# Electronic Supporting Information

## *De novo* Fabrication of Higher Arene Ring Incorporated Contorted Calix[2]phyrin(**2**.**2**.*1*.*1*.*1*) and Its $F^-$ Bound Complex

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# 1. Mass spectral analyses:

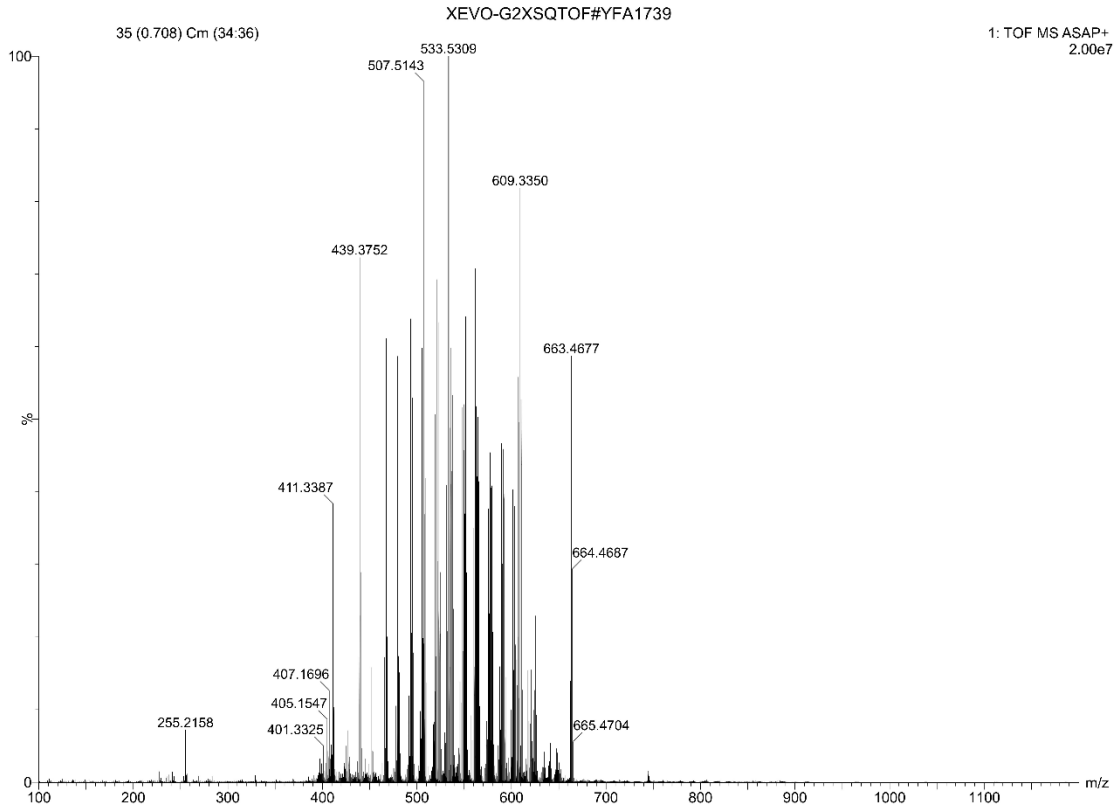


**Fig. S1.** Complete Mass (ESI-MS) spectrum of **1**.

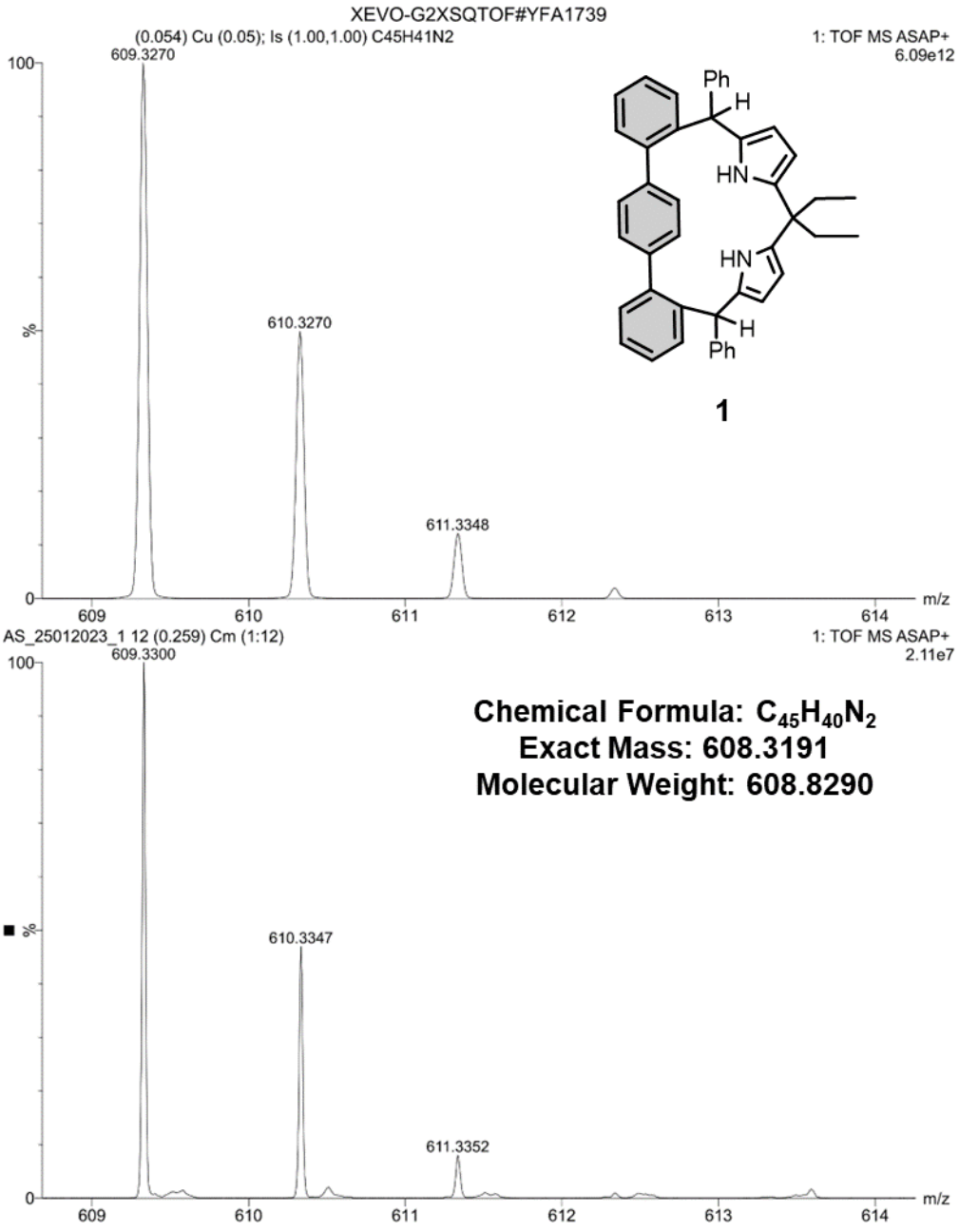


**Fig. S2.** (HR-ESI) Mass spectrum of **1**.

## 2. NMR spectral analyses:

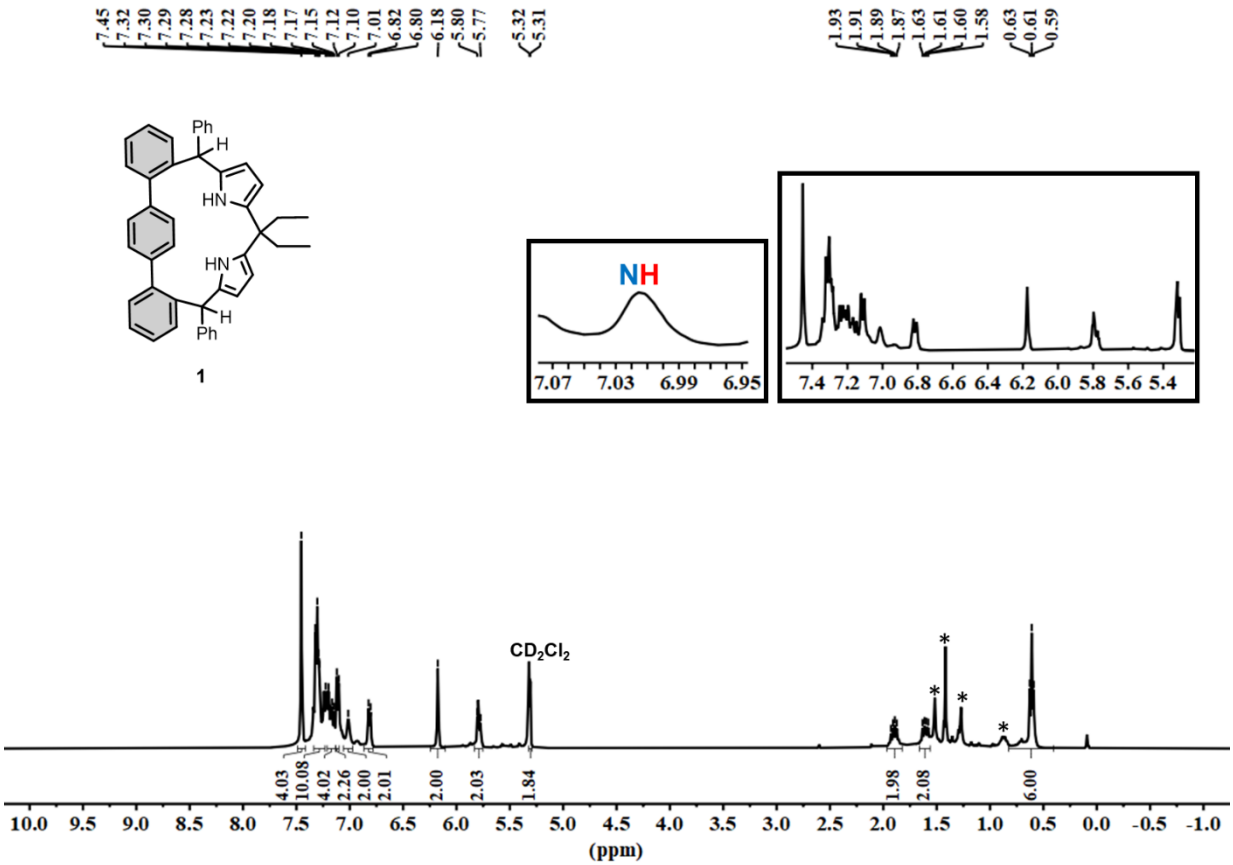


**Fig. S3.** $^{1}$H (400 MHz) NMR spectrum of **1** in $CD_2Cl_2$ at 298K (*Residual solvents and impurity grease).

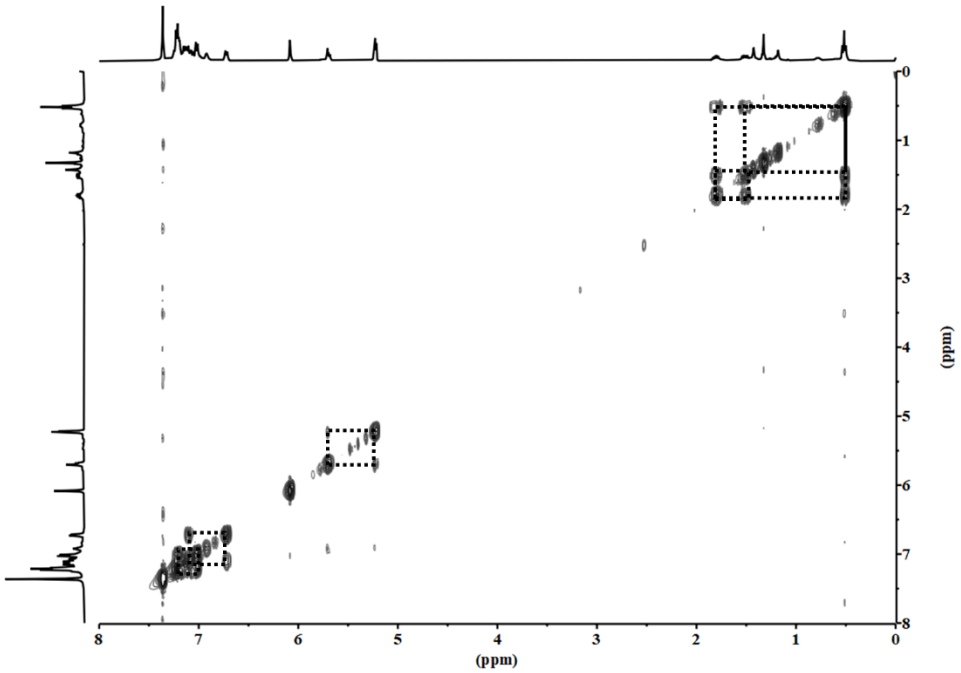


**Fig. S4.** $^{1}$H-$^{1}$H COSY spectrum of **1** in $CD_2Cl_2$ at 298K.

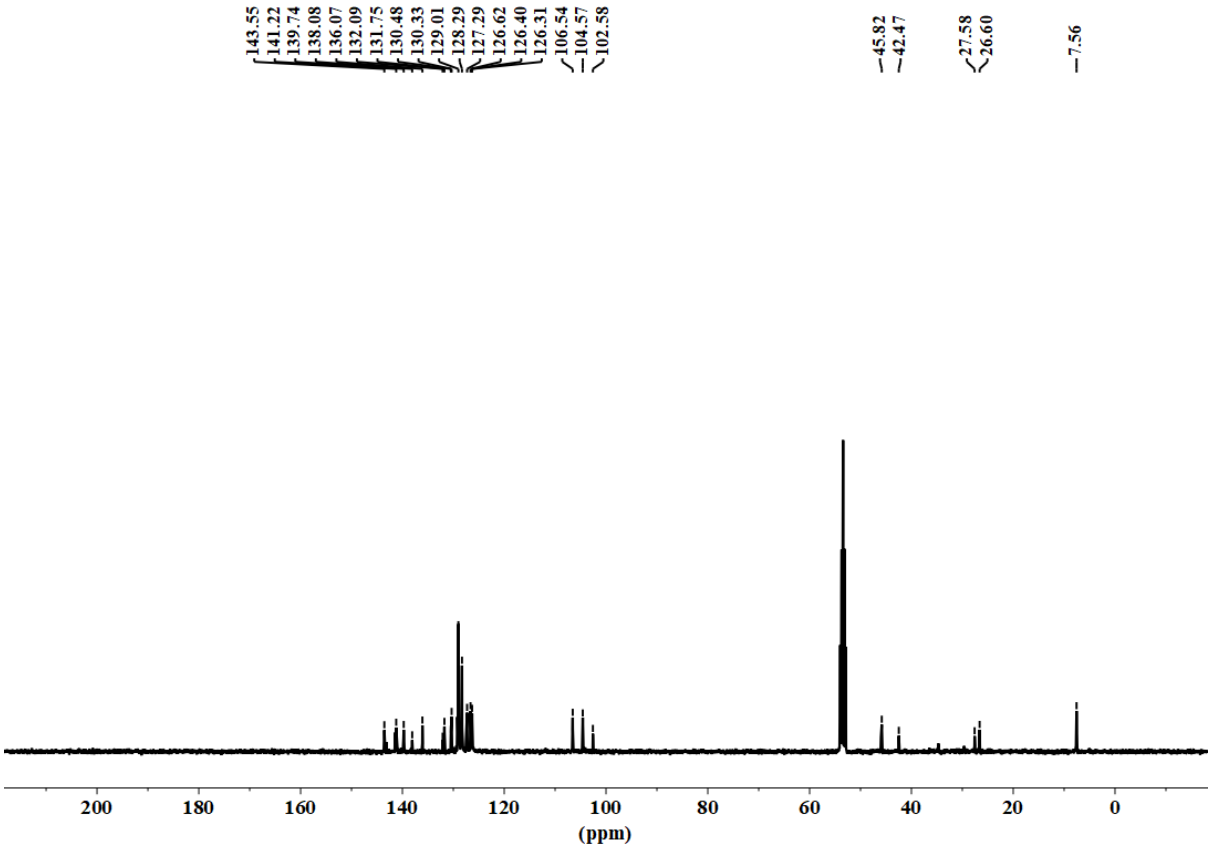


**Fig. S5**. $^{13}C\{^{1}H\}$ (101 MHz) NMR spectrum of **1** in $CD_2Cl_2$ at 298K.

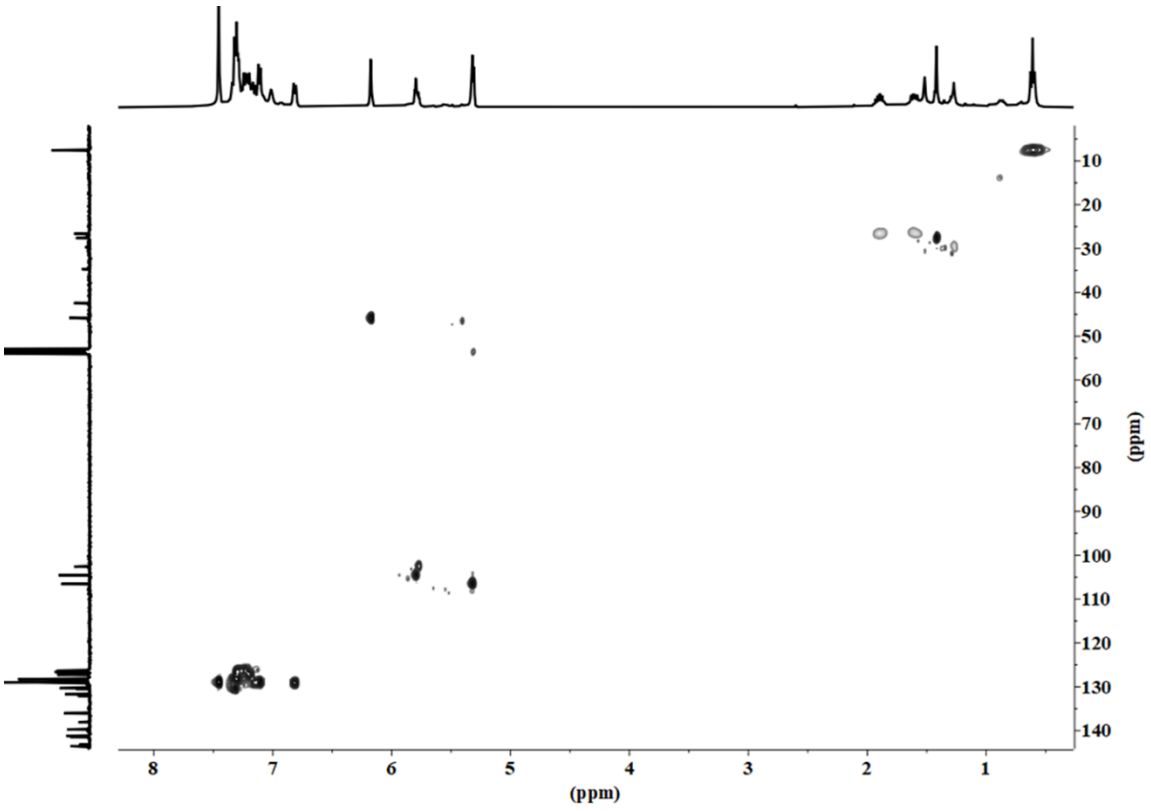


**Fig. S6.** $^{1}H$-$^{13}C$ HSQC spectrum of **1** in $CD_2Cl_2$ at 298K.

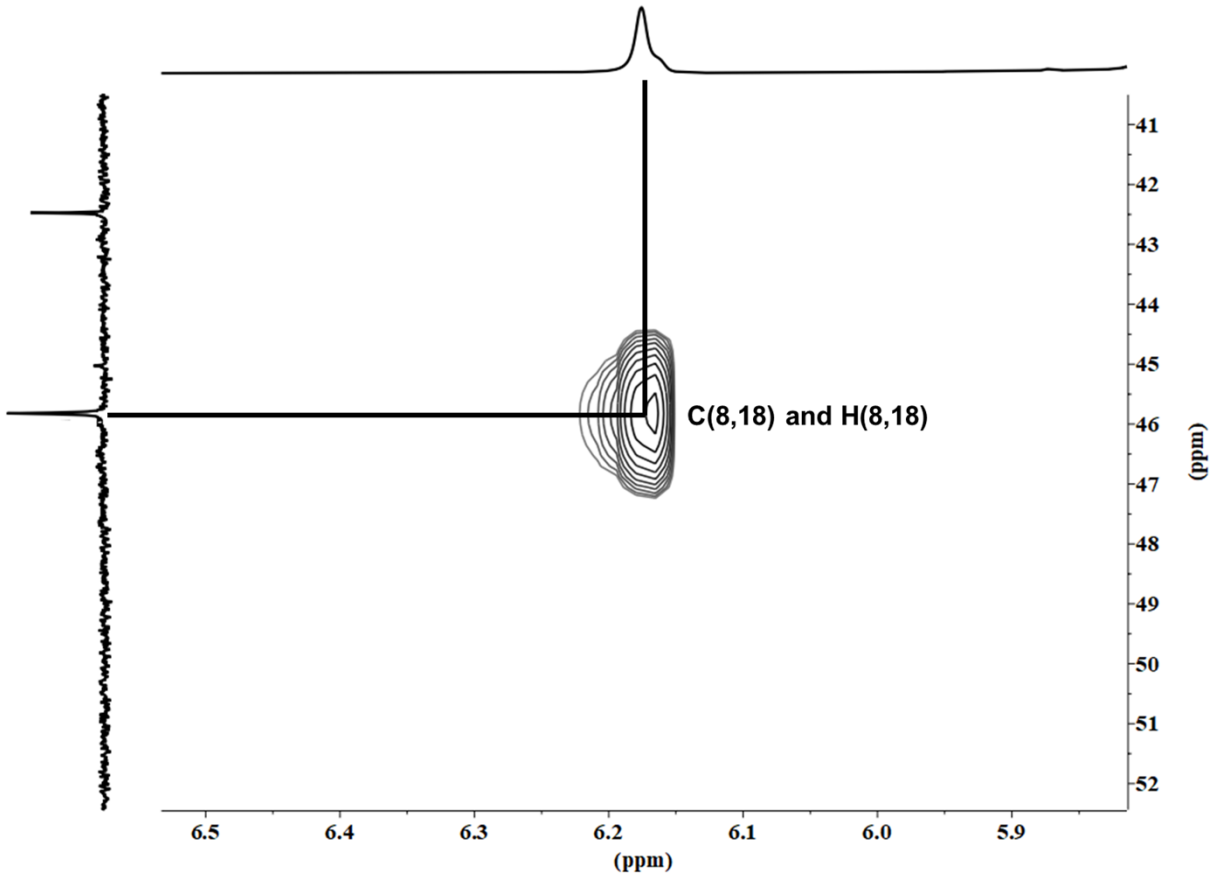


**Fig. S7.** $^{1}H$-$^{13}C$ HSQC spectrum of **1** with correlation between C(8,18) and H(8,18) in $CD_2Cl_2$ at 298K.

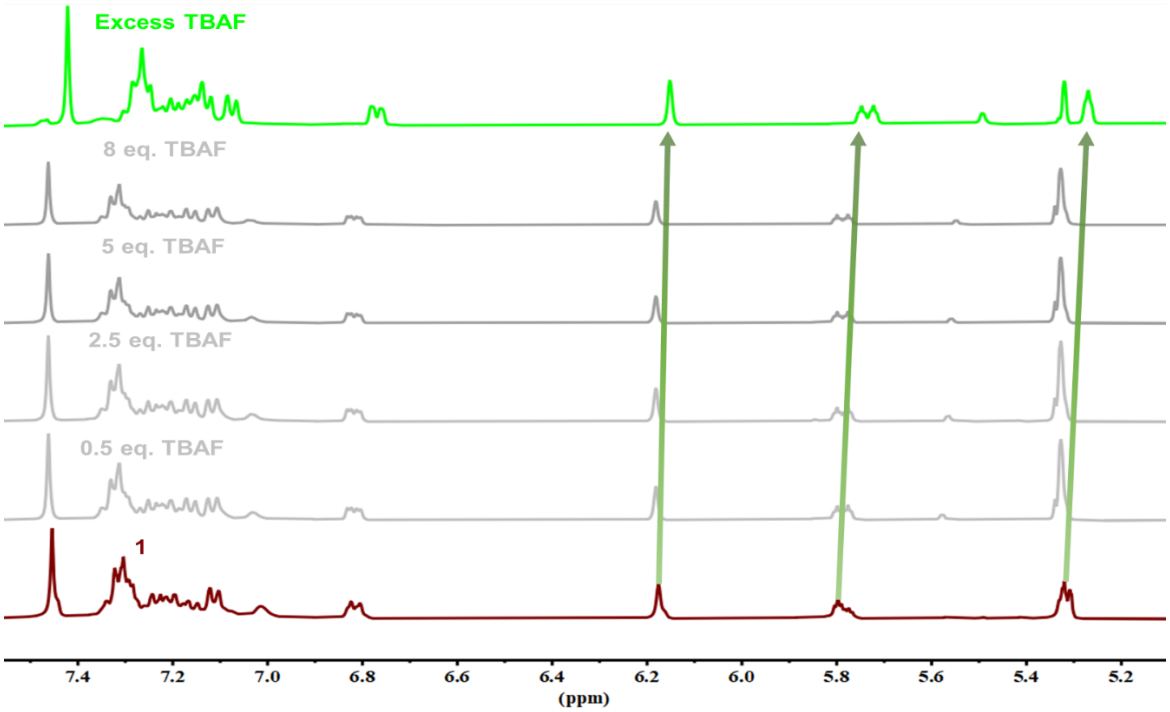


**Fig. S8**. $^{1}H$-NMR spectra of **1** with increasing concentration of TBAF in $CD_2Cl_2$ at 298 K (5.2-7.5 ppm region).

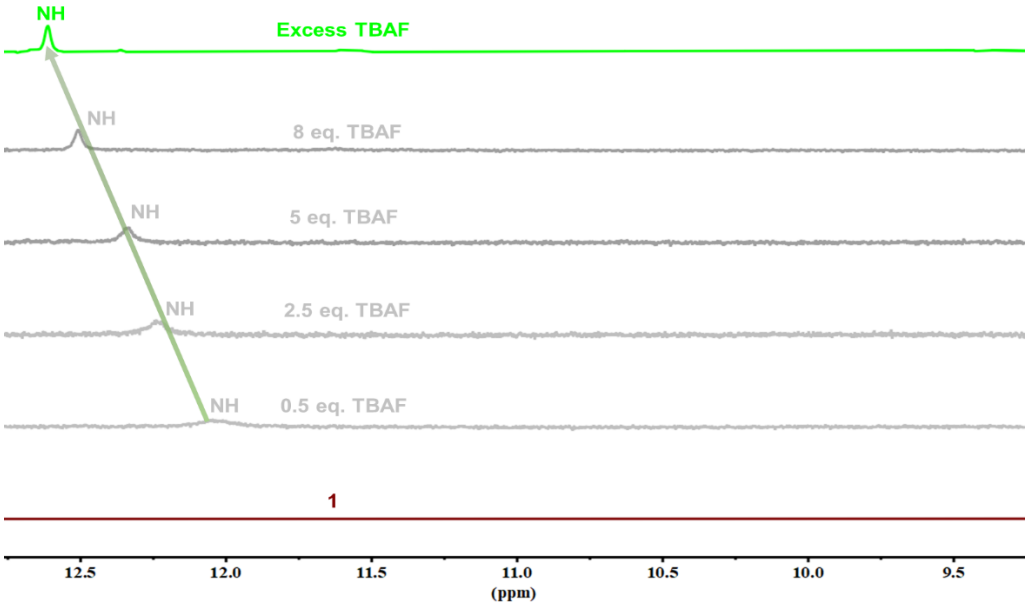


**Fig. S9**. $^{1}$H-NMR spectra of **1** with increasing concentration of TBAF in $CD_2Cl_2$ at 298 K (9.5-13 ppm region showing change in the NH peak).

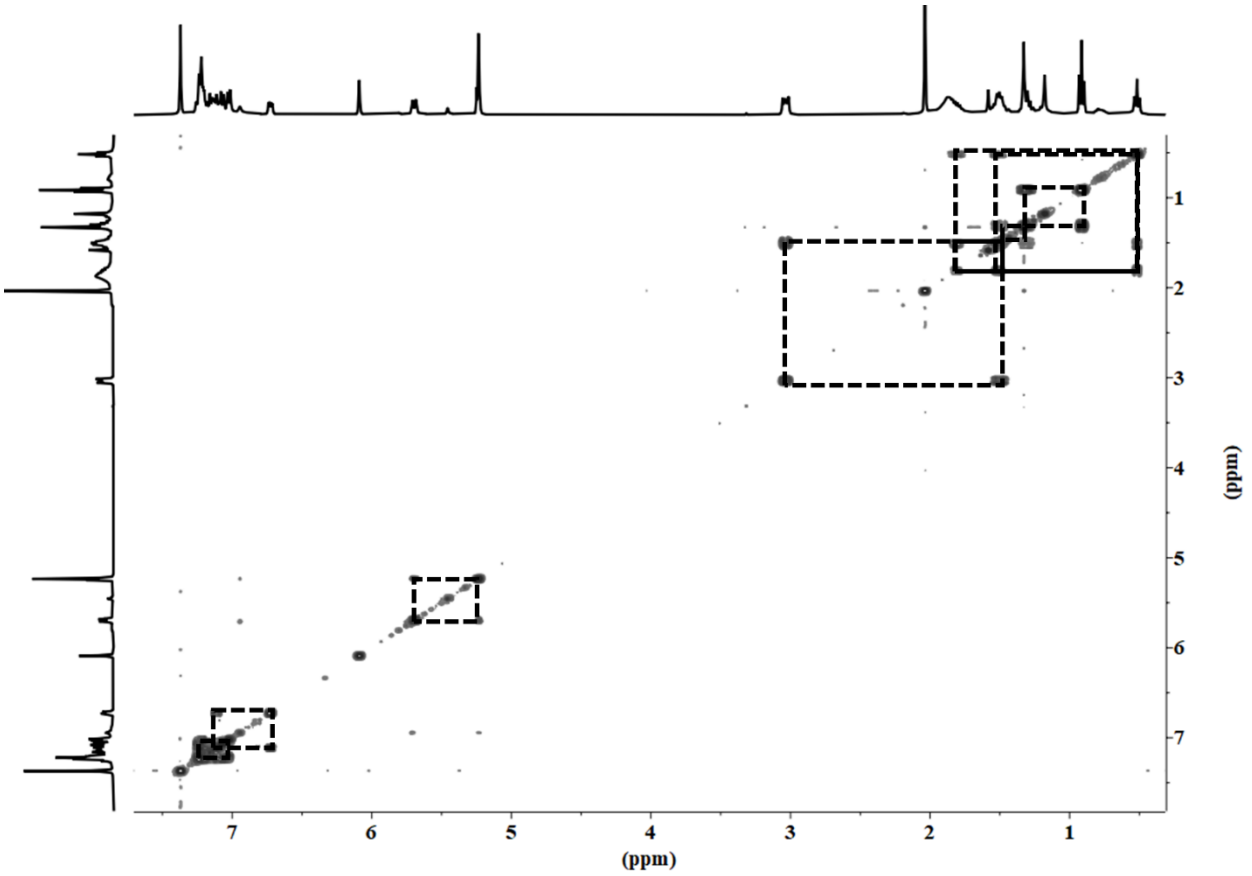


**Fig. S10.** $^{1}$H-$^{1}$H COSY spectrum of **1** after the addition of 8 eq. TBAF in $CD_2Cl_2$ at 223K.

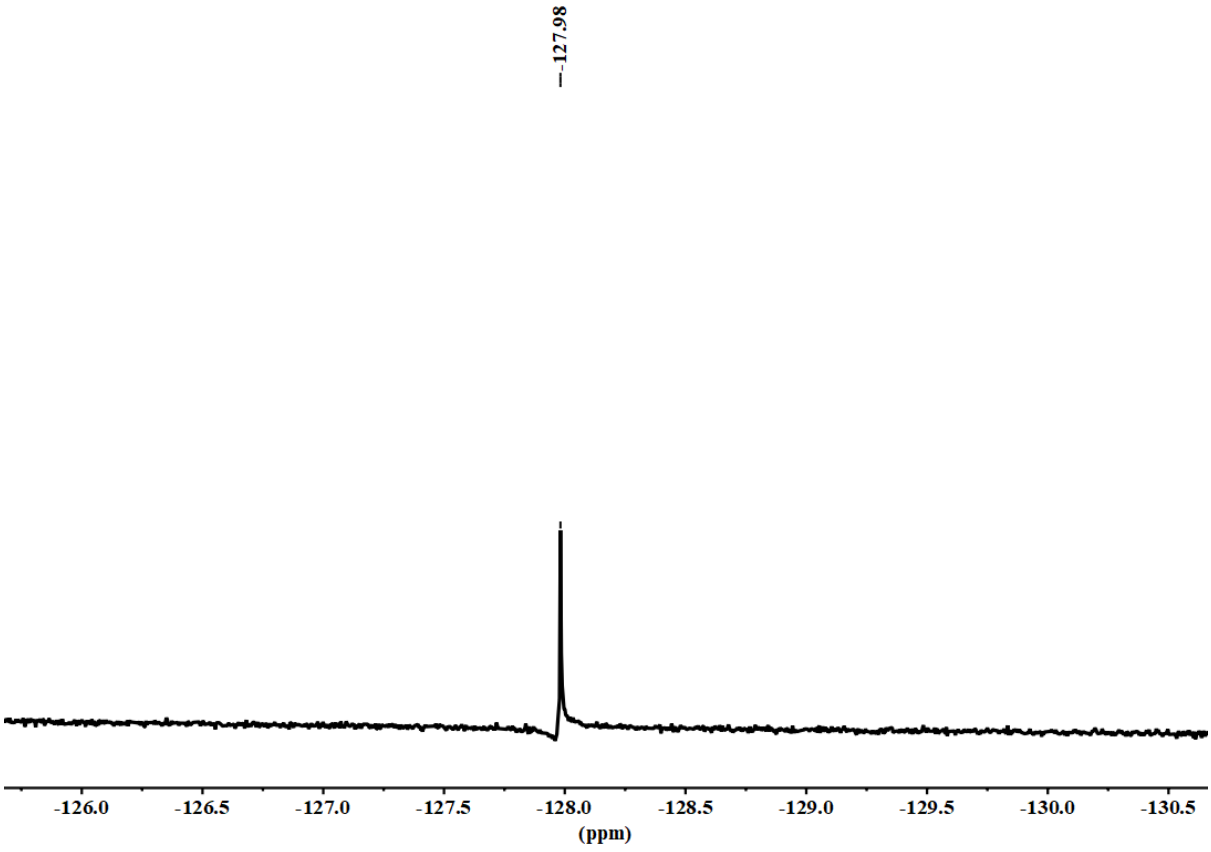


**Fig. S11.** $^{19}F$ (376 MHz) NMR spectrum of **1.F** in $CDCl_3$ at 298 K.

## 3. Single crystal X-ray analyses of 1 and 1.F:

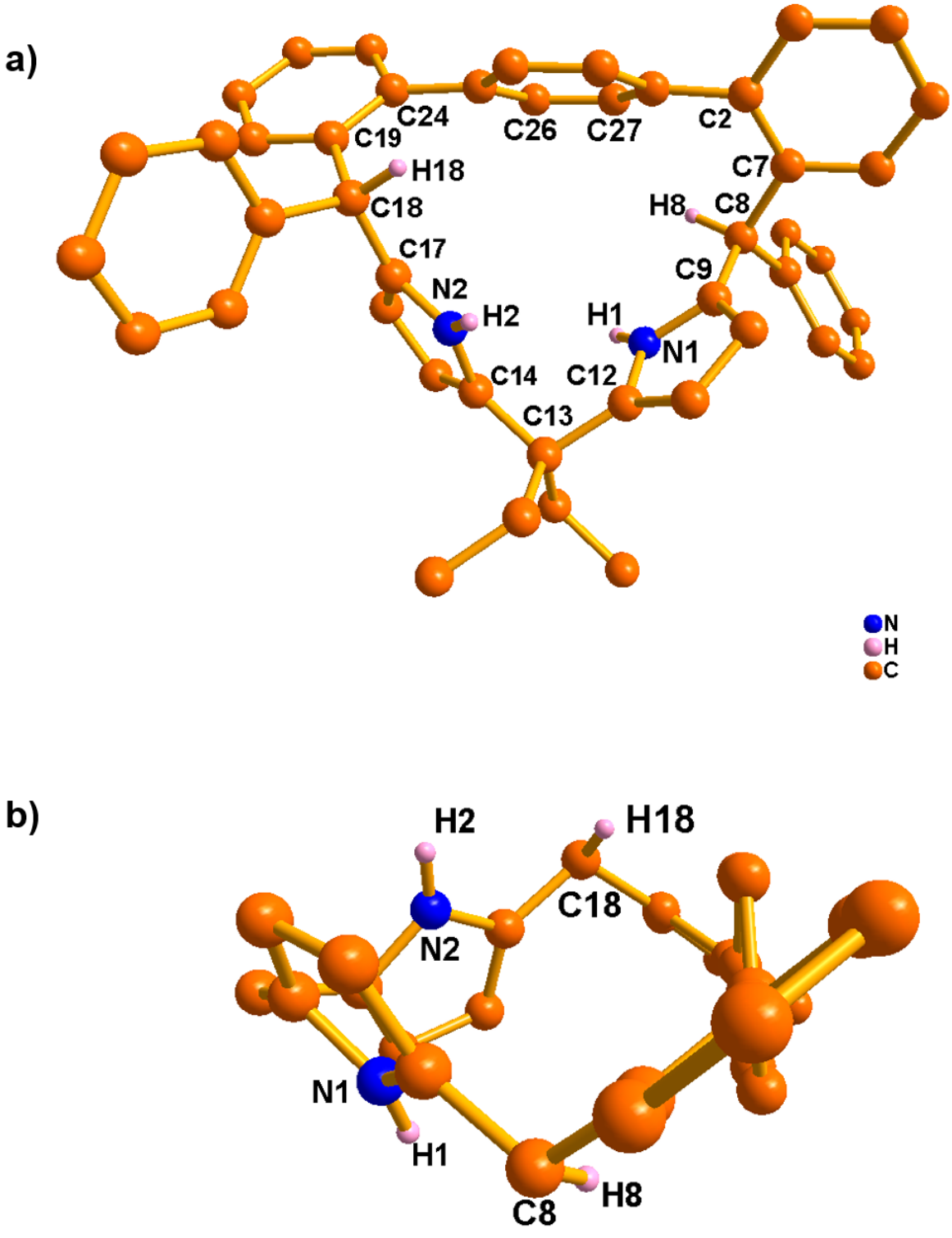


**Fig. S12.** Single crystal X-ray structure of **1**. **a**) Top view and **b**) Side view. Peripheral hydrogen atoms in a), b) and *meso*-aryl groups in b) are omitted for clarity.

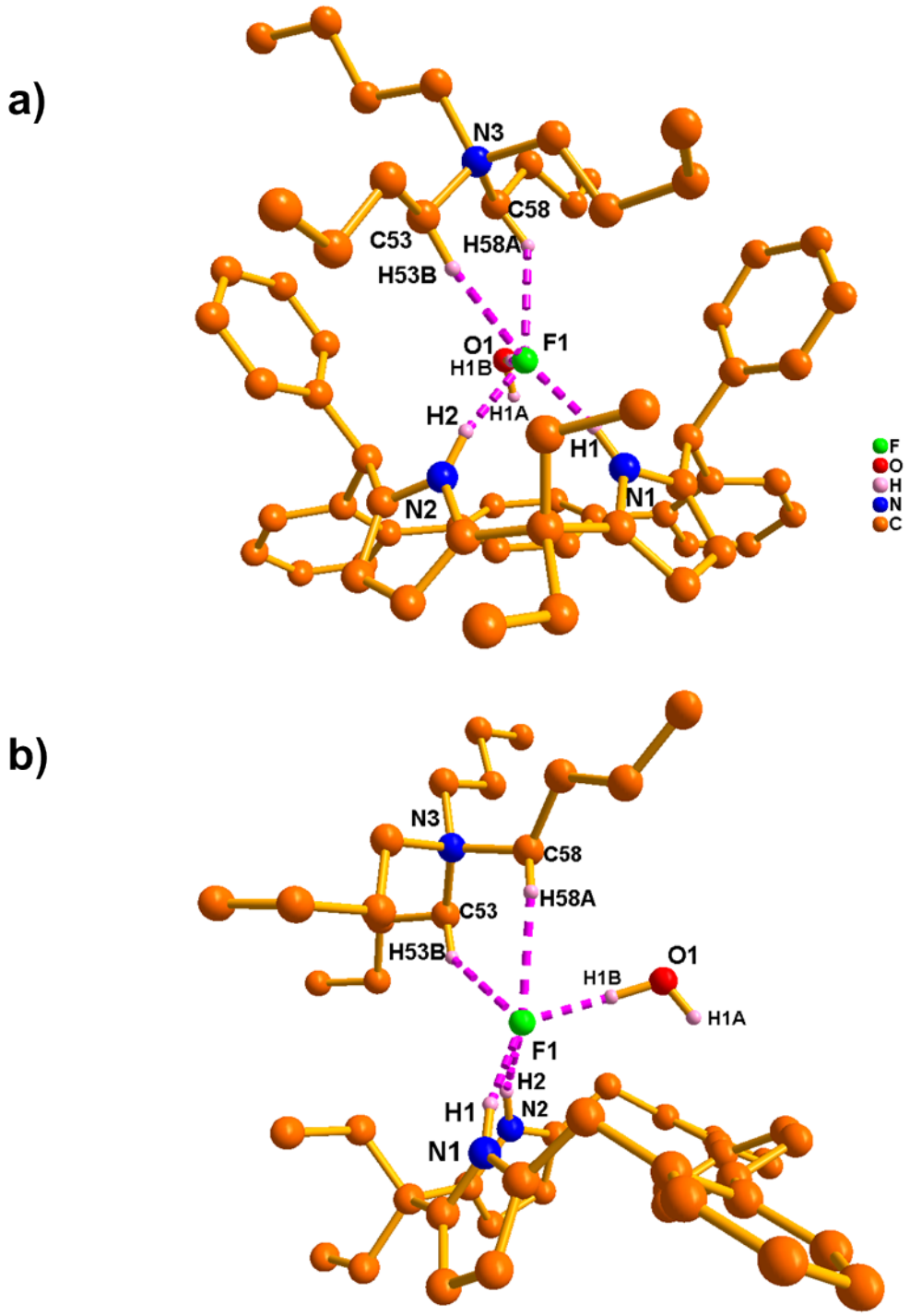


**Fig. S13.** Single crystal X-ray structure of **1.F**. **a**) Top view and **b**) Side view. Peripheral hydrogen atoms and hydrogen atoms not involved in intermolecular hydrogen bond with fluoride anion in a), b) and *meso*-phenyl groups in b) are omitted for clarity.

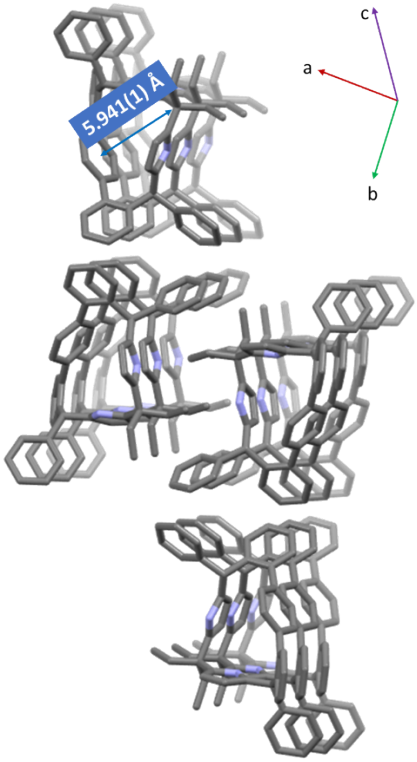


**Fig. S14.** Top view of **1** (peripheral hydrogens are omitted for clarity) with the tubular representation of the solid-state superstructures, displaying the nanometer-sized cavity with a dimension of 5.941(1) Å. The hydrogen atoms are omitted for the sake of clarity.

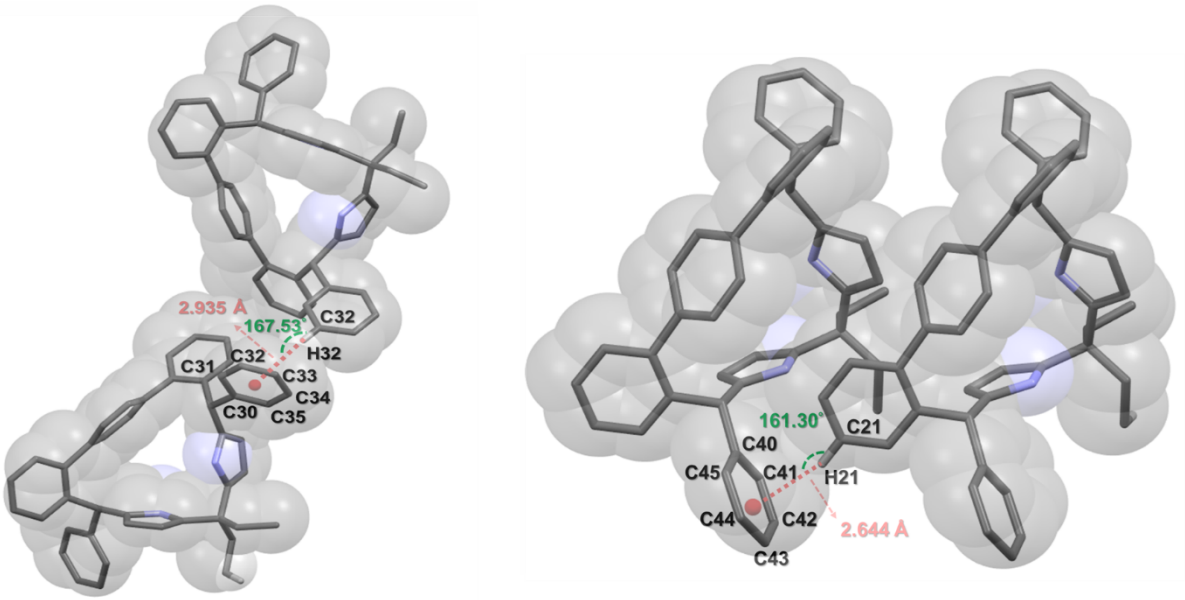


**Fig. S15.** Side-on view showing molecular packing of two sets of the supramolecular dimer of **1** molecules as a part of columnar superstructure held together employing multiple inter and intra-layer CH···π interaction. Bond lengths are shown in red and torsional angles in green.

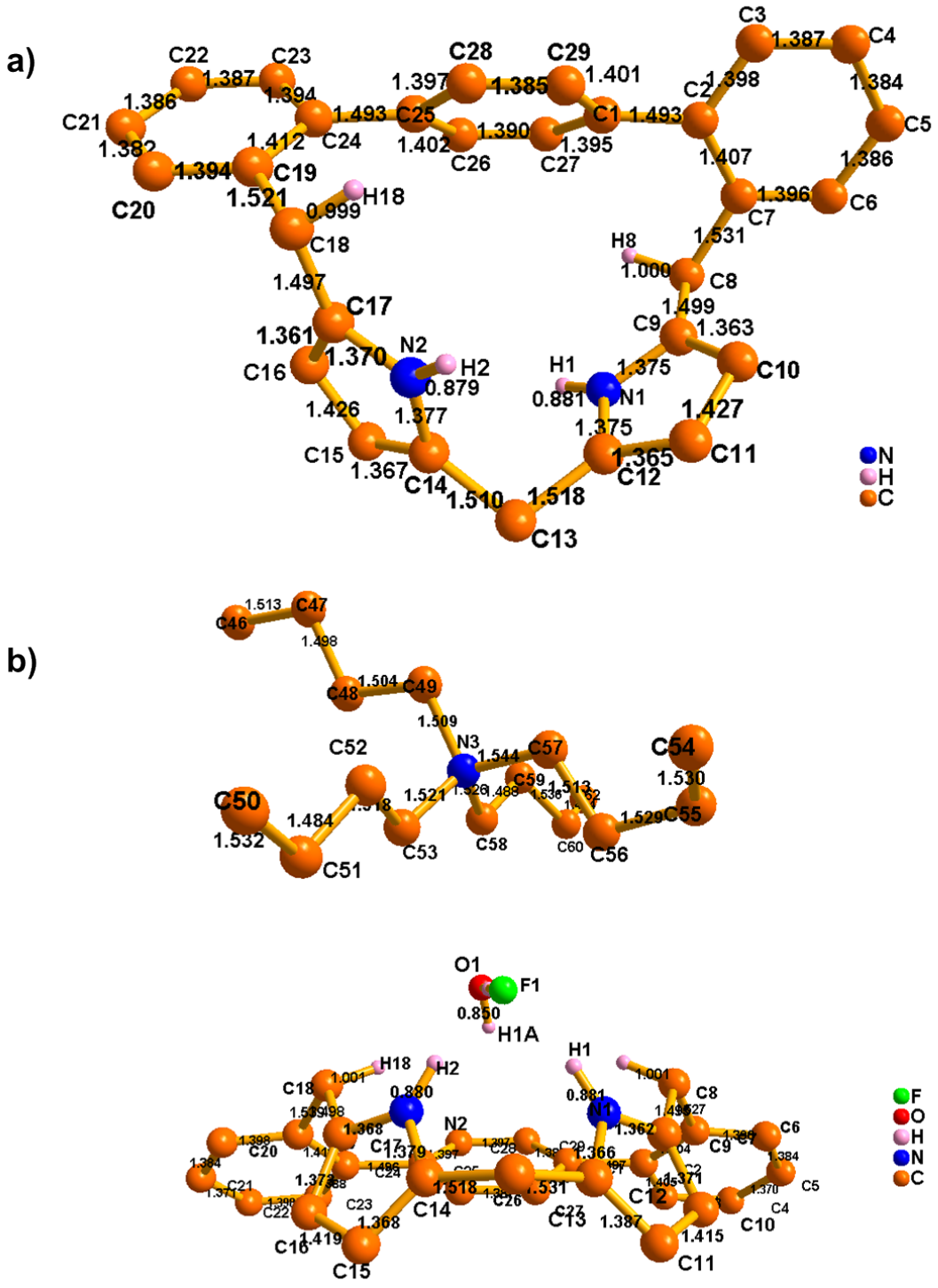


**Fig. S16**. Bond Lengths in (a) **1** and (b) **1.F** (Å) respectively.

| **Crystal parameters** | **1** | **1.F** |
|---|---|---|
| Formula | $C_{45}H_{40}N_2$ | $C_{61}H_{78}FN_3O$ |
| *M*/g mol$^{-1}$ | 608.79 | 888.26 |
| *T*/K | 111.5(10) K | 100.00(10) K |
| Crystal dimensions/mm$^3$ | 0.2 × 0.1 × 0.1 | 0.2 × 0.1 × 0.1 |
| Crystal system | monoclinic | monoclinic |
| Space group | *P* $2_1$/c | *P* $2_1$/n |
| a/Å | 18.0411(2) | 14.0491(11) |
| b/Å | 25.9133(3) | 21.1710(12) |
| c/Å | 7.63460(10) | 18.6212(16) |
| α/° | 90 | 90 |
| β/° | 95.6400(10) | 106.367(9) |
| γ/° | 90 | 90 |
| V/Å$^3$ | 3551.93(7) | 5314.1(7) |
| Z | 4 | 4 |
| ρcalcd/mg m$^{-3}$ | 1.138 | 1.110 |
| μ/mm$^{-1}$ | 0.497 | 0.516 |
| F(000) | 1296.0 | 1928.0 |
| Reflns. collected | 26987 | 35027 |
| Indep.reflns.[*R*(int)] | 7285 [0.0546] | 10615 [0.0564] |
| Max/min transmission | 1.000, 0.589 | 1.000,0.831 |
| Data/restraints/parameters | 7285/0/427 | 10615/2/600 |
| GOF on $F^2$ | 1.104 | 1.069 |
| Final R indices[I > 2σ(I)] | R1 = 0.0538, wR2 = 0.1537 | R1 = 0.1198, wR2 = 0.2606 |
| R indices (all data) | R1 = 0.0595, wR2 = 0.1579 | $R_1$ = 0.1620, wR2 = 0.2856 |
| Largest diff peak and hole [e Å$^{-3}$] | 0.27 and -0.26 | 0.68 and -1.24 |

**Table S1.** Crystal data for **1** and **1.F**

The crystals have been deposited in the Cambridge Crystallographic Data Centre with reference no. **CCDC 2350180 (1)** and **CCDC 2350181 (1.F)**. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

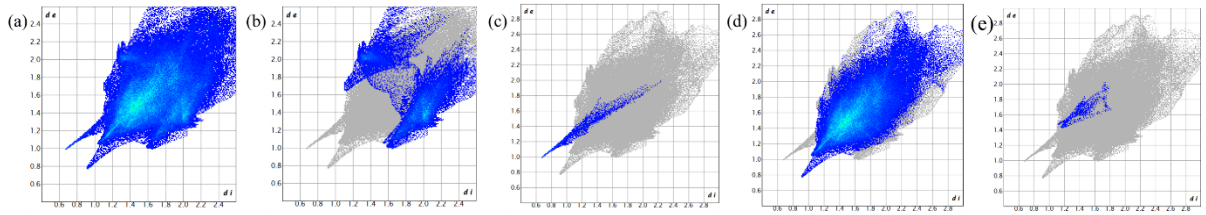

**Fig. S17.** The full Hirshfeld surface fingerprint (HS-FP) of **1**.**F** (a) as well as the contributions from H···C (b), H···F (c), H···H (d), and H···O (e) contacts.

**Table S2.** The % surface area of particular atom-atom interactions to the overall surface.

| Interaction type | % |
|---|---|
| H···C | 20.2 |
| H···F | 1.7 |
| H···H | 77.2 |
| H···O | 0.8 |

## 4. Electronic absorption spectral analysis

| Compd. | $\lambda_{max}$/nm ($\varepsilon$[$M^{-1}cm^{-1}$]×$10^4$) |
|---|---|
| **1** | 252 (4.47), 264 (3.89) |
| **1.F** | 252 (7.37), 266 (10.19), 363 (1.13) |

**Table S3.** The electronic absorption spectral data of **1** and **1**.**F**

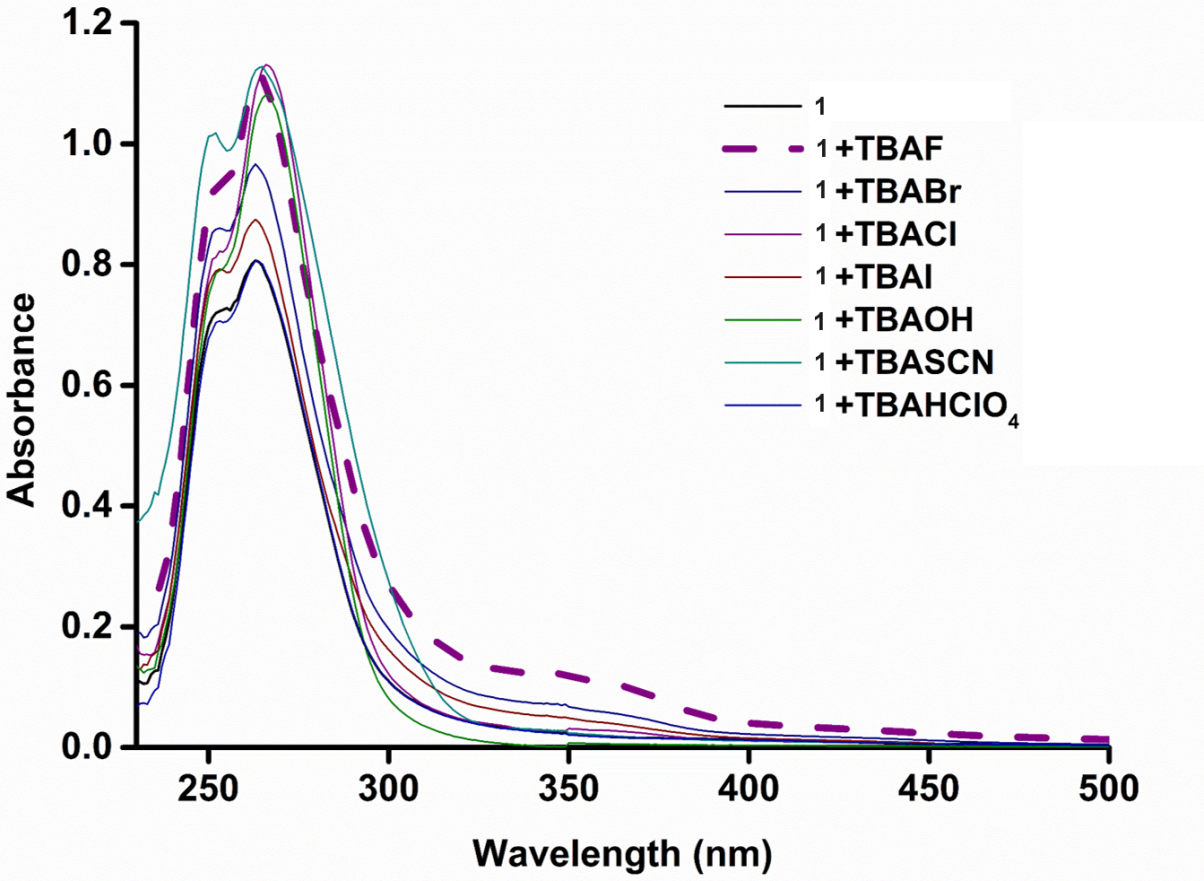


**Fig. S18**. Electronic absorption spectra of **1** with different anion salts (excess) in $CH_3CN$.

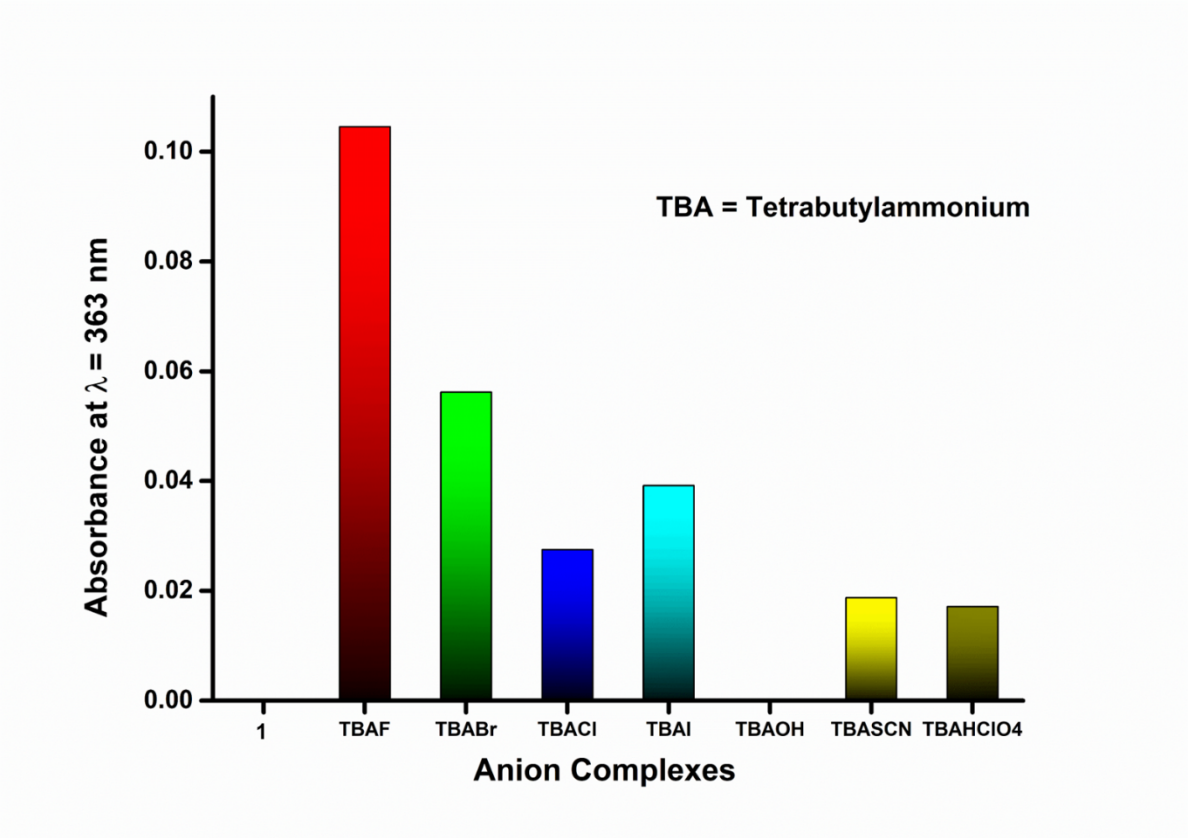


**Fig. S19**. Bar graph of intensities at 363 nm wavelength of **1** with different anion salts. (~20 eq. of each anion salts were taken)

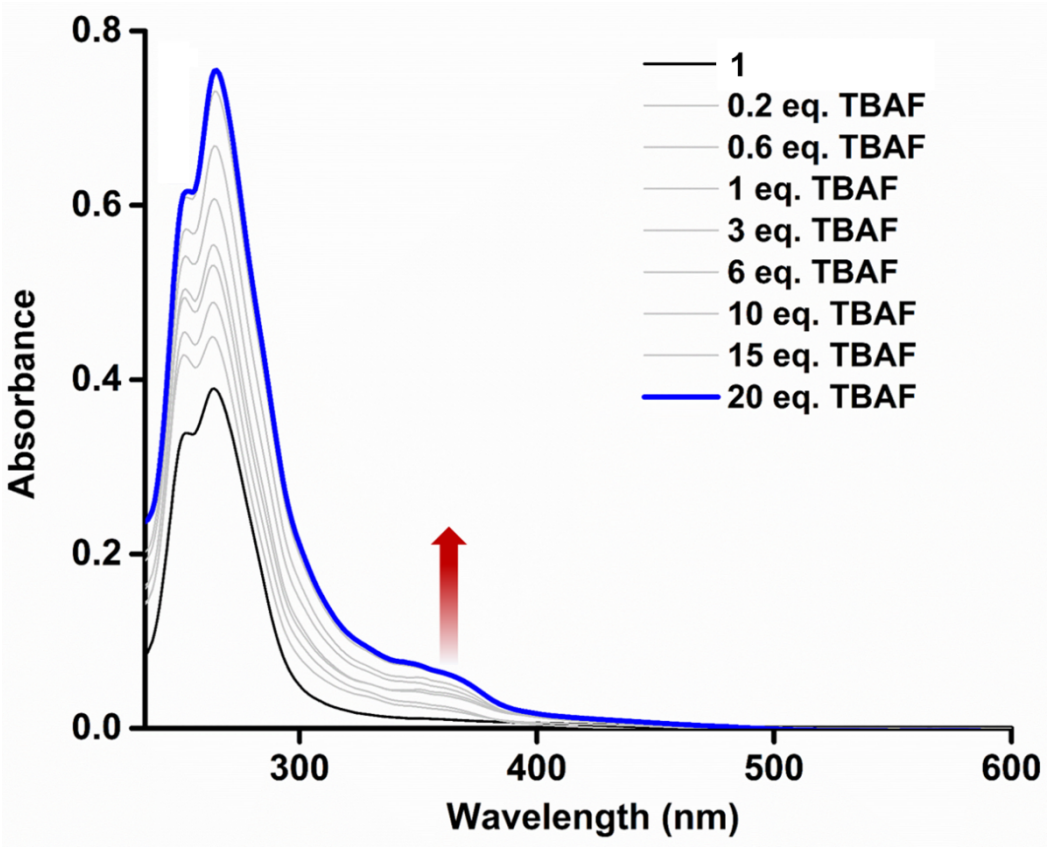


**Fig. S20**. Electronic absorption spectra of **1** in different equivalents of TBAF in $CH_3CN$.

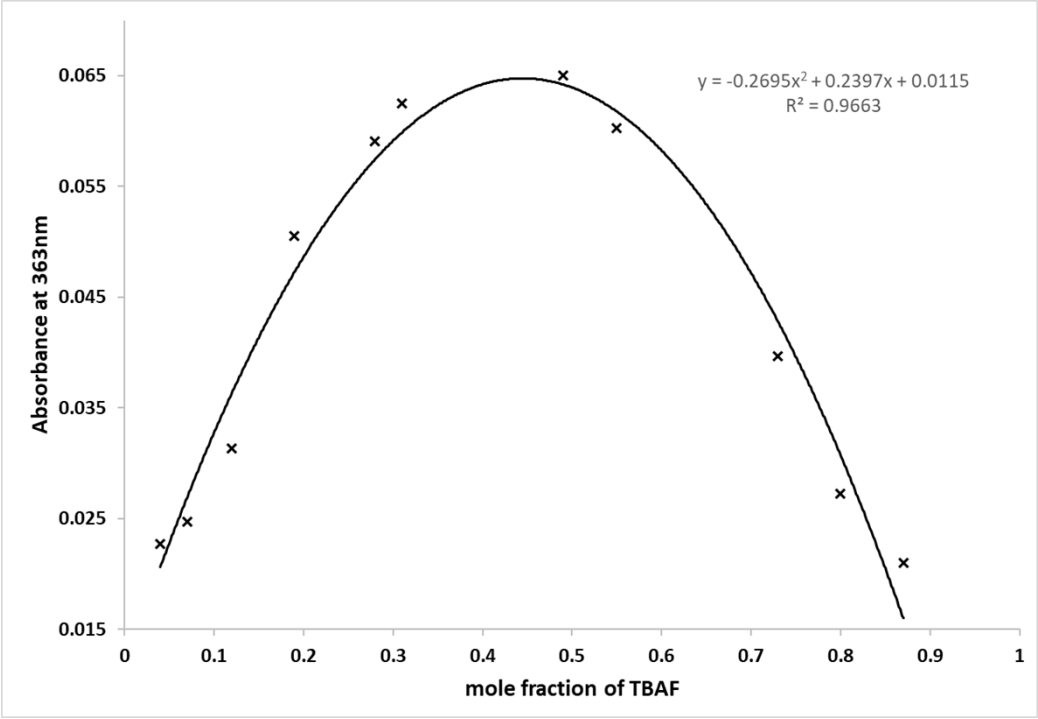


**Fig. S21**. Job's plot analysis of **1** with TBAF salt in $CH_3CN$ at 25 °C.

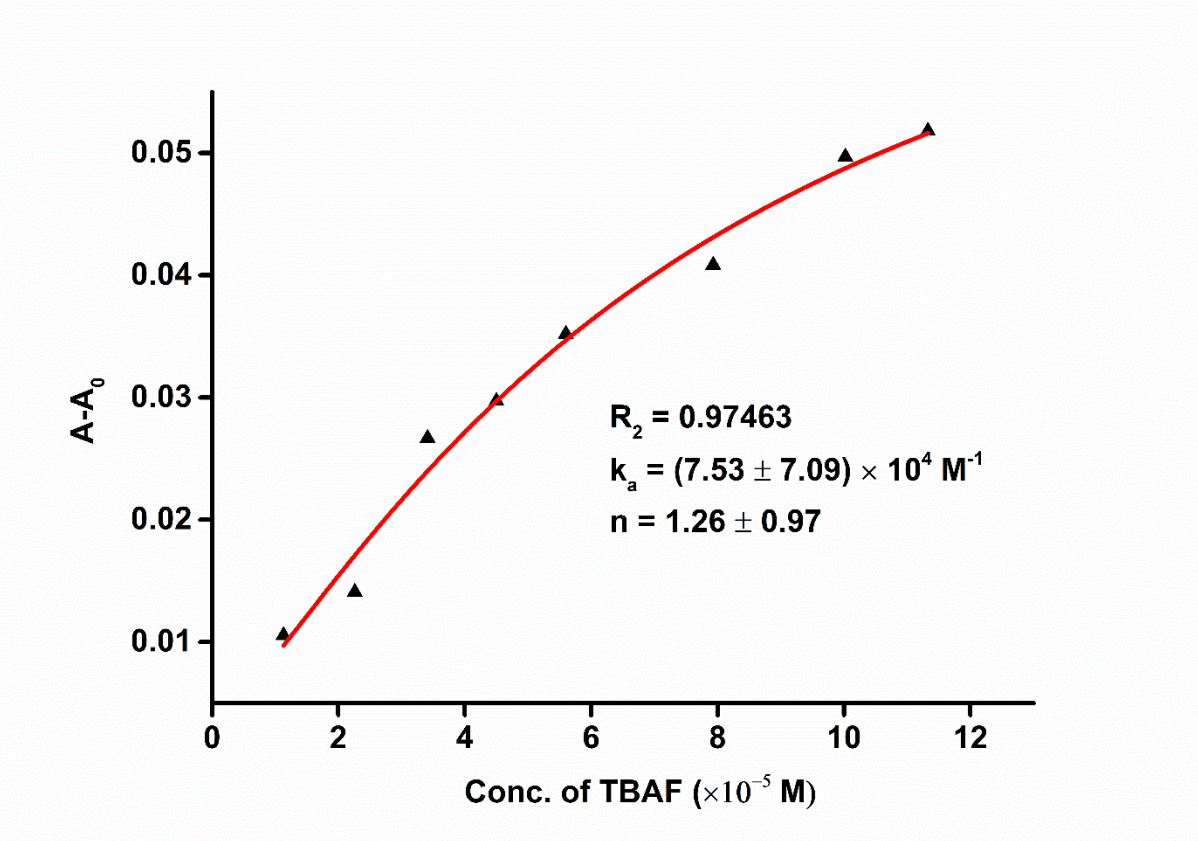


**Fig. S22**. The nonlinear fit to Hill equation of UV-Vis titration experiments based on the absorption band centered at 363 nm for **1** at different TBAF concentrations.

## 5. Theoretical Calculations:

Geometry optimization for all analysed structures were carried out with the Gaussian 09W[S1] software package within unconstrained C1 symmetry, with starting coordinates derived from X-ray analysis if available. The structure of the **1** and **1.F** in ground ($S_0$) states were optimized with the use of the density functional theory (DFT) approach, Becke's three-parameter hybrid exchange functional and the Lee–Yang–Parr correlation functional (B3LYP), and basis set 6-311G(d, p) for C, H, N, F atoms. While TD-DFT methods were employed to acquire the vertical excitation energies for $S_0$-$S_n$ transitions, similar basis sets was used to obtain oscillator strengths using the B3LYP method. On the basis of the optimized structures in the $S_0$ state, the electronic absorption spectra and oscillator strengths were fully studied using TD-DFT method. The GIAO chemical shifts were calculated using the B3LYP method with the same basis sets. The polarizable continuum model of solvation was used (IEFPCM [Integral Equation Formalism Polarizable Continuum Model] as standard acetonitrile parametrization) for all optimizations.

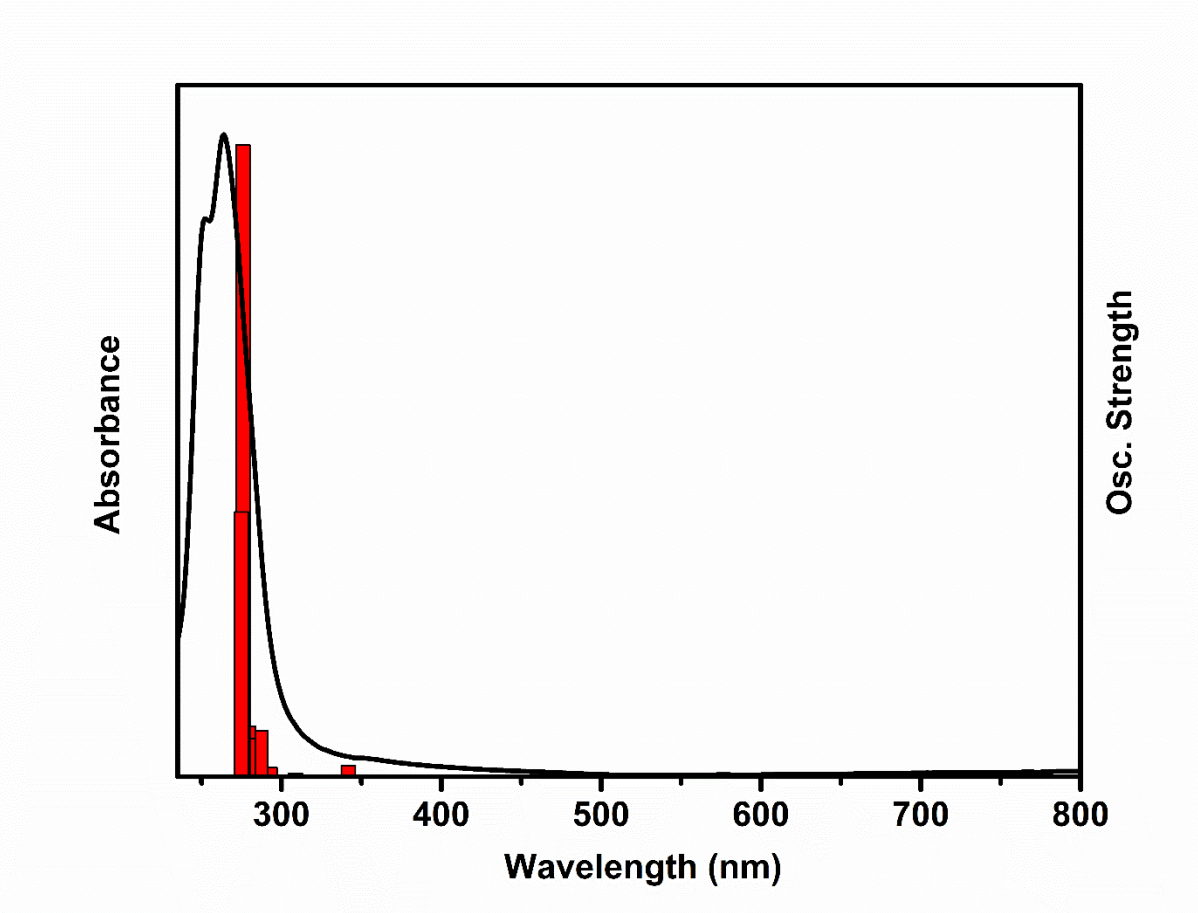


**Fig. S23**. Absorption spectrum of **1** along with the calculated vertical transitions (red) obtained by TD-DFT (B3LYP/6-311G (d, p), solvent=acetonitrile) method.

**Table S4**: Selected TD-DFT calculated energies, oscillator strengths and compositions of the major electronic transitions of **1**. The terms H and L refer to HOMO and LUMO, respectively.

| **Energy(eV)** | **Wavelength(nm)** | **Oscillator strength, f** | **Major Transitions** |
|---|---|---|---|
| 3.6269 | 341.84 | 0.0023 | H -> L (99.06%) |
| 4.0158 | 308.74 | 0.0007 | H-1 -> L (91.66%)<br>H-> L+2 (7.55%) |
| 4.2344 | 292.80 | 0.0019 | H -> L+1 (97.84%) |
| 4.3202 | 286.99 | 0.0093 | H-1 -> L (7.49%)<br>H-> L+2 (89.07%) |
| 4.4353 | 279.54 | 0.0102 | H-2 -> L (13.46%)<br>H-1-> L+2 (4.10%)<br>H-1 -> L+5 (3.86%)<br>H-> L+3 (75.08%) |

| | | | |
|---|---|---|---|
| | | | H -> L+6 (2.44%) |
| 4.4386 | 279.33 | 0.0077 | H-1 -> L+1 (8.68%)<br>H-1-> L+6 (2.13%)<br>H -> L+4 (85.31%) |
| 4.4950 | 275.83 | 0.1279 | H-2 -> L (27.29%)<br>H-1-> L+2 (2.50%)<br>H-1 -> L+4 (4.16%)<br>H-> L+3 (10.41%)<br>H -> L+6 (54.19%) |
| 4.5120 | 274.79 | 0.0536 | H-1 -> L+3 (3.91%)<br>H -> L+5 (90.99%) |

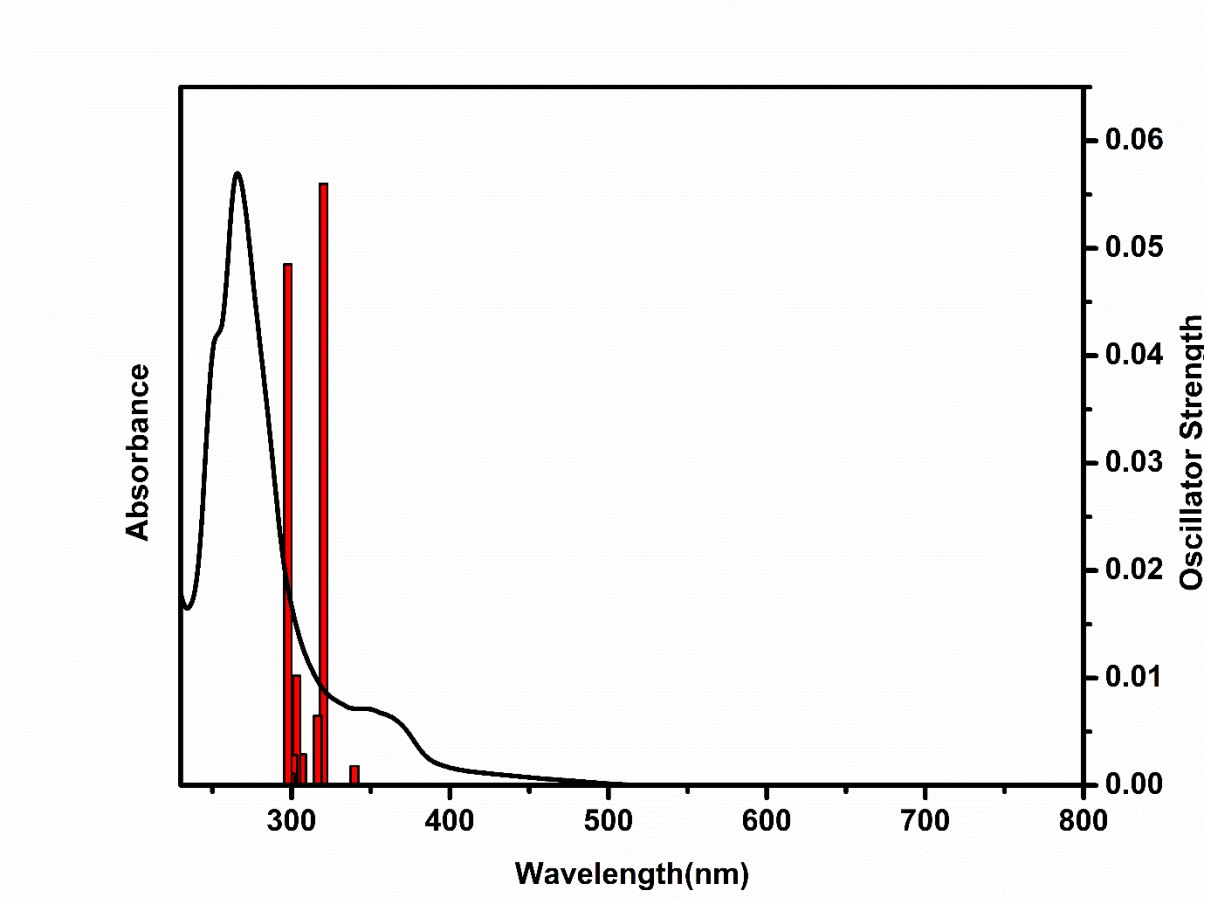


**Fig. S24**. Absorption spectrum of **1.F** along with the calculated vertical transitions (red) obtained by TD-DFT (B3LYP/6-311G(d,p)) method.

**Table S5:** Selected TD-DFT calculated energies, oscillator strengths and compositions of the major electronic transitions of **1.F**. The terms H and L refer to HOMO and LUMO, respectively.

| **Energy(eV)** | **Wavelength(nm)** | **Oscillator strength, f** | **Major Transitions** |
|---|---|---|---|
| 3.6498 | 339.70 | 0.0018 | H -> L (98.03%) |
| 3.8726 | 320.16 | 0.0560 | H-1 -> L (2.68%)<br>H-> L+1 (95.04%) |
| 3.9177 | 316.47 | 0.0065 | H-1 -> L (13.44%)<br>H -> L+2 (83.54%) |
| 4.0420 | 306.74 | 0.0029 | H-1 -> L+1 (4.88%)<br>H-1 -> L+3 (2.37%)<br>H -> L+3 (84.59%)<br>H-> L+4 (2.83%)<br>H-> L+5 (2.55%) |
| 4.0895 | 303.17 | 0.0102 | H-1 -> L+1 (2.25%)<br>H-1 -> L+3 (3.69%)<br>H -> L+3 (4.77%)<br>H-> L+4 (79.32%)<br>H-> L+5 (5.52%) |
| 4.1160 | 301.22 | 0.0028 | H-1 -> L (13.78%)<br>H-1 -> L+2 (4.18%)<br>H-1 -> L+4 (2.31%)<br>H-> L+2 (2.15%)<br>H-> L+4 (4.87%)<br>H -> L+5 (65.80%)<br>H -> L+6 (2.67%) |
| 4.1377 | 299.64 | 0.0011 | H-1 -> L (65.87%)<br>H-1 -> L+5 (2.33%)<br>H -> L+2 (10.95%)<br>H-> L+4 (3.53%)<br>H-> L+5 (13.00%) |
| 4.1664 | 297.58 | 0.0485 | H-1 -> L+1 (7.45%)<br>H-1 -> L+2 (4.94%)<br>H -> L+5 (2.18%)<br>H-> L+6 (81.23%) |

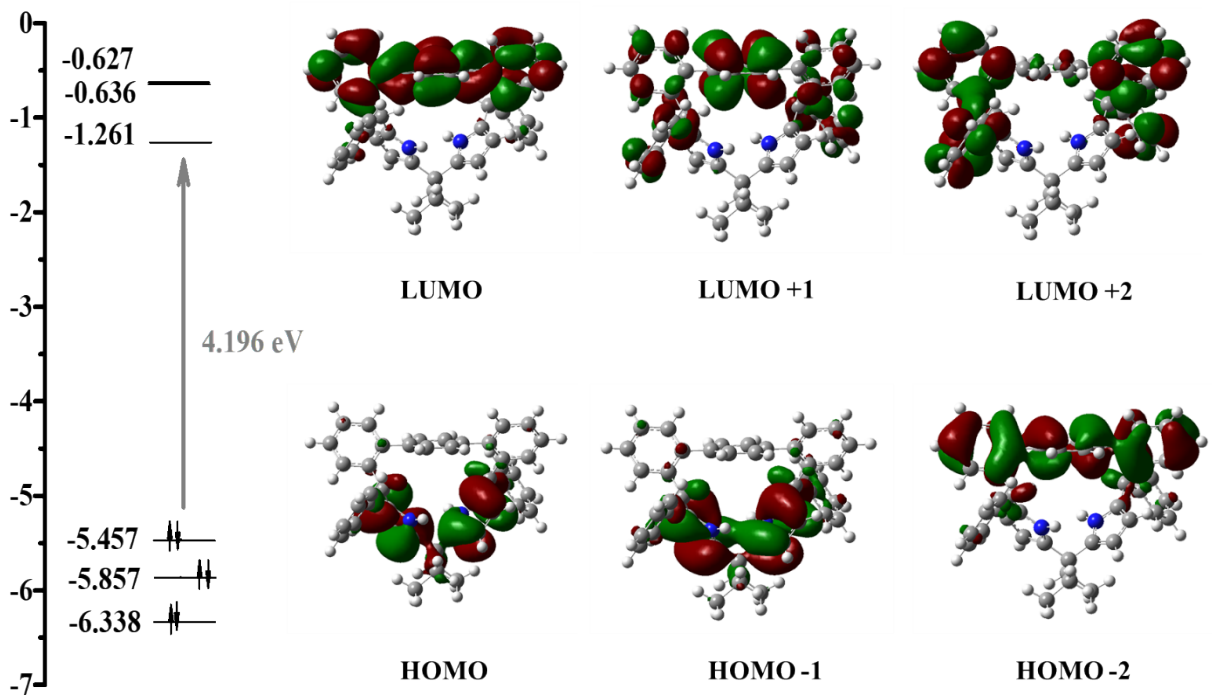


**Fig. S25**. Kohn−Sham orbital energy level diagram of **1** selected orbitals calculated at the B3LYP/6-311G(d, p) level of theory and contour plots of selected orbitals (isovalue of 0.02 au).

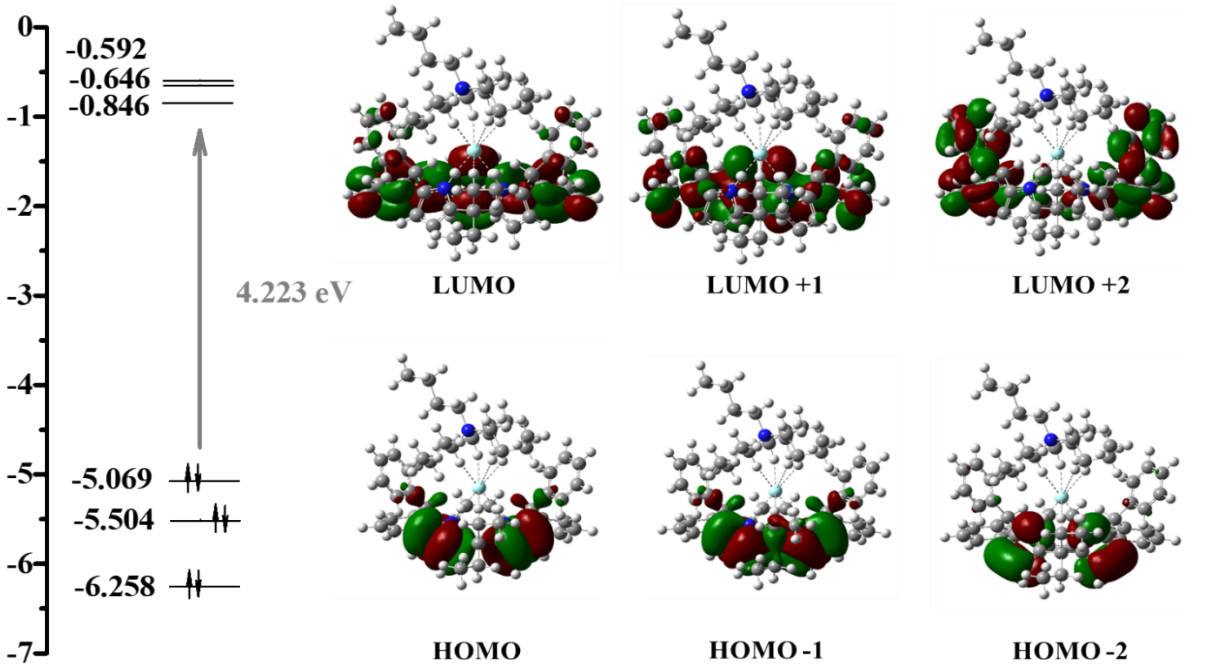


**Fig. S26**. Kohn−Sham orbital energy level diagram of **1.F** selected orbitals calculated at the B3LYP/6-311G (d, p) level of theory and contour plots of selected orbitals (isovalue of 0.02 au).

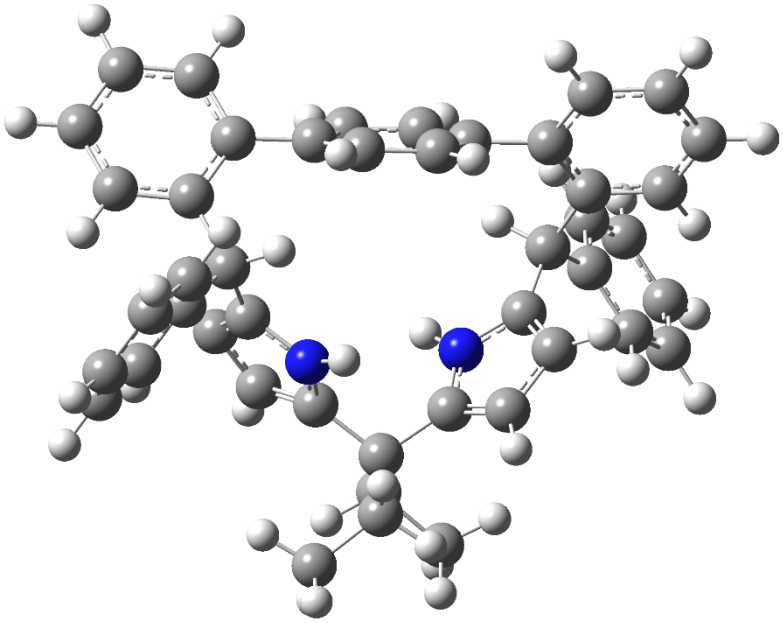

**Fig. S27**. Optimized structure of **1** calculated at the B3LYP/(6-311G (d, p)) level (Solvent = Acetonitrile).

**Table S6**: Cartesian coordinates of the optimized geometry of **1** optimized at B3LYP/(6-311G (d, p)) level (Solvent = Acetonitrile).

# Sum of imaginary frequencies = 0

# Total Energy (Hartree) = -1848.845865 Hartree

Optimized structure coordinates:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.706519 | 1.386174 | 0.166934 |
| 2 | 1 | 0 | 1.501644 | 1.218768 | 1.140590 |
| 3 | 7 | 0 | -1.706508 | 1.386175 | -0.166928 |
| 4 | 1 | 0 | -1.501612 | 1.218755 | -1.140578 |
| 5 | 6 | 0 | 4.680391 | 0.100564 | 0.731552 |
| 6 | 6 | 0 | 3.674096 | -1.622185 | -0.878692 |
| 7 | 6 | 0 | 2.570066 | 0.625696 | -0.588942 |
| 8 | 6 | 0 | 3.406593 | -0.442899 | 0.070021 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 1 | 0 | 2.802240 | -0.829523 | 0.892074 |
| 10 | 6 | 0 | -1.065949 | 2.327395 | 0.608331 |
| 11 | 6 | 0 | -1.319608 | -2.590349 | 0.534097 |
| 12 | 6 | 0 | 1.319591 | -2.590362 | -0.534043 |
| 13 | 6 | 0 | 1.065947 | 2.327389 | -0.608322 |
| 14 | 6 | 0 | 1.096963 | -2.621479 | 0.849057 |
| 15 | 1 | 0 | 1.936596 | -2.673013 | 1.532389 |
| 16 | 6 | 0 | -2.686854 | -2.603800 | 1.138273 |
| 17 | 6 | 0 | -2.570073 | 0.625707 | 0.588938 |
| 18 | 6 | 0 | 0.000005 | 3.229567 | 0.000011 |
| 19 | 6 | 0 | 5.217037 | -0.578584 | 1.832812 |
| 20 | 1 | 0 | 4.722746 | -1.471308 | 2.202827 |
| 21 | 6 | 0 | -3.674113 | -1.622161 | 0.878701 |
| 22 | 6 | 0 | -0.193592 | -2.608399 | 1.369953 |
| 23 | 1 | 0 | -0.330276 | -2.612570 | 2.445387 |
| 24 | 6 | 0 | 2.686833 | -2.603830 | -1.138227 |
| 25 | 6 | 0 | -2.979654 | -3.633582 | 2.044897 |
| 26 | 1 | 0 | -2.227785 | -4.392343 | 2.230703 |
| 27 | 6 | 0 | 4.900182 | -1.715883 | -1.544619 |
| 28 | 1 | 0 | 5.660441 | -0.968972 | -1.352964 |
| 29 | 6 | 0 | -1.546566 | 2.169831 | 1.895006 |
| 30 | 1 | 0 | -1.253038 | 2.749518 | 2.756014 |
| 31 | 6 | 0 | -3.406591 | -0.442893 | -0.070028 |
| 32 | 1 | 0 | -2.802222 | -0.829531 | -0.892064 |
| 33 | 6 | 0 | 0.193574 | -2.608443 | -1.369899 |
| 34 | 1 | 0 | 0.330258 | -2.612647 | -2.445332 |
| 35 | 6 | 0 | 2.979622 | -3.633634 | -2.044830 |
| 36 | 1 | 0 | 2.227751 | -4.392400 | -2.230608 |

| | | | | | |
|---|---|---|---|---|---|
| 37 | 6 | 0 | -1.096981 | -2.621509 | -0.849002 |
| 38 | 1 | 0 | -1.936614 | -2.673066 | -1.532332 |
| 39 | 6 | 0 | 5.331153 | 1.251492 | 0.279092 |
| 40 | 1 | 0 | 4.923473 | 1.796209 | -0.564693 |
| 41 | 6 | 0 | -4.207537 | -3.712044 | 2.695270 |
| 42 | 1 | 0 | -4.404901 | -4.524557 | 3.385229 |
| 43 | 6 | 0 | -2.491715 | 1.099097 | 1.882361 |
| 44 | 1 | 0 | -3.048778 | 0.720415 | 2.725679 |
| 45 | 6 | 0 | -4.900209 | -1.715845 | 1.544611 |
| 46 | 1 | 0 | -5.660465 | -0.968939 | 1.352927 |
| 47 | 6 | 0 | -4.680374 | 0.100564 | -0.731592 |
| 48 | 6 | 0 | 4.207495 | -3.712111 | -2.695219 |
| 49 | 1 | 0 | 4.404849 | -4.524641 | -3.385161 |
| 50 | 6 | 0 | -5.172875 | -2.743154 | 2.445563 |
| 51 | 1 | 0 | -6.135548 | -2.783725 | 2.942591 |
| 52 | 6 | 0 | 6.374819 | -0.125573 | 2.460304 |
| 53 | 1 | 0 | 6.770911 | -0.664412 | 3.314013 |
| 54 | 6 | 0 | 0.621143 | 4.110422 | 1.124260 |
| 55 | 1 | 0 | -0.181223 | 4.672130 | 1.610135 |
| 56 | 1 | 0 | 1.029978 | 3.449804 | 1.894478 |
| 57 | 6 | 0 | -0.621122 | 4.110446 | -1.124226 |
| 58 | 1 | 0 | 0.181252 | 4.672139 | -1.610105 |
| 59 | 1 | 0 | -1.029981 | 3.449843 | -1.894445 |
| 60 | 6 | 0 | 5.172835 | -2.743213 | -2.445551 |
| 61 | 1 | 0 | 6.135501 | -2.783794 | -2.942593 |
| 62 | 6 | 0 | 2.491682 | 1.099072 | -1.882369 |
| 63 | 1 | 0 | 3.048727 | 0.720379 | -2.725694 |
| 64 | 6 | 0 | 7.019364 | 1.021496 | 1.996064 |

| | | | | | |
|---|---|---|---|---|---|
| 65 | 1 | 0 | 7.919150 | 1.378186 | 2.484486 |
| 66 | 6 | 0 | 1.546537 | 2.169809 | -1.895006 |
| 67 | 1 | 0 | 1.252992 | 2.749487 | -2.756014 |
| 68 | 6 | 0 | 6.492772 | 1.707697 | 0.904085 |
| 69 | 1 | 0 | 6.982705 | 2.603112 | 0.537490 |
| 70 | 6 | 0 | -5.331137 | 1.251506 | -0.279171 |
| 71 | 1 | 0 | -4.923468 | 1.796240 | 0.564609 |
| 72 | 6 | 0 | 1.716663 | 5.076985 | 0.667797 |
| 73 | 1 | 0 | 2.529109 | 4.549898 | 0.161031 |
| 74 | 1 | 0 | 2.141664 | 5.595088 | 1.531504 |
| 75 | 1 | 0 | 1.334721 | 5.839745 | -0.015255 |
| 76 | 6 | 0 | -5.217004 | -0.578605 | -1.832848 |
| 77 | 1 | 0 | -4.722711 | -1.471340 | -2.202835 |
| 78 | 6 | 0 | -1.716615 | 5.077031 | -0.667746 |
| 79 | 1 | 0 | -2.141622 | 5.595139 | -1.531446 |
| 80 | 1 | 0 | -1.334646 | 5.839786 | 0.015296 |
| 81 | 1 | 0 | -2.529062 | 4.549962 | -0.160962 |
| 82 | 6 | 0 | -6.492742 | 1.707704 | -0.904195 |
| 83 | 1 | 0 | -6.982675 | 2.603130 | -0.537631 |
| 84 | 6 | 0 | -7.019317 | 1.021482 | -1.996169 |
| 85 | 1 | 0 | -7.919092 | 1.378166 | -2.484617 |
| 86 | 6 | 0 | -6.374771 | -0.125601 | -2.460372 |
| 87 | 1 | 0 | -6.770850 | -0.664457 | -3.314077 |

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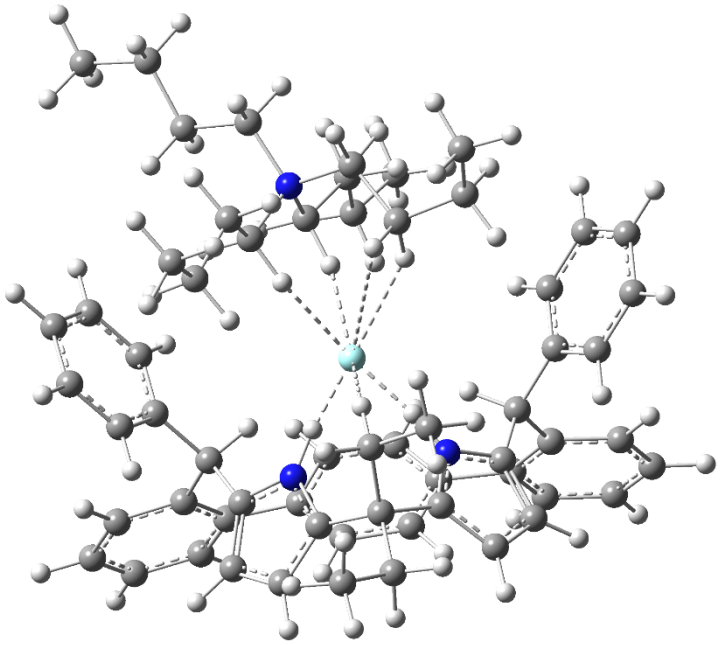

**Fig. S28**. Optimized structure of **1.F** calculated at the B3LYP/(6-311G (d, p)) level. (Solvent = Acetonitrile)

**Table S7**: Cartesian coordinates of the optimized geometry of **1.F** optimized at B3LYP/(6-311G (d, p)) level (Solvent = Acetonitrile).

# Sum of imaginary frequencies = 0

# Total Energy (Hartree) = -2635.077509 Hartree

Optimized structure coordinates:

---

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 9 | 0 | 0.232299 | -0.571193 | 0.561391 |
| 2 | 7 | 0 | -2.232505 | -0.263721 | 1.609108 |
| 3 | 1 | 0 | -1.310082 | -0.442136 | 1.164874 |
| 4 | 7 | 0 | 0.069690 | 1.841082 | 1.725001 |
| 5 | 1 | 0 | 0.202603 | 0.926810 | 1.246586 |
| 6 | 6 | 0 | -3.269671 | 2.228769 | -0.690718 |
| 7 | 1 | 0 | -3.895194 | 2.075142 | 0.179741 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 6 | 0 | -2.251897 | 3.174309 | -0.645154 |
| 9 | 1 | 0 | -2.095615 | 3.747324 | 0.260183 |
| 10 | 6 | 0 | -1.427253 | 3.401454 | -1.754204 |
| 11 | 6 | 0 | -0.390308 | 4.479945 | -1.709496 |
| 12 | 6 | 0 | -2.683690 | 1.703083 | -2.959645 |
| 13 | 1 | 0 | -2.845990 | 1.136547 | -3.870263 |
| 14 | 6 | 0 | -3.503909 | 1.475372 | -1.847876 |
| 15 | 6 | 0 | 1.121441 | 3.100520 | -0.158859 |
| 16 | 1 | 0 | 0.691210 | 2.277720 | -0.740185 |
| 17 | 6 | 0 | -1.660483 | 2.651578 | -2.913309 |
| 18 | 1 | 0 | -1.039486 | 2.810671 | -3.788310 |
| 19 | 6 | 0 | 0.783982 | 4.385931 | -0.929186 |
| 20 | 6 | 0 | 0.445020 | 3.049820 | 1.190886 |
| 21 | 6 | 0 | 2.632269 | 2.839366 | -0.117022 |
| 22 | 6 | 0 | -3.480403 | -1.158338 | -0.360620 |
| 23 | 1 | 0 | -2.597426 | -0.775151 | -0.883207 |
| 24 | 6 | 0 | -4.658924 | 0.525002 | -1.902743 |
| 25 | 6 | 0 | 1.653168 | 5.481961 | -0.896979 |
| 26 | 1 | 0 | 2.561321 | 5.417727 | -0.309861 |
| 27 | 6 | 0 | -4.695641 | -0.684675 | -1.173417 |
| 28 | 6 | 0 | -3.440847 | -0.547214 | 1.020344 |
| 29 | 6 | 0 | -0.627794 | 5.646479 | -2.449112 |
| 30 | 1 | 0 | -1.527155 | 5.707492 | -3.052162 |
| 31 | 6 | 0 | 0.251212 | 6.725526 | -2.409215 |
| 32 | 1 | 0 | 0.041591 | 7.618586 | -2.987139 |
| 33 | 6 | 0 | -2.422687 | 0.340160 | 2.831860 |
| 34 | 6 | 0 | -6.909112 | 0.094264 | -2.737161 |
| 35 | 1 | 0 | -7.752495 | 0.398444 | -3.346809 |
| 36 | 6 | 0 | -5.764267 | 0.885061 | -2.685678 |
| 37 | 1 | 0 | -5.724381 | 1.811104 | -3.248829 |
| 38 | 6 | 0 | -4.434631 | -0.140056 | 1.890370 |
| 39 | 1 | 0 | -5.497829 | -0.214735 | 1.716850 |

| | | | | | |
|---|---|---|---|---|---|
| 40 | 6 | 0 | -5.856577 | -1.463786 | -1.232898 |
| 41 | 1 | 0 | -5.893187 | -2.398273 | -0.686251 |
| 42 | 6 | 0 | 0.035651 | 4.037940 | 2.066013 |
| 43 | 1 | 0 | 0.174743 | 5.100321 | 1.932235 |
| 44 | 6 | 0 | 1.392537 | 6.645653 | -1.617512 |
| 45 | 1 | 0 | 2.085792 | 7.477932 | -1.567494 |
| 46 | 6 | 0 | 3.274518 | 2.360625 | -1.266619 |
| 47 | 1 | 0 | 2.689962 | 2.161090 | -2.159298 |
| 48 | 6 | 0 | 3.405096 | 3.084081 | 1.020807 |
| 49 | 1 | 0 | 2.921964 | 3.445324 | 1.921433 |
| 50 | 6 | 0 | -3.347553 | -2.686641 | -0.376534 |
| 51 | 6 | 0 | -6.958447 | -1.081391 | -1.994938 |
| 52 | 1 | 0 | -7.843458 | -1.707596 | -2.015875 |
| 53 | 6 | 0 | -0.602190 | 2.026909 | 2.912970 |
| 54 | 6 | 0 | -3.792622 | 0.418835 | 3.034388 |
| 55 | 1 | 0 | -4.284974 | 0.843077 | 3.895679 |
| 56 | 6 | 0 | 5.413413 | 2.401364 | -0.142555 |
| 57 | 1 | 0 | 6.484752 | 2.235399 | -0.153053 |
| 58 | 6 | 0 | -1.245136 | 0.856924 | 3.663322 |
| 59 | 6 | 0 | -0.626252 | 3.393621 | 3.151313 |
| 60 | 1 | 0 | -1.078241 | 3.884737 | 3.998904 |
| 61 | 6 | 0 | 4.784716 | 2.869860 | 1.008983 |
| 62 | 1 | 0 | 5.366434 | 3.070284 | 1.902129 |
| 63 | 6 | 0 | -0.189633 | -0.278785 | 3.850684 |
| 64 | 1 | 0 | 0.168254 | -0.575627 | 2.863199 |
| 65 | 1 | 0 | 0.673580 | 0.141818 | 4.375745 |
| 66 | 6 | 0 | 4.650252 | 2.144458 | -1.282936 |
| 67 | 1 | 0 | 5.127352 | 1.776368 | -2.184547 |
| 68 | 6 | 0 | -3.736419 | -3.486095 | 0.701253 |
| 69 | 1 | 0 | -4.116141 | -3.014642 | 1.600425 |
| 70 | 6 | 0 | -0.687698 | -1.522159 | 4.594022 |
| 71 | 1 | 0 | -0.977160 | -1.302443 | 5.625029 |

| | | | | | |
|---|---|---|---|---|---|
| 72 | 1 | 0 | 0.100449 | -2.279861 | 4.630265 |
| 73 | 1 | 0 | -1.551762 | -1.966477 | 4.092829 |
| 74 | 6 | 0 | -1.787778 | 1.341696 | 5.034788 |
| 75 | 1 | 0 | -2.452533 | 2.192423 | 4.859931 |
| 76 | 1 | 0 | -2.421369 | 0.551187 | 5.445364 |
| 77 | 6 | 0 | -2.847874 | -3.315407 | -1.524482 |
| 78 | 1 | 0 | -2.538473 | -2.710213 | -2.370815 |
| 79 | 6 | 0 | -3.643970 | -4.877402 | 0.629874 |
| 80 | 1 | 0 | -3.955390 | -5.479966 | 1.476276 |
| 81 | 6 | 0 | -3.154245 | -5.491459 | -0.520632 |
| 82 | 1 | 0 | -3.081840 | -6.571816 | -0.576159 |
| 83 | 6 | 0 | -2.751827 | -4.702742 | -1.599551 |
| 84 | 1 | 0 | -2.362770 | -5.168128 | -2.498626 |
| 85 | 6 | 0 | -0.742179 | 1.727183 | 6.088210 |
| 86 | 1 | 0 | -1.240378 | 2.139695 | 6.970441 |
| 87 | 1 | 0 | -0.043719 | 2.480246 | 5.718534 |
| 88 | 1 | 0 | -0.158081 | 0.865264 | 6.420101 |
| 89 | 7 | 0 | 3.085858 | -2.573336 | -0.662572 |
| 90 | 6 | 0 | 3.411143 | -1.561325 | 0.437968 |
| 91 | 1 | 0 | 3.830688 | -0.693763 | -0.070903 |
| 92 | 1 | 0 | 2.443075 | -1.257308 | 0.837826 |
| 93 | 6 | 0 | 4.343914 | -3.017619 | -1.405437 |
| 94 | 1 | 0 | 4.985192 | -3.478527 | -0.655458 |
| 95 | 1 | 0 | 4.028370 | -3.807694 | -2.086333 |
| 96 | 6 | 0 | 2.472815 | -3.845404 | -0.078830 |
| 97 | 1 | 0 | 2.172737 | -4.447409 | -0.935691 |
| 98 | 1 | 0 | 3.292741 | -4.369436 | 0.409103 |
| 99 | 6 | 0 | 5.113592 | -1.941764 | -2.165427 |
| 100 | 1 | 0 | 4.496638 | -1.506895 | -2.956034 |
| 101 | 1 | 0 | 5.406835 | -1.126693 | -1.498401 |
| 102 | 6 | 0 | 2.101987 | -1.859567 | -1.596613 |
| 103 | 1 | 0 | 1.293856 | -1.494307 | -0.957524 |

| | | | | | |
|---|---|---|---|---|---|
| 104 | 1 | 0 | 2.640593 | -0.984989 | -1.959728 |
| 105 | 6 | 0 | 0.592835 | -4.987707 | 1.171998 |
| 106 | 1 | 0 | -0.295911 | -4.764693 | 1.769162 |
| 107 | 1 | 0 | 0.226214 | -5.420388 | 0.234574 |
| 108 | 6 | 0 | 1.299266 | -3.652522 | 0.877613 |
| 109 | 1 | 0 | 0.582991 | -2.935187 | 0.474381 |
| 110 | 1 | 0 | 1.651769 | -3.227263 | 1.821823 |
| 111 | 6 | 0 | 6.377447 | -2.546038 | -2.799030 |
| 112 | 1 | 0 | 6.092525 | -3.377289 | -3.453613 |
| 113 | 1 | 0 | 7.008644 | -2.972709 | -2.011901 |
| 114 | 6 | 0 | 4.356788 | -2.040328 | 1.535733 |
| 115 | 1 | 0 | 3.982545 | -2.954714 | 2.004130 |
| 116 | 1 | 0 | 5.345999 | -2.269449 | 1.128548 |
| 117 | 6 | 0 | 1.450268 | -6.017154 | 1.917343 |
| 118 | 1 | 0 | 0.860207 | -6.902768 | 2.167349 |
| 119 | 1 | 0 | 1.838226 | -5.601506 | 2.852736 |
| 120 | 1 | 0 | 2.304180 | -6.354857 | 1.323129 |
| 121 | 6 | 0 | 7.180379 | -1.517697 | -3.599690 |
| 122 | 1 | 0 | 7.508436 | -0.689678 | -2.964363 |
| 123 | 1 | 0 | 6.582869 | -1.097980 | -4.414364 |
| 124 | 1 | 0 | 8.070881 | -1.973663 | -4.039570 |
| 125 | 6 | 0 | 4.504841 | -0.957911 | 2.616819 |
| 126 | 1 | 0 | 3.517811 | -0.726230 | 3.031218 |
| 127 | 1 | 0 | 4.871514 | -0.034051 | 2.157597 |
| 128 | 6 | 0 | 1.569179 | -2.673463 | -2.771805 |
| 129 | 1 | 0 | 2.382538 | -3.112842 | -3.357292 |
| 130 | 1 | 0 | 0.943007 | -3.497693 | -2.419362 |
| 131 | 6 | 0 | 0.728773 | -1.775671 | -3.694280 |
| 132 | 1 | 0 | -0.079456 | -1.317054 | -3.114918 |
| 133 | 6 | 0 | 5.449101 | -1.382765 | 3.744496 |
| 134 | 1 | 0 | 5.086454 | -2.285962 | 4.244477 |
| 135 | 1 | 0 | 5.537526 | -0.596699 | 4.498737 |

| | | | | | |
|---|---|---|---|---|---|
| 136 | 1 | 0 | 6.452438 | -1.593023 | 3.361847 |
| 137 | 6 | 0 | 0.140272 | -2.540697 | -4.882508 |
| 138 | 1 | 0 | -0.517701 | -3.347917 | -4.547177 |
| 139 | 1 | 0 | 0.929285 | -2.986202 | -5.495981 |
| 140 | 1 | 0 | -0.445956 | -1.877424 | -5.523620 |
| 141 | 1 | 0 | 1.351630 | -0.952619 | -4.061844 |

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## 6. References:

[S1] Gaussian 09, Revision E.01; M. J. Frisch et al., Gaussian, Inc.: Wallingford CT, 2009.