90857221
H	2.43960568	6.44588405	1.44380074
H	3.01076914	8.07099087	1.05930616
H	1.29544264	7.78435873	1.39335744
C	3.61271518	8.28535909	-3.81485177
H	3.51849249	9.37577834	-3.73211359
H	4.66211496	8.03959600	-3.60891289
H	3.40286573	8.01096677	-4.85368420
C	0.28006812	5.21790093	3.06903825
H	0.82062585	4.60457863	2.34711661
H	1.01420686	5.85516978	3.57988380
H	-0.13966842	4.54580992	3.82726236
C	-2.18363228	7.36993918	-0.90751437
H	-1.29444676	7.78552551	-1.39208138
H	-2.43915253	6.44752809	-1.44328169
H	-3.00964765	8.07263566	-1.05778054
C	-3.61139150	8.28403541	3.81654688
H	-3.51735040	9.37448117	3.73398794
H	-4.66083547	8.03816812	3.61094226
H	-3.40113489	8.00945433	4.85524695
C	-4.86160210	-3.28627180	-0.17747076
C	-5.90154407	-3.91978674	-0.20652736
C	4.86136992	-3.28665944	0.17668612
C	5.90121810	-3.92031538	0.20601330
C	-7.11256435	-4.66299225	-0.23233580
C	-8.16159782	-4.33083318	-1.11233242
C	-7.31005309	-5.76740446	0.62021444
C	-9.34377037	-5.05548125	-1.13910733
H	-8.03746458	-3.48931264	-1.78756504
C	-8.48838599	-6.49791143	0.60118019
H	-6.51711088	-6.05375376	1.30483610

C	-9.54795119	-6.15730009	-0.27383789
H	-10.11470468	-4.76046840	-1.84071410
H	-8.58332393	-7.34221564	1.27326058
C	7.11212434	-4.66369720	0.23212693
C	8.16100328	-4.33165067	1.11235605
C	7.30964075	-5.76819209	-0.62030148
C	9.34305471	-5.05648154	1.13945017
H	8.03683518	-3.49007742	1.78751625
C	8.48785898	-6.49888131	-0.60094448
H	6.51681047	-6.05447645	-1.30507992
C	9.54727845	-6.15837199	0.27428102
H	10.11386742	-4.76154997	1.84122528
H	8.58279327	-7.34326780	-1.27292173
C	-10.84295275	-8.09458281	0.49493693
H	-11.85222283	-8.49706105	0.39019298
H	-10.12861384	-8.86685715	0.16814436
H	-10.67180074	-7.90491457	1.56160447
C	-11.72583530	-6.60996699	-1.31059776
H	-12.06566928	-5.56756157	-1.27995528
H	-11.34551947	-6.81400556	-2.32404100
H	-12.59688005	-7.24509939	-1.13868711
C	10.84212929	-8.09597740	-0.49394326
H	10.67099935	-7.90648395	-1.56063793
H	11.85138699	-8.49847465	-0.38913715
H	10.12775091	-8.86816576	-0.16701726
C	11.72470064	-6.61149980	1.31179511
H	12.06470046	-5.56914418	1.28144112
H	11.34394189	-6.81563818	2.32505311
H	12.59572512	-7.24672777	1.14013129
N	10.73671999	-6.86973412	0.27817384
N	-10.73746719	-6.86851251	-0.27743464

Table S6: Spatial coordinate for optimized 2



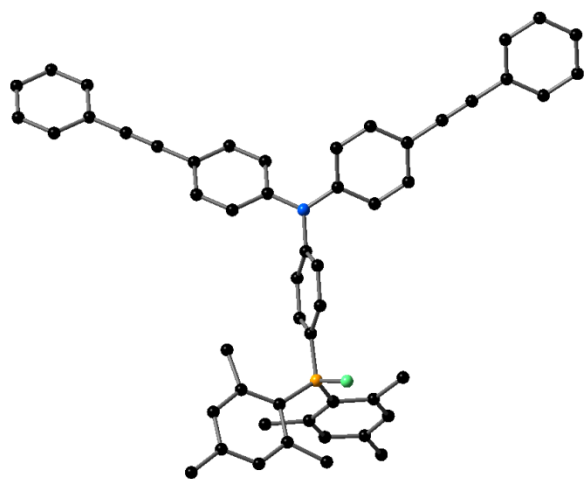
Atom	X	Y	Z
C	-2.06744471	-1.22392439	0.07781971
C	-3.19470719	-1.44119744	-0.73201345
C	-1.66940988	-2.23384276	0.96995161
C	-3.90391134	-2.63198946	-0.65079773
H	-3.50828569	-0.67024416	-1.42846433
C	-2.37043725	-3.43000538	1.04029662
H	-0.80618747	-2.07315471	1.60761364
C	-3.50492731	-3.65523522	0.23350757
H	-4.77021027	-2.78918045	-1.28580660
H	-2.05363587	-4.20157639	1.73510732
C	-2.06735598	1.22399065	-0.07793108
C	-3.19439721	1.44146405	0.73215151
C	-1.66943103	2.23376518	-0.97027205
C	-3.90350989	2.63231405	0.65096722
H	-3.50787624	0.67061732	1.42876635
C	-2.37036087	3.42998690	-1.04059079
H	-0.80637044	2.07291655	-1.60811404
C	-3.50464005	3.65541304	-0.23355824

H	-4.76963986	2.78966410	1.28616699
H	-2.05365279	4.20145090	-1.73556248
C	0.06689738	-0.00002908	-0.00009952
C	0.78525153	1.02540109	0.64270883
C	0.78519360	-1.02548853	-0.64292890
C	2.17384944	1.01310205	0.64155500
H	0.24673063	1.81948688	1.14966642
C	2.17379164	-1.01326927	-0.64179022
H	0.24662545	-1.81955053	-1.14987364
C	2.92203340	-0.00010432	-0.00012067
H	2.70198442	1.80827232	1.16072763
H	2.70186397	-1.80847483	-1.16096789
N	-1.34849417	0.00000219	-0.00007201
B	4.48849334	-0.00011957	-0.00002390
C	5.25747395	0.88093653	1.07493772
C	5.07468669	0.69606098	2.46868978
C	6.13588386	1.92344524	0.65930333
C	5.74024592	1.52202465	3.38683061
C	6.76746337	2.73209777	1.60423524
C	6.58755289	2.54836251	2.98026882
H	5.58726935	1.35018321	4.45149562
H	7.41949298	3.53272861	1.25822157
C	5.25759407	-0.88117624	-1.07489423
C	5.07479119	-0.69640648	-2.46868125
C	6.13595948	-1.92368749	-0.65919821
C	5.74020179	-1.52255018	-3.38675168
C	6.76743236	-2.73249673	-1.60408218
C	6.58744981	-2.54892181	-2.98011442
H	5.58716526	-1.35084768	-4.45142948
H	7.41942043	-3.53313311	-1.25800287
C	4.23504132	0.42378693	-3.05379185

H	4.87848723	1.20842088	-3.47404934
H	3.60729682	0.05505610	-3.87371459
H	3.57972061	0.89475490	-2.31976192
C	6.38593938	-2.22117025	0.80549493
H	5.46552297	-2.51362721	1.32580987
H	7.09781809	-3.04530725	0.91726832
H	6.79009495	-1.35194861	1.33379683
C	7.29436420	-3.43453148	-3.97889543
H	8.38454712	-3.33258538	-3.90262586
H	7.06070704	-4.49336368	-3.81123293
H	7.00814530	-3.18722374	-5.00618039
C	4.23467975	-0.42398023	3.05373807
H	3.58013444	-0.89554197	2.31940501
H	4.87791127	-1.20819124	3.47510235
H	3.60606376	-0.05487506	3.87282986
C	6.38578279	2.22104554	-0.80537920
H	6.79026032	1.35196386	-1.33368200
H	5.46527929	2.51318954	-1.32570439
H	7.09738395	3.04542796	-0.91712269
C	7.29453449	3.43388444	3.97908078
H	8.38474170	3.33319637	3.90159427
H	7.05954402	4.49260848	3.81255419
H	7.00961578	3.18542096	5.00644741
C	-4.22457049	4.87979544	-0.30862919
C	-4.83902052	5.92845157	-0.37082657
C	-4.22494517	-4.87956463	0.30859314
C	-4.83946964	-5.92817730	0.37079824
C	-5.55619220	7.15708028	-0.44228899
C	-5.15189807	8.17304429	-1.33220511
C	-6.68196504	7.37991269	0.37658681
C	-5.85451048	9.37291692	-1.39718482

H	-4.28561309	8.00677262	-1.96513465
C	-7.37820382	8.58310480	0.30465980
H	-6.99767531	6.60092864	1.06376771
C	-6.96864052	9.58344062	-0.58069777
H	-5.53156477	10.14750679	-2.08760527
H	-8.24399934	8.74136859	0.94207495
H	-7.51448426	10.52139401	-0.63418195
C	-5.55679139	-7.15671588	0.44231410
C	-5.15237016	-8.17285733	1.33196983
C	-6.68284020	-7.37928434	-0.37625498
C	-5.85512395	-9.37264519	1.39699093
H	-4.28587531	-8.00678855	1.96466532
C	-7.37921809	-8.58239343	-0.30428920
H	-6.99865265	-6.60016207	-1.06323236
C	-6.96952446	-9.58290784	0.58080600
H	-5.53207579	-10.14737370	2.08720793
H	-8.24522507	-8.74045243	-0.94146798
H	-7.51547499	-10.52079726	0.63432092

Table S7: Spatial coordinate for optimized 2+F⁻ adduct



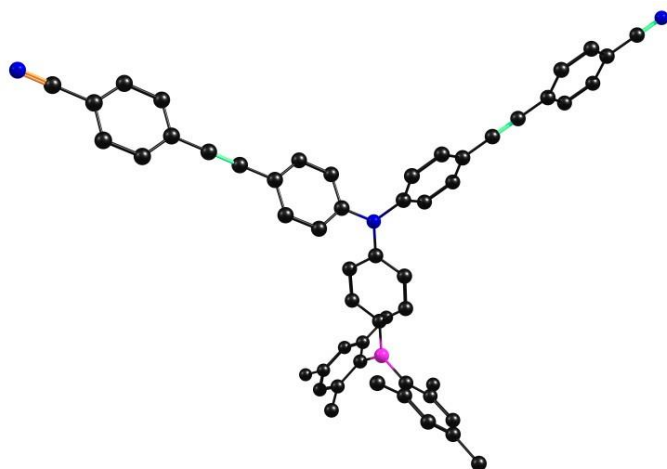
Atom	X	Y	Z
C	-2.06744471	-1.22392439	0.07781971
C	-3.19470719	-1.44119744	-0.73201345
C	-1.66940988	-2.23384276	0.96995161
C	-3.90391134	-2.63198946	-0.65079773
H	-3.50828569	-0.67024416	-1.42846433
C	-2.37043725	-3.43000538	1.04029662
H	-0.80618747	-2.07315471	1.60761364
C	-3.50492731	-3.65523522	0.23350757
H	-4.77021027	-2.78918045	-1.28580660
H	-2.05363587	-4.20157639	1.73510732
C	-2.06735598	1.22399065	-0.07793108
C	-3.19439721	1.44146405	0.73215151
C	-1.66943103	2.23376518	-0.97027205
C	-3.90350989	2.63231405	0.65096722
H	-3.50787624	0.67061732	1.42876635
C	-2.37036087	3.42998690	-1.04059079
H	-0.80637044	2.07291655	-1.60811404
C	-3.50464005	3.65541304	-0.23355824
H	-4.76963986	2.78966410	1.28616699
H	-2.05365279	4.20145090	-1.73556248
C	0.06689738	-0.00002908	-0.00009952
C	0.78525153	1.02540109	0.64270883
C	0.78519360	-1.02548853	-0.64292890
C	2.17384944	1.01310205	0.64155500
H	0.24673063	1.81948688	1.14966642
C	2.17379164	-1.01326927	-0.64179022
H	0.24662545	-1.81955053	-1.14987364
C	2.92203340	-0.00010432	-0.00012067
H	2.70198442	1.80827232	1.16072763
H	2.70186397	-1.80847483	-1.16096789

N	-1.34849417	0.00000219	-0.00007201
B	4.48849334	-0.00011957	-0.00002390
C	5.25747395	0.88093653	1.07493772
C	5.07468669	0.69606098	2.46868978
C	6.13588386	1.92344524	0.65930333
C	5.74024592	1.52202465	3.38683061
C	6.76746337	2.73209777	1.60423524
C	6.58755289	2.54836251	2.98026882
H	5.58726935	1.35018321	4.45149562
H	7.41949298	3.53272861	1.25822157
C	5.25759407	-0.88117624	-1.07489423
C	5.07479119	-0.69640648	-2.46868125
C	6.13595948	-1.92368749	-0.65919821
C	5.74020179	-1.52255018	-3.38675168
C	6.76743236	-2.73249673	-1.60408218
C	6.58744981	-2.54892181	-2.98011442
H	5.58716526	-1.35084768	-4.45142948
H	7.41942043	-3.53313311	-1.25800287
C	4.23504132	0.42378693	-3.05379185
H	4.87848723	1.20842088	-3.47404934
H	3.60729682	0.05505610	-3.87371459
H	3.57972061	0.89475490	-2.31976192
C	6.38593938	-2.22117025	0.80549493
H	5.46552297	-2.51362721	1.32580987
H	7.09781809	-3.04530725	0.91726832
H	6.79009495	-1.35194861	1.33379683
C	7.29436420	-3.43453148	-3.97889543
H	8.38454712	-3.33258538	-3.90262586
H	7.06070704	-4.49336368	-3.81123293
H	7.00814530	-3.18722374	-5.00618039
C	4.23467975	-0.42398023	3.05373807

H	3.58013444	-0.89554197	2.31940501
H	4.87791127	-1.20819124	3.47510235
H	3.60606376	-0.05487506	3.87282986
C	6.38578279	2.22104554	-0.80537920
H	6.79026032	1.35196386	-1.33368200
H	5.46527929	2.51318954	-1.32570439
H	7.09738395	3.04542796	-0.91712269
C	7.29453449	3.43388444	3.97908078
H	8.38474170	3.33319637	3.90159427
H	7.05954402	4.49260848	3.81255419
H	7.00961578	3.18542096	5.00644741
C	-4.22457049	4.87979544	-0.30862919
C	-4.83902052	5.92845157	-0.37082657
C	-4.22494517	-4.87956463	0.30859314
C	-4.83946964	-5.92817730	0.37079824
C	-5.55619220	7.15708028	-0.44228899
C	-5.15189807	8.17304429	-1.33220511
C	-6.68196504	7.37991269	0.37658681
C	-5.85451048	9.37291692	-1.39718482
H	-4.28561309	8.00677262	-1.96513465
C	-7.37820382	8.58310480	0.30465980
H	-6.99767531	6.60092864	1.06376771
C	-6.96864052	9.58344062	-0.58069777
H	-5.53156477	10.14750679	-2.08760527
H	-8.24399934	8.74136859	0.94207495
H	-7.51448426	10.52139401	-0.63418195
C	-5.55679139	-7.15671588	0.44231410
C	-5.15237016	-8.17285733	1.33196983
C	-6.68284020	-7.37928434	-0.37625498
C	-5.85512395	-9.37264519	1.39699093
H	-4.28587531	-8.00678855	1.96466532

C	-7.37921809	-8.58239343	-0.30428920
H	-6.99865265	-6.60016207	-1.06323236
C	-6.96952446	-9.58290784	0.58080600
H	-5.53207579	-10.14737370	2.08720793
H	-8.24522507	-8.74045243	-0.94146798
H	-7.51547499	-10.52079726	0.63432092
F	4.49914449	-1.12925361	0.92547211

Table S8: Spatial coordinate for optimized compound 3



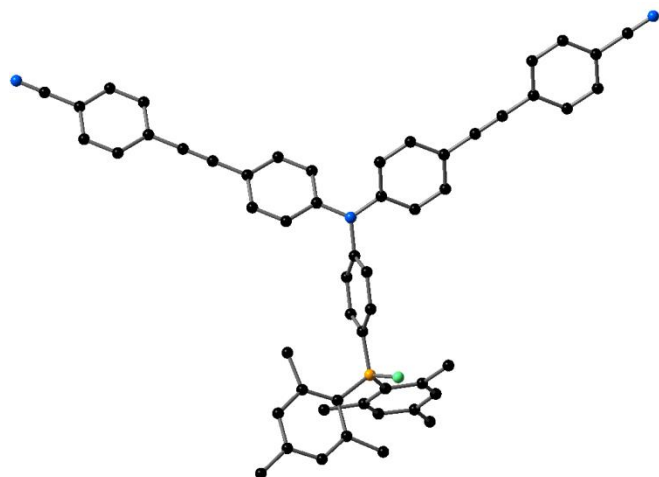
Atom	X	Y	Z
C	1.41260469	0.16132960	0.00063520
C	2.01962814	1.13962140	0.80499056
C	2.22382906	-0.65489476	-0.80446353
C	3.40386890	1.30002797	0.79388307
H	1.40089636	1.77019707	1.43547629
C	3.60860377	-0.49916974	-0.79458952
H	1.76248862	-1.40880087	-1.43435756
C	4.20848884	0.48068343	-0.00074553
H	3.85563518	2.06258205	1.42313387
H	4.22003018	-1.14026963	-1.42442074
C	-0.84588512	1.14262393	0.00064333

C	-0.54275565	2.25512967	-0.80142534
C	-1.99869839	1.17740030	0.80214202
C	-1.37029512	3.37631427	-0.79141510
H	0.34228497	2.23393644	-1.42925096
C	-2.83022022	2.29557282	0.79066659
H	-2.23657908	0.32513058	1.43061940
C	-2.52112917	3.40378967	-0.00082520
H	-1.11939413	4.22775175	-1.41881726
H	-3.71812818	2.30411546	1.41762269
C	-0.56620519	-1.30384527	0.00037244
C	-1.68090897	-1.59733160	-0.80201396
C	-0.02052343	-2.31960918	0.80231648
C	-2.23855720	-2.87438950	-0.79181039
H	-2.10481046	-0.82040230	-1.43022274
C	-0.57377380	-3.59860227	0.79133445
H	0.83660210	-2.09953080	1.43070685
C	-1.68804158	-3.88471391	-0.00036709
H	-3.10118865	-3.08270899	-1.41951141
H	-0.13767657	-4.37170548	1.41875804
N	0.00013985	0.00006776	0.00108464
B	-2.34595684	-5.39787201	-0.00064286
C	-1.90305693	-6.48984126	-1.15560729
C	-0.83907718	-7.36068784	-0.92082771
C	-2.59326852	-6.54239962	-2.36691050
C	-0.46489567	-8.28407804	-1.89745976
C	-2.21892992	-7.46522142	-3.34354121
C	-1.15416285	-8.33608320	-3.10883417
H	0.37446096	-8.96997911	-1.71235990
H	-2.76228079	-7.50645075	-4.29871989
C	-3.44677202	-5.81906087	1.15404580
C	-4.80900072	-5.63049267	0.92097254

C	-3.01491027	-6.36435876	2.36340742
C	-5.73963785	-5.98690960	1.89737048
C	-3.94523750	-6.72027398	3.33980519
C	-5.30801268	-6.53113908	3.10680659
H	-6.81347472	-5.83740625	1.71361818
H	-3.60515742	-7.14945085	4.29345560
C	-5.28584191	-5.02901331	-0.41410987
H	-5.83444352	-5.76652581	-0.96184301
H	-5.91618067	-4.18629409	-0.22072591
H	-4.43821309	-4.71630921	-0.98738252
C	-1.51084948	-6.57292544	2.62011946
H	-1.17114113	-5.86364409	3.34566630
H	-1.34568170	-7.56465967	2.98629267
H	-0.97069680	-6.43538569	1.70676417
C	-6.33512865	-6.92377656	4.18498496
H	-6.55430101	-7.96805621	4.10533897
H	-5.93161343	-6.71693158	5.15415503
H	-7.23311676	-6.35914831	4.04458448
C	-0.07742690	-7.30307169	0.41639675
H	-0.04858276	-6.29261745	0.76718194
H	-0.57573935	-7.91683974	1.13741927
H	0.92123979	-7.65972590	0.27369912
C	-3.76829683	-5.58113170	-2.62550759
H	-4.68519168	-6.05426844	-2.34205484
H	-3.63363492	-4.68997832	-2.04878250
H	-3.80247930	-5.33125467	-3.66536000
C	-0.74065403	-9.35470441	-4.18726882
H	-1.34239098	-10.23475861	-4.09606982
H	-0.88209216	-8.92482511	-5.15685587
H	0.28982905	-9.61227253	-4.05818244
C	-3.43802723	4.64108398	-0.00168503

C	-4.15320772	5.60617354	-0.00235570
C	5.73853974	0.65545070	-0.00155927
C	6.93197943	0.79176918	-0.00219399
C	-5.07010578	6.84346785	-0.00321553
C	-5.32004734	7.52732296	1.18649853
C	-5.65035490	7.28066554	-1.19425668
C	-6.15056041	8.64835746	1.18545169
H	-4.86248212	7.18299353	2.12522860
C	-6.48105849	8.40114199	-1.19529806
H	-5.45277802	6.74152075	-2.13221216
C	-6.73149815	9.08496717	-0.00497052
H	-6.34802656	9.18682042	2.12369822
H	-6.93917192	8.74561435	-2.13379005
C	8.46203033	0.96653645	-0.00300774
C	9.13406940	1.22431810	-1.19777141
C	9.17590915	0.86752903	1.19155680
C	10.52019444	1.38283809	-1.19824493
H	8.57144186	1.30269648	-2.13928610
C	10.56175650	1.02552882	1.19108898
H	8.64572135	0.66468015	2.13348432
C	11.23411465	1.28291255	-0.00427903
H	11.04980886	1.58529600	-2.14045571
H	11.12486309	0.94684225	2.13237306
C	12.76428706	1.45661234	-0.00515088
C	-7.64925797	10.32162246	-0.00574839
N	13.90356998	1.58593972	-0.00580001
N	-8.33257187	11.24236854	-0.00632754

Table S9: Spatial coordinate for optimized 3+F⁻ adduct



Atom	X	Y	Z
C	-1.97353132	1.12516685	-0.17738784
C	-2.59253494	2.24565772	-0.77255809
C	-2.79863229	0.11808513	0.36674558
C	-3.97276810	2.36301042	-0.80087603
H	-1.98072480	3.01568901	-1.22956697
C	-4.17787092	0.23700324	0.33309093
H	-2.34010018	-0.75623907	0.81419038
C	-4.80094479	1.36377986	-0.24664832
H	-4.42956160	3.22800407	-1.27274561
H	-4.79417568	-0.54544309	0.76529526
C	0.30157603	2.06834642	-0.07502894
C	-0.04196652	3.24502054	0.62574413
C	1.58204004	1.99291451	-0.66344915
C	0.84484231	4.30594260	0.71073693
H	-1.00568940	3.31275229	1.11834957
C	2.46722811	3.05398670	-0.57289309
H	1.86899028	1.09055039	-1.19107013
C	2.12044666	4.23997118	0.11060926
H	0.56456266	5.19846122	1.26247096
H	3.44393152	2.97887321	-1.04122151
C	-0.02341620	-0.35879778	-0.22492461

C	0.72358827	-0.86650520	0.84284068
C	-0.25127969	-1.16035404	-1.34845158
C	1.24166163	-2.15991247	0.77035026
H	0.88214363	-0.25115278	1.72587603
C	0.27211747	-2.45222699	-1.39215635
H	-0.84297089	-0.76900672	-2.17351255
C	1.05223755	-2.99262967	-0.34940575
H	1.79211186	-2.54274356	1.62671776
H	0.07139415	-3.07741004	-2.25742579
N	-0.57658966	0.97594765	-0.15833833
B	1.56843820	-4.56290154	-0.46061614
C	1.44882321	-5.22052900	1.07055127
C	0.18854580	-5.68319178	1.55147985
C	2.52769315	-5.28645145	1.99364555
C	0.05567133	-6.21810880	2.83946616
C	2.35622183	-5.82367188	3.27985929
C	1.13065266	-6.31308209	3.72342016
H	-0.92680695	-6.56273628	3.16474161
H	3.21296841	-5.85522455	3.95391326
C	3.02053819	-4.85054698	-1.24047127
C	3.95346363	-3.88575353	-1.70237117
C	3.32641981	-6.20926614	-1.55924408
C	5.10172431	-4.26423019	-2.41962110
C	4.48119270	-6.55040512	-2.27275007
C	5.39236453	-5.59137513	-2.71718892
H	5.78943178	-3.48740729	-2.75542841
H	4.67132300	-7.60210019	-2.49043727
C	3.80637654	-2.39233241	-1.46407686
H	3.69996892	-2.14492287	-0.40316448
H	4.68858945	-1.86042681	-1.84106054
H	2.92634588	-1.97720241	-1.96576335

C	2.43062153	-7.36270935	-1.14363334
H	2.84006911	-8.31679778	-1.49757672
H	2.32863124	-7.42101918	-0.05460394
H	1.42205895	-7.23679686	-1.54170725
C	6.64438065	-5.98173659	-3.46935953
H	7.39637449	-6.43479233	-2.80710664
H	6.43210596	-6.71725005	-4.25626488
H	7.11222457	-5.11121648	-3.94404528
C	-1.08576424	-5.60951115	0.72705388
H	-1.23039527	-4.61633471	0.29248516
H	-1.07158679	-6.30669122	-0.11468750
H	-1.95502750	-5.84072001	1.35610855
C	3.92606322	-4.78806232	1.66870089
H	4.44176188	-5.44125935	0.95761655
H	3.92178730	-3.78957014	1.22186740
H	4.53294268	-4.73984767	2.58159061
C	0.97120860	-6.92549125	5.09647166
H	1.02953720	-8.02341529	5.06457847
H	1.75493827	-6.58165854	5.78209061
H	0.00097152	-6.67177902	5.54187446
C	3.02489486	5.32833091	0.19648663
C	3.80132926	6.26579624	0.26773501
C	-6.21323233	1.48469286	-0.27783911
C	-7.42798812	1.58694585	-0.30286616
C	4.70494097	7.35438629	0.34797648
C	5.98330396	7.27891154	-0.25047712
C	4.34921072	8.54196709	1.02702095
C	6.86728429	8.34434992	-0.17470976
H	6.26743061	6.37151797	-0.77326238
C	5.23173456	9.60843133	1.10392698
H	3.37060182	8.61040982	1.49090148

C	6.50144861	9.52217475	0.50317908
H	7.84669343	8.27601636	-0.63765879
H	4.94866816	10.51603948	1.62778803
C	-8.84010523	1.70212554	-0.33111707
C	-9.65947773	0.68780459	0.21464428
C	-9.46300279	2.83350927	-0.90541923
C	-11.04119450	0.79955936	0.18838572
H	-9.19202747	-0.18588071	0.65684312
C	-10.84446244	2.94712433	-0.93263965
H	-8.84370157	3.61788089	-1.32823208
C	-11.65003695	1.93119832	-0.38541409
H	-11.66111200	0.01461618	0.61004425
H	-11.31288770	3.82016621	-1.37611856
C	-13.07603941	2.04920967	-0.41219747
C	7.41186108	10.62363936	0.58092385
N	-14.23622058	2.14720497	-0.43397683
N	8.15122589	11.52110249	0.64419394
F	0.58448338	-5.18801952	-1.33977463

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