Supporting Information

Solvatochromism and pH effect on emission of triphenyl imidazole-phenylacrylonitrile derivative. Experimental and DFT studies

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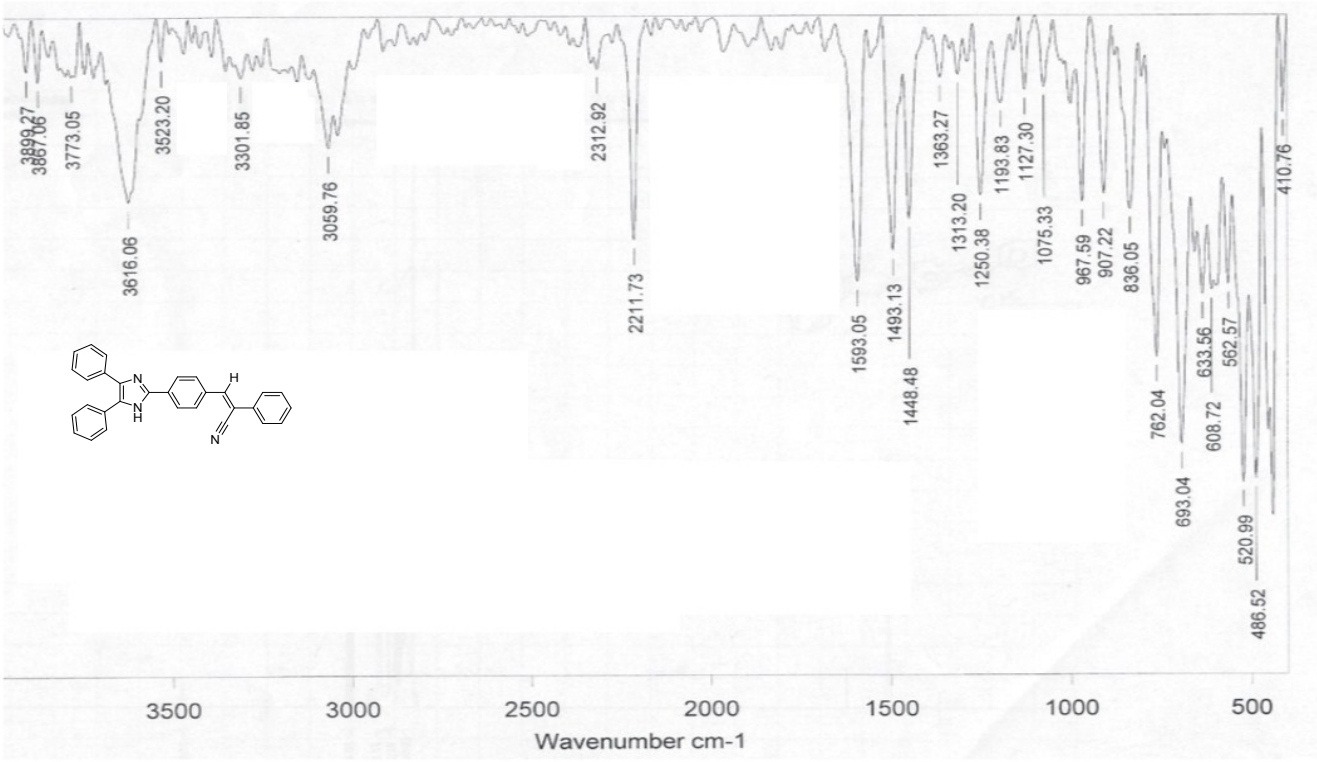
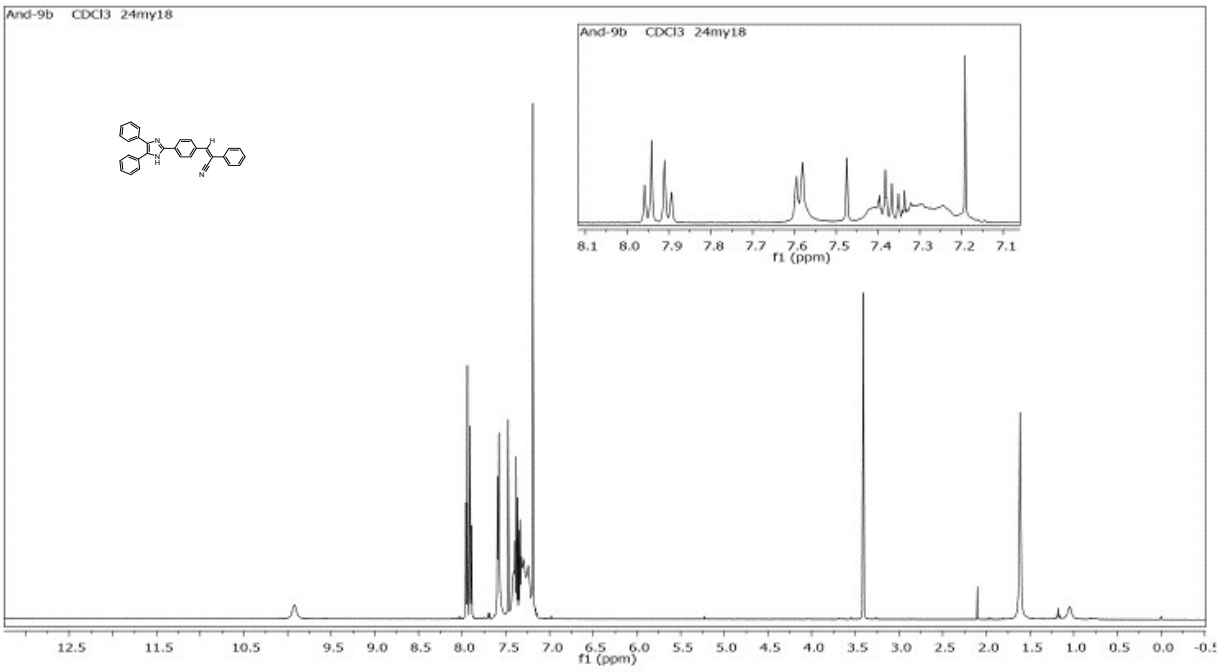
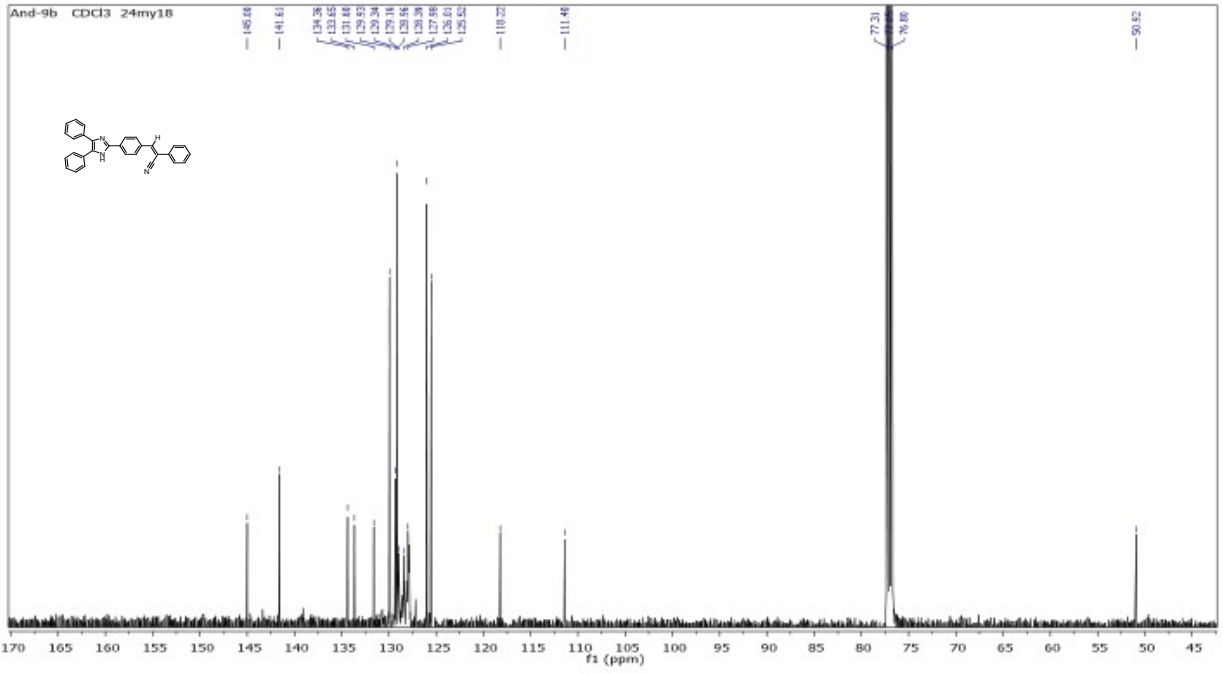
IR spectrum of the (Z)-3-(4-(4,5-diphenyl-1H-imidazol-2-yl)phenyl)-2-phenylacrylonitrile (**2**).

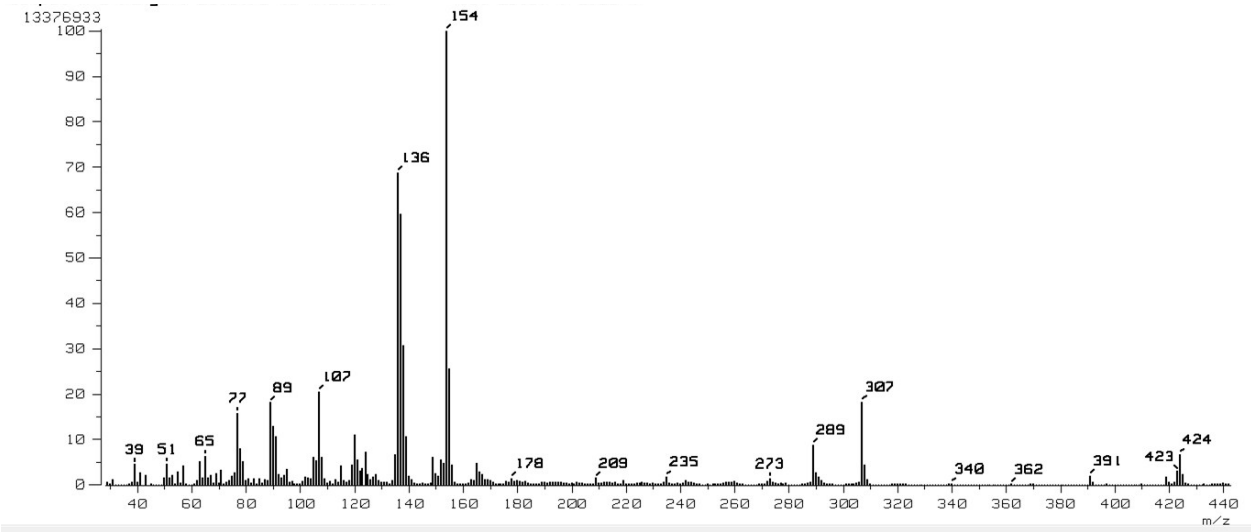


^{1}H-and ^{13}C -NMR spectra of the (Z)-3-(4-(4,5-diphenyl-1H-imidazol-2-yl)phenyl)-2-phenylacrylonitrile (**2**).





MS-(ESI) spectra of the (Z)-3-(4-(4,5-diphenyl-1H-imidazol-2-yl)phenyl)-2-phenylacrylonitrile (**2**).



The Lippert-Mataga plot

The expression for Δf (ε, n), given as,

$$\Delta f\ (\varepsilon,n) = \frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1} \qquad (1)$$

Where ε and n are the dielectric constant and refractive index of the solvents, respectively.

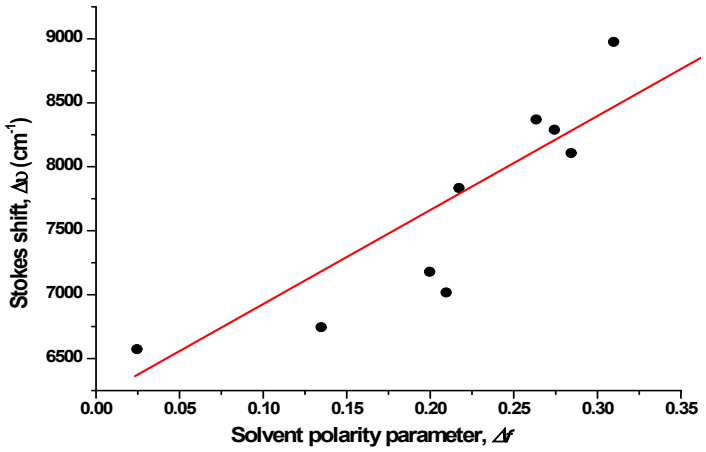


Figure S1. The relationship between stokes shift (nm) and the solvent polarity parameter for the compound **2** in different solvent.

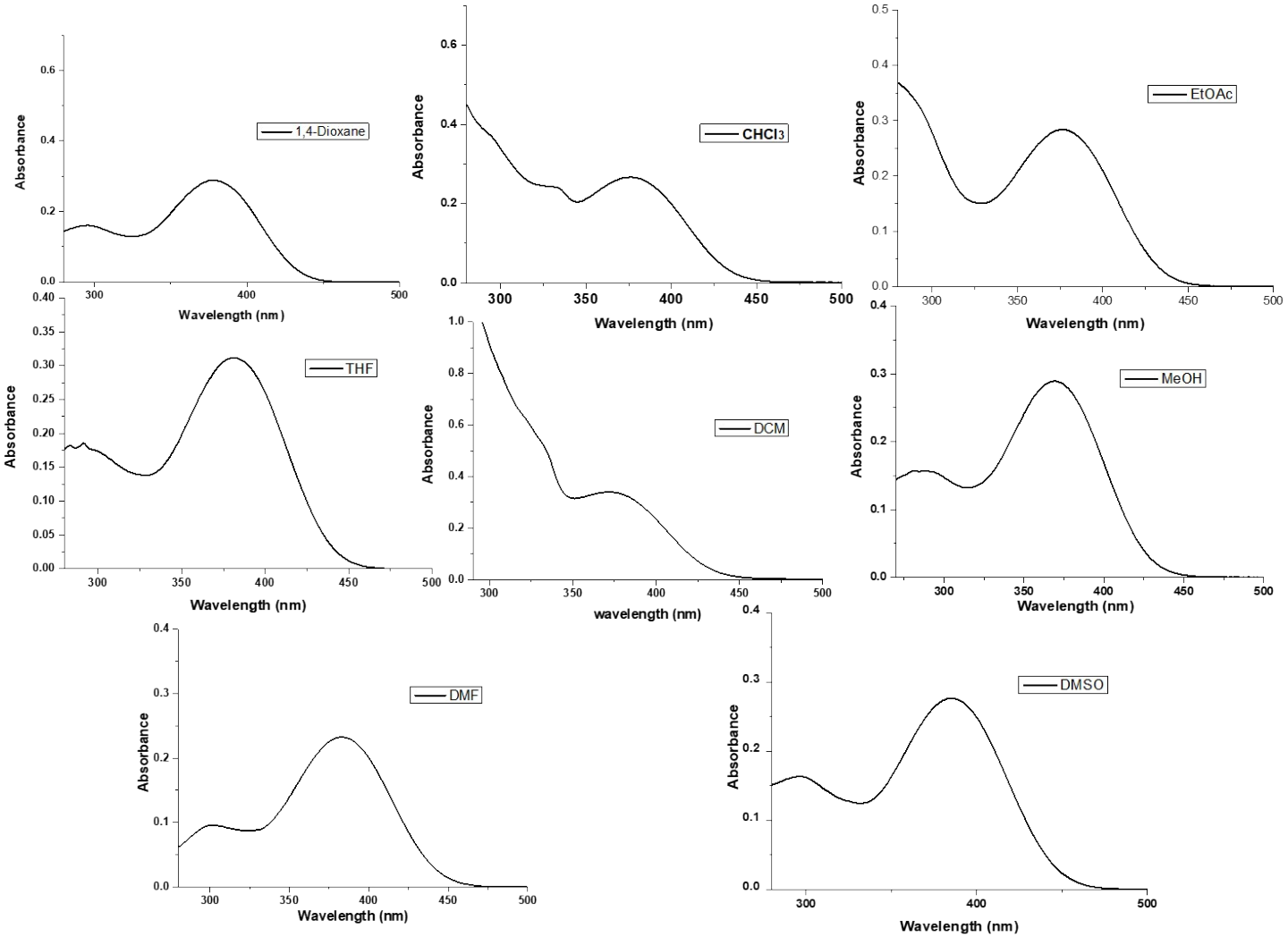
Optical band gap calculation

$$\alpha h\nu = (h\nu - Eg)^n \qquad (2)$$

Where α is the absorbance, E_{gap} is the band gap corresponding to absorption of photon energy at $h\nu$ and n is ½ for allowed direct, 3/2 for forbidden direct, 2 for allowed indirect and 3 for forbidden indirect transitions in the materials. The direct band where obtained from extrapolation of the straight-line portion of their $(\alpha h\nu)^2$ versus hν plots to α = 0

For E_{gap} values are calculated from spectra, it was used a straight line was fitted to the edge of spectra and its intersection with the corrected baseline was determined.

Figure -S2 absorption spectra of the compound 2 in the various solvents.



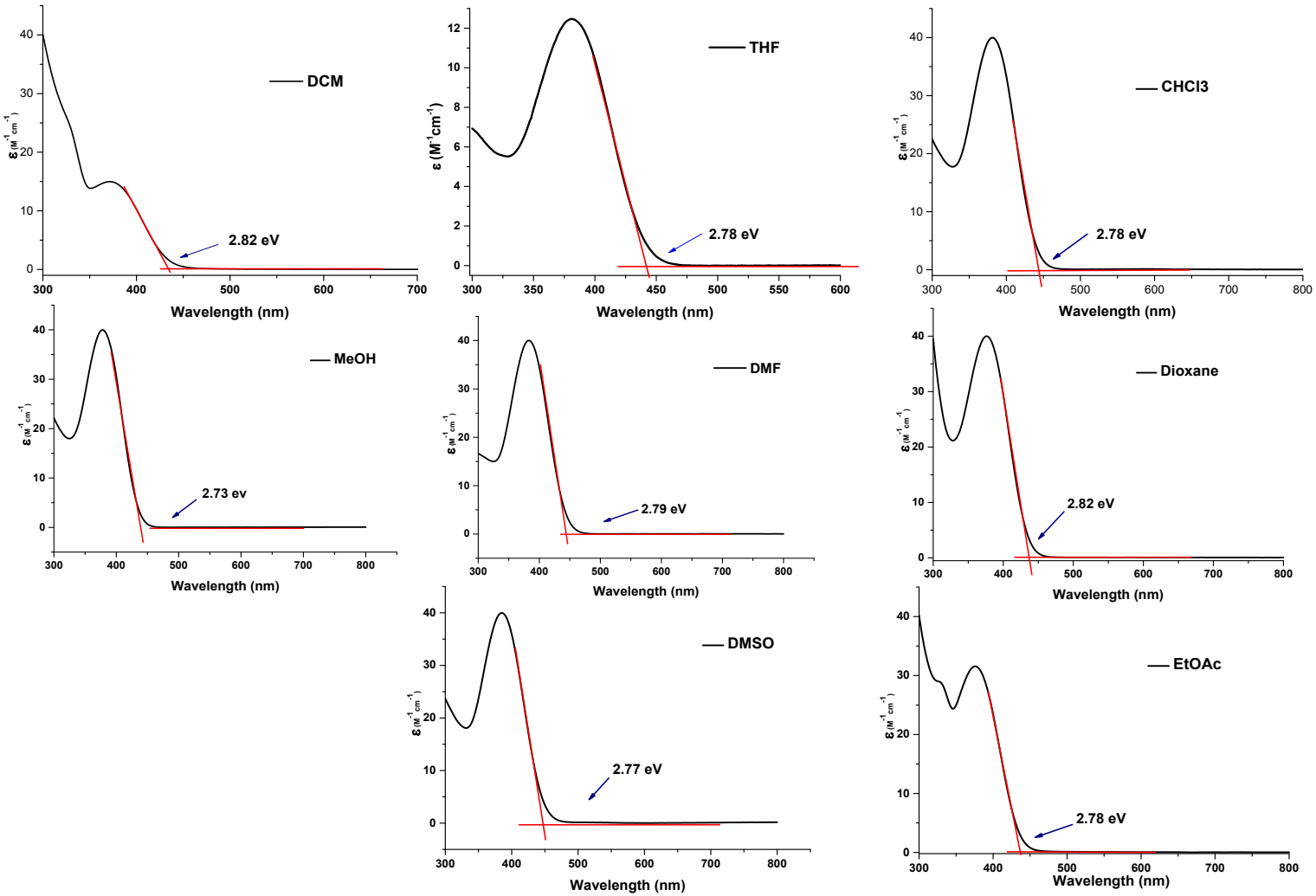
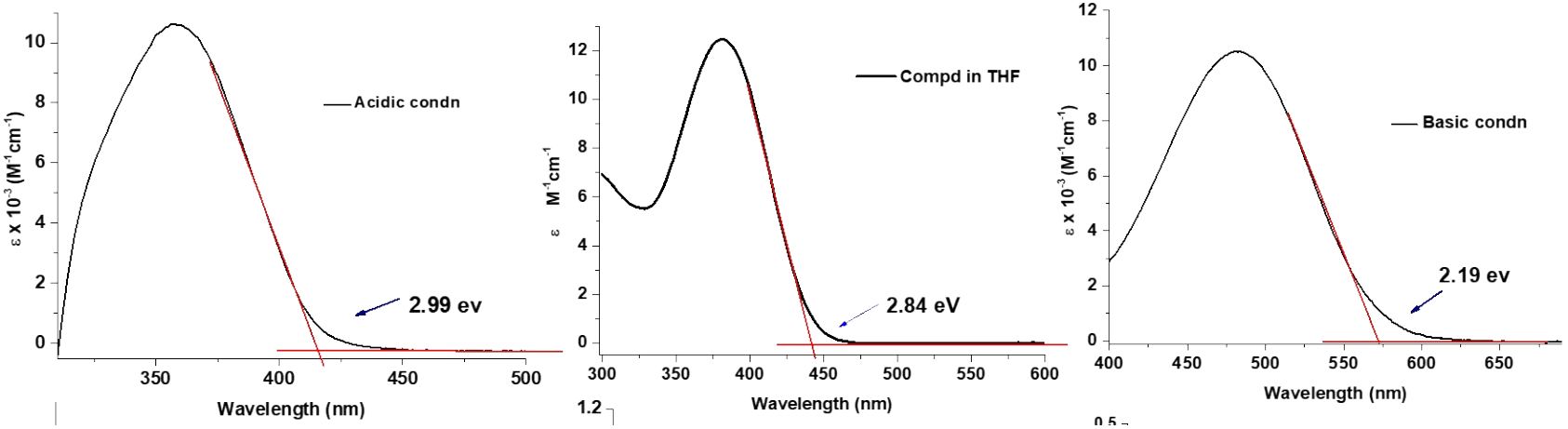


Figure S3 Absorption onset, spectroscopically determined the energy gap for the compound **2** in different solvents.

Figure S4. Absorption onset, spectroscopically determined the energy gap for the compound **2** in pH 2, pH 7 and pH 14



Fluorescence quantum yield

The PL quantum yield (ϕ_F) were evaluated according to the following equation (1) and using a fluorescein solution of 0.1 M NaOH as reference (r).

$$\Phi_x = \Phi_r\left(\frac{Grad_x}{Grad_r}\right)\left(\frac{\eta_x^2}{\eta_r^2}\right) \quad (3)$$

Where Φ is the fluorescence quantum yield, *Grad* refers to the gradient from the plot of integrated fluorescence intensity (excited at 405 nm) against the absorbance, η is the refractive index of the solvent, and the subscripts r and x mean the standard and test sample respectively.[1]

The Cyclo voltagrammetric studies

Electrochemical properties of the compound **2** were evaluated by cyclovoltammetry (CV) in DCM with 0.1 M tetrabutylammonium hexafluorophosphate as supporting electrolyte at a scan rate of 50 $mV^{-1}s$. The Pt acted as the working and saturated calomel electrode (SCE) as the reference electrode. This method is widely used for estimating the energy level of the organic compound. From the oxidation (Ip) and reduction (Ea) potential, the HOMO and LUMO energy levels were calculated using the equation (**3**) and (**4**) and the band gap Egap deduced from equation (**5**). [2,3]

$$Ip = -(Eox + 4.4)\ eV, \quad (3)$$

$$Ea = -(Ered + 4.4)\ eV, \quad (4)$$

$$Eg = Ip - Ea \quad (5)$$

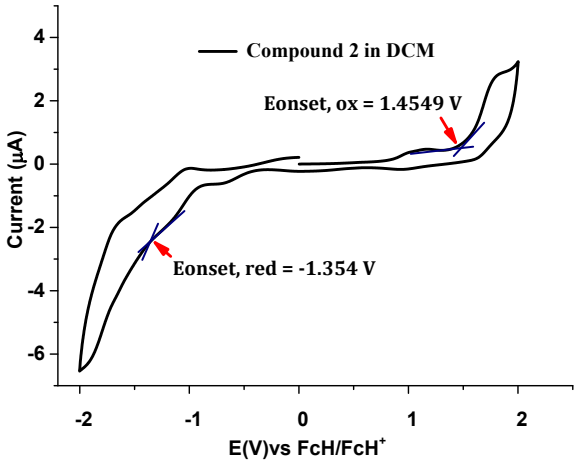


Fig S5 Cyclic Voltagrams of the compound **2** in DCM (50mV/s scan rate)

Table S1 Crystal data and refinement parameters for compound 2

Parameters	Values
Chemical formula	C30H21N3·2(H2O)
Mw	459.53
Crystal system, space group	Monoclinic, P21/c
Temperature (K)	110
a, b, c (Å)	19.3734 (9), 7.6646 (4), 16.9594 (6)
β (°)	110.353 (4)
V (Å3)	2361.07 (19)
Z	4
Radiation type	Cu Kα
μ (mm-1)	0.65
Crystal size (mm)	0.18 × 0.06 × 0.02
Data collection	
Diffractometer	SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid.[4] Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
Tmin, Tmax	0.937, 0.990
No. of measured, independent and observed [I > 2σ(I)] reflections	15779, 4639, 3338
Rint	0.056
(sin θ/λ)max (Å-1)	0.616
Refinement	
R[F2 > 2σ(F2)], wR(F2), S	0.044, 0.111, 1.01
No. of reflections	4639
No. of parameters	331
No. of restraints	7
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρmax, Δρmin (e Å-3)	0.25, -0.26

Table S2. Selected dihedral angles (°) for compound **2**

Bond	Angle (°)
C(1)C(6)-C(7)-N(1)	136.66(18)
C(5)-C(6)-C(7)-N(1)	-41.3(3)
C(1)-C(6)-C(7)-C(8)	-40.2(3)
C(5)-C(6)-C(7)-C(8)	141.9(2)
N(1)-C(7)-C(8)-N(2)	-1.1(2)
N(2)-C(15)-N(1)-C(7)	-0.8(2)
C(8)-C(7)-N(1)-C(15)	1.2(2)
N(1)-C(15)-N(2)-C(8)	0.1(2)
C(7)-C(8)-N(2)-C(15)	0.7(2)
C(6)-C(7)-C(8)-C(9)	-5.3(4)
N(2)-C(8)-C(9)-C(10)	-22.0(3)
C(7)-C(8)-C(9)-C(14)	-20.2(3)
C(8)-C(9)-C(14)-C(13)	176.91(18)
N(2)-C(15)-C(16)-C(21)	21.8(3)
N(1)-C(15)-C(16)-C(17)	22.3(3)
C(18)-C(19)-C(22)-C(23)	-25.6(3)
C(19)-C(22)-C(23)-C(24)	-9.3(3)
C(22)-C(23)-C(25)-C(30)	-21.3(3)
C(24)-C(23)-C(25)-C(26)	-17.1(2)

Table S3. Bond lengths (Å) for data of compound **2**

C(1)-C(2)	1.382(3)
C(1)-C(6)	1.397(3)
C(2)-C(3)	1.392(3)
C(3)-C(4)	1.387(3)
C(4)-C(5)	1.388(3)
C(5)-C(6)	1.400(2)
C(6)-C(7)	1.469(3)
C(7)-N(1)	1.383(2)
C(7)-C(8)	1.391(2)
C(8)-N(2)	1.380(2)
C(8)-C(9)	1.475(2)
C(9)-C(10)	1.398(3)
C(9)-C(14)	1.400(3)
C(10)-C(11)	1.392(2)
C(11)-C(12)	1.384(3)
C(12)-C(13)	1.392(3)
C(13)-C(14)	1.391(2)
C(15)-N(2)	1.329(2)
C(15)-N(1)	1.349(2)
C(15)-C(16)	1.468(2)
C(16)-C(21)	1.389(3)
C(16)-C(17)	1.405(2)
C(17)-C(18)	1.379(3)
C(18)-C(19)	1.396(3)
C(19)-C(20)	1.410(2)
C(19)-C(22)	1.456(3)
C(20)-C(21)	1.385(3)
C(22)-C(23)	1.358(2)
C(23)-C(24)	1.439(3)
C(23)-C(25)	1.482(3)
C(24)-N(3)	1.149(3)
C(25)-C(30)	1.398(3)
C(25)-C(26)	1.402(2)
C(26)-C(27)	1.380(3)
C(27)-C(28)	1.384(3)
C(28)-C(29)	1.397(3)
C(29)-C(30)	1.386(3)
N(1)-C(1N)	0.880(18)
O(1W)-H1(W1)	0.84(2)
O(1W)-H1(W2)	0.86(2)
O(2W)-H(2W1)	0.86(2)
C(2W)-H(2W2)	0.84(2)

Table S4. Bond angles (º) for compound **2**

C(2)-C(1)-C(6)	120.60(16)
C(2)-C(1)-H(1)	119.7
C(6)-C(1)-H(1)	119.7
C(1)-C(2)-C(3)	120.55(18)
C(1)-C(2)-H(2)	119.7
C(3)-C(2)-H(2)	119.7
C(4)-C(3)-C(2)	119.32(19)
C(4)-C(3)-H(3)	120.3
C(2)-C(3)-H(3)	120.3
C(3)-C(4)-C(5)	120.41(17)
C(3)-C(4)-H(4)	119.8
C(5)-C(4)-H(4)	119.8
C(4)-C(5)-C(6)	120.52(17)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(1)-C(6)-C(5)	118.59(17)
C(1)-C(6)-C(7)	121.24(15)
C(5)-C(6)-C(7)	120.13(16)
N(1)-C(7)-C(8)	104.66(16)
N(1)-C(7A)-C(6)	120.46(14)
C(8)-C(7)-C(6)	134.83(15)
N(2)-C(8)-C(7)	109.72(14)
N(2)-C(8)-C(8)	119.67(16)
C(7)-C(8)-C(9)	130.59(18)
C(10)-C(9)-C(14)	118.25(15)
C(10)-C(9)-C(8)	119.48(17)
C(14)-C(9)-C(9)	122.27(16)
C(11)-C(10)-C(9)	120.89(18)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(12)-C(11)-C(10)	120.26(17)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	119.56(15)
C(11)-C(12)-H(12)	120.2
C(13)-C(12)-H(12)	120.2
C(14)-C(13)-C(12)	120.25(18)
C(14)-C(13)-H(13)	119.9
C(12)-C(13)-H(13)	119.9
C(13)-C(14)-C(9)	120.68(17)
C(13)-C(14)-H(14)	119.7
C(9)-C(14)-H(14)	119.7
N(2)-C(15)-N(1)	111.01(16)
N(2)-C(15)-C(16)	124.79(17)
N(1)-C(15)-C(16)	124.19(14)
C(21)-C(16)-C(17)	119.15(16)
C(21)-C(16)-C(15)	121.03(14)
C(17)-C(16)-C(15)	119.80(17)
C(18)-C(17)-C(16)	120.18(17)
C(18)-C(17)-H(17)	119.9
C(16)-C(17)-H(17)	119.9
C(17)-C(18)-C(19)	121.21(15)
C(17)-C(18)-H(18)	119.4
C(19)-C(18)-H(18)	119.4
C(18)-C(19)-C(20)	118.27(17)
C(18)-C(19)-C(22)	122.91(15)
C(20)-C(19)-C(22)	118.78(17)
C(21)-C(20)-H(19)	120.50(18)
C(21)-C(20)-H(20)	119.7
C(19)-C(20)-H(20)	119.7
C(20)-C(21)-C(16)	120.65(15)
C(20)-C(21)-H(21)	119.7
C(16)-C(21)-H(21)	119.7
C(23)-C(22)-C(19)	127.72(18)
C(23)-C(22)-H(22)	116.1
C(19)-C(22)-H(22)	116.1
C(22)-C(23)-C(24)	120.07(17)
C(22)-C(23)-C(25)	124.11(18)
C(24)-C(23)-C(25)	115.75(14)
N(3)-C(24)-C(23)	177.5(2)
C(30)-C(25)-C(26)	118.54(17)
C(30)-C(25)-C(23)	120.98(15)
C(26)-C(25)-C(23)	120.47(17)
C(27)-C(26)-C(25)	120.75(18)
C(27)-C(26)-H(26)	119.6
C(25)-C(26)-H(26)	119.6
C(26)-C(27)-C(28)	120.51(16)
C(26)-C(27)-H(27)	119.7
C(28)-C(27)-H(27)	119.7
C(27)-C(28)-C(29)	119.39(18)
C(27)-C(28)-H(28)	120.3
C(29)-C(28)-H(28)	120.3
C(30)-C(29)-C(28)	120.35(19)
C(30)-C(29)-H(29)	119.8
C(28)-C(29)-H(29)	119.8
C(29)-C(30)-C(25)	120.43(16)
C(29)-C(30)-H(30)	119.8
C(25)-C(30)-H(30)	119.8
C(15)-N(1)-C(7)	108.52(13)
C(15)-N(1)-N(1N)	125.4(15)
C(7)-N(1)-N(N1)	126.1(15)
C(15)-N(2)-C(8)	106.07(15)
H(1W1)-O(1W)-H(1W2)	108(2)
H(2W1)-O(2W)-H(2W2)	112(2)

Table S5 Torsion angles (º) for compound **2**

C(6)-C(1)-C(2)-C(3)	0.0(3)
C(1)-C(2)-C(3)-C(4)	0.7(3)
C(2)-C(3)-C(4)-C(5)	-0.6(3)
C(3)-C(4)-C(5)-C(6)	-0.2(3)
C(2)-C(1)-C(6)-C(5)	-0.8(3)
C(2)-C(1)-C(6)-C(7)	-178.73(17)
C(4)-C(5)-C(6)-C(1)	0.9(3)
C(4)-C(5)-C(6)-C(7)	178.87(17)
C(1)C(6)-C(7)-N(1)	136.66(18)
C(5)-C(6)-C(7)-N(1)	-41.3(3)
C(1)-C(6)-C(7)-C(8)	-40.2(3)
C(5)-C(7)-C(7)-C(8)	141.9(2)
N(1)-C(7)-C(8)-N(2)	-1.1(2)
C(6)-C(7)-C(8)-N(2)	176.1(2)
N(1)-C(7)-C(8)-C(9)	177.52(18)
C(6)-C(7)-C(8)-C(9)	-5.3(4)
N(2)-C(8)-C(9)-C(10)	-22.0(3)
C(7)-C(8)-C(9)-C(10)	159.4(2)
N(2)-C(8)-C(9)-C(14)	158.29(18)
C(7)-C(8)-C(9)-C(14)	-20.2(3)
C(14)-C(9)-C(10)-C(11)	3.1(3)
C(8)-C(9)-C(10)-C(11)	-176.63(18)
C(9)-C(10)-C(11)-C(12)	-0.6(3)
C(10)-C(11)-C(12)-C(13)	-2.2(3)
C(11)-C(12)-C(13)-C(14)	2.4(3)
C(12)-C(13)-C(14)-C(9)	0.1(3)
C(10)-C(9)-C(14)-C(13)	-2.8(3)
C(8)-C(9)-C(14)-C(13)	176.91(18)
N(2)-C(15)-C(16)-C(21)	21.8(3)
N(1)-C(15)-C(16)-C(21)	-159.52(18)
N(2)-C(15)-C(16)-C(17)	-156.48(18)
N(1)-C(15)-C(16)-C(17)	22.3(3)
C(21)-C(16)-C(17)-C(18)	0.5(3)
C(15)-C(16)-C(17)-C(18)	178.76(17)
C(16)-C(16)-C(18)-C(19)	0.3(3)
C(17)-C(18)-C(19)-C(20)	-1.7(3)
C(17)-C(18)-C(19)-C(22)	-179.49(18)
C(18)-C(19)-C(20)-C(21)	2.3(3)
C(22)-C(19)-C(20)-C(21)	-179.83(18)
C(19)-C(20)-C(21)-C(16)	-1.5(3)
C(17)-C(16)-C(21)-C(20)	0.1(3)
C(15)-C(16)-C(21)-C(20)	-178.13(17)
C(18)-C(19)-C(22)-C(23)	-25.6(3)
C(20)-C(19)-C(22)-C(23)	156.7(2)
C(19)-C(22)-C(23)-C(24)	-9.3(3)
C(19)-C(22)-C(23)-C(25)	173.71(17)
C(22)-C(23)-C(25)-C(30)	-21.3(3)
C(24)-C(23)-C(25)-C(30)	161.58(17)
C(22)-C(23)-C(25)-C(26)	160.00(18)
C(24)-C(23)-C(25)-C(26)	-17.1(2)
C(30)-C(25)-C(26)-C(27)	1.8(3)
C(23)-C(25)-(26)-C(27)	-179.43(17)
C(25)-C(26)-C(27)-C(28)	-0.7(3)
C(26)-C(27)-C(28)-C(29)	-0.6(3)
C(27)-C(28)-C(29)-C(30)	0.7(3)
C(28)-C(29)-C(29)-C(25)	0.5(3)
C(26)-C(25)-C(30)-C(29)	-1.7(3)
C(23)-C(25)-C(30)-C(29)	179.53(17)
N(15)-C(15)-N(1)-C(7)	-0.8(2)
C(16)-C(15)-N(1)-C(7)	-179.70(17)
C(8)-C(7)-N(1)-C(15)	1.2(2)
C(6)-C(7)-N(1)-C(15)	-176.54(17)
N(1)-C(15)-N(2)-C(8)	0.1(2)
C(16)-C(15)-N(2)-C(8)	178.97(17)
C(7)-C(8)-N(2)-C(15)	0.7(2)
C(9)-C(8)-N(2)-C(15)	-178.15(16)

Table S6. The data of absorption, emission for the compound **2** in the solid state.

Nature	**λ_{abs} (nm)**	**λ_{em} (nm)**	**Φ_F**
Powder	420 br	563	0.16
Thin film	388	540	ND

λ_{abs} = Maximum absorption wavelength; λ_{em} = Maximum absorption wavelength[1]; ΦF= Quantum yield; ND = Not determined.

Table S7. Optoelectronic properties for Compound **2** at B3LYP/MIDIX level of theory.

Parameters	Values
Oxidation Potential (eV)	1.2822
Reduction Potential (eV)	-1.4001
Hole Reorganization Energy (HER) (eV)	0.2174
Electron Reorganization Energy (ERE)(eV)	0.3238
Triplet Energy (eV)	1.8327
Lmax (nm)	412
Emax (nm)	458
Stokes Shift	46
Triplet Stabilization Energy (eV)	0.5449
Hole Extraction Potential (eV)	6.3368
Electron Extraction Potential (eV)	-1.2032
Scaled HOMO (eV)	-5.8121
Scaled LUMO (eV)	-3.1299
Electron Small Polaron Stabilization Energy (eV)	0.1859
Hole Small Polaron Stabilization Energy (eV)	0.1191
Triplet Reorganization Energy (eV)	2.008
T1 Vertical Emission (eV)	0.3019
T1 Vertical Absorption (eV)	2.3100
T1 Raw Triplet Energy (eV)	1.7651
S1-T1 Gap (eV)	1.8530
S1-T2 Gap (eV)	0.2558
S1-T3 Gap (eV)	-0.7439
Dipole (D)	1.0851

All torsion angles follow the convention defined by Allen & Rogers (Allen, F.H. & Rogers, D. (1969) *Acta Cryst*. **B25**, 1326-1330)

Table S8. Experimental and computed absorption wavelength (λ, in nm) for compound **2**. (The B3LYP/6-311+G(d,p) level) of the was used for this calculation.

λ_{abs} (DFT)	eV	*f*	Major Transition (%)	λ_{exp}	λ_{abs} (DFT)	eV	*f*	Major Transition (%)	λ_{exp}
Gas					**Cloroform**				
444	2.79	0.999	H→ L (99)		458	2.71	1.180	H→ L (99)	
341	3.63	0.573	H-1→ L (87)		345	3.60	0.418	H-1→ L (95)	375
329	3.81	0.246	H→ L+1 (86)		325	3.81	0.263	H→ L+1 (94)	297
1,4-Dioxane					**Ethyl acetate**				
457	2.71	1.175	H→ L (99)		456	2.72	1.162	H→ L (99)	
345	3.59	0.435	H-1→ L (95)	378	344	3.60	0.421	H-1→ L (95)	376
327	3.79	0.256	H→ L+1 (93)	300	324	3.82	0.255	H→ L+1 (94)	293
Major Transition					**Major Transition**				
457	2.72	1.170	H→ L (99)		457	2.71	1.174	H→ L (99)	
344	3.60	0.416	H-1→ L (95)	381	344	3.60	0.413	H-1→ L (96)	371
324	3.82	0.260	H→ L+1 (94)	305	324	3.82	0.263	H→ L+1 (94)	281
Metanol					**DMF**				
455	2.73	1.149	H→ L (99)		457	2.71	1.176	H→ L (99)	
343	3.61	0.415	H-1→ L (95)	370	344	3.60	0.407	H-1→ L (96)	382
323	3.84	0.252	H→ L+1 (94)	290	324	3.83	0.265	H→ L+1 (94)	300
DMSO									
457	2.72	1.173	H→ L (99)						
344	3.60	0.407	H-1→ L (96)	385					
324	3.83	0.264	H→ L+1 (94)	297					

Table S9 Computed absorption wavelength (λ, in nm) for compound 2 in cation and anion environment. The B3LYP/6-311+G(d,p) level of the was used for this calculation.

Cation				**Anion**			
λ_{abs} (DFT)	**eV**	*f*	**Major Transition (%)**	λ_{abs} (DFT)	**eV**	*f*	**Major Transition (%)**
Gas							
441	2.81	1.229	H→ L (99)	582	2.13	1.293	H→ L (96)
365	3.39	0.083	H-2→ L (98)	389	3.19	0.027	H→ L+3 (63)
317	3.91	0.058	H→ L+1 (98)				H→ L+2 (17)
				372	3.33	0.114	H→ L+2 (71)
							H→ L+3 (12)
THF							
418	2.97	1.456	H→ L (99)	563	2.20	1.303	H→ L (100)
356	3.48	0.033	H-1→ L (98)	370	3.35	0.209	H→ L+1 (96)
300	4.13	0.050	H-4→ L (85)	350	3.54	0.361	H-2→ L (69)
							H-3→ L (15)

Table S10 The selected second order perturbation energy (E^2 in kcal mol^{-1}) for compound **2** at neutral environment.

Donor NBO (i)	Acceptor NBO (j)	E^2	Donor NBO (i)	Acceptor NBO (j)	E^2
Phenyl Ring 1 (atoms 1-11)			**Phenylacrylnitrile moiety**		
BD (2) C 1 - C 3	BD*(2) C 9 - C 11	20.58	BD (1) C 38 - C 40	BD*(2) C 40 - C 41	753.42
BD (2) C 5 - C 7	BD*(2) C 9 - C 11	20.37	BD (1) C 38 - C 39	BD*(1) C 40 - C 41	706.11
BD (2) C 9 - C 11	BD*(2) C 5 - C 7	20.31	BD (1) C 36 - C 38	BD*(1) C 40 - C 41	437.57
BD (2) C 1 - C 3	BD*(2) C 5 - C 7	20.25	BD (2) C 39 - N 54	BD*(3) C 39 - N 54	252.49
BD (2) C 5 - C 7	BD*(2) C 1 - C 3	19.80	BD (1) C 41 - C 43	BD*(2) C 40 - C 41	119.45
BD (2) C 9 - C 11	BD*(2) C 1 - C 3	18.80	BD (2) C 40 - C 41	BD*(2) C 43 - C 45	74.72
Phenyl Ring 2 (atoms 14-24)			BD (1) C 41 - H 42	BD*(3) C 39 - N 54	59.00
BD (2) C 14 - C 23	BD*(2) C 19 - C 21	20.92	BD (1) C 39 - N 54	BD*(1) C 40 - C 41	49.06
BD (2) C 15 - C 17	BD*(2) C 19 - C 21	20.64	BD (1) C 40 - C 49	BD*(2) C 40 - C 41	45.89
BD (2) C 15 - C 17	BD*(2) C 14 - C 23	20.06	BD (2) C 36 - C 38	BD*(3) C 39 - N 54	35.96
BD (2) C 14 - C 23	BD*(2) C 15 - C 17	19.45	BD (2) C 47 - C 49	BD*(2) C 43 - C 45	35.30
BD (2) C 19 - C 21	BD*(2) C 14 - C 23	16.17	BD (2) C 36 - C 38	BD*(2) C 43 - C 45	32.08
BD (2) C 19 - C 21	BD*(2) C 15 - C 17	15.85	BD (1) C 40 - C 41	BD*(3) C 39 - N 54	32.06
Phenyl Ring 3 (atoms 26-35)			BD (1) C 38 - C 39	BD*(3) C 39 - N 54	28.95
BD (2) C 26 - C 34	BD*(2) C 31 - C 32	23.10	BD (1) C 39 - N 54	BD*(2) C 36 - C 38	18.98
BD (2) C 31 - C 32	BD*(2) C 36 - C 38	22.28	BD (1) C 38 - C 39	BD*(3) C 39 - N 54	16.82
BD (2) C 31 - C 32	BD*(2) C 26 - C 34	20.74	BD (2) C 40 - C 41	BD*(2) C 36 - C 38	15.31
BD (2) C 27 - C 29	BD*(2) C 26 - C 34	19.80			
BD (2) C 26 - C 34	BD*(2) C 25 - N 53	19.35	**Lone pair electrons in nitrogen atoms**		
BD (2) C 31 - C 32	BD*(2) C 27 - C 29	19.79	LP (1) N 51	BD*(2) C 12 - C 13	32.07
BD (2) C 26 - C 34	BD*(2) C 27 - C 29	18.77	LP (1) N 51	D*(2) C 25 - N 53	47.01
BD (2) C 27 - C 29	BD*(2) C 31 - C 32	17.54	LP (1) N 53	BD*(1) C 25 - N 51	8.49
Imidazole ring (atoms 12,13,25,51-53)			LP (1) N 53	BD*(1) C 12 - C 13	5.78
BD (2) C 25 - N 53	BD*(2) C 12 - C 13	21.75	LP (1) N 54	BD*(2) C 36 - C 38	6.23
BD (1) C 12 - C 13	BD*(2) C 25 - N 53	15.44			
BD (2) C 14 - C 23	BD*(2) C 12 - C 13	12.33			
BD (1) C 12 - C 13	BD*(2) C 14 - C 23	8.99			
BD (2) C 25 - N 53	BD*(2) C 26 - C 34	8.74			
BD (1) C 12 - C 13	BD*(2) C 9 - C 11	8.27			
BD (1) C 13 - N 53	BD*(1) C 25 - C 26	6.12			
BD (1) C 12 - C 13	BD*(1) C 11 - C 12	4.81			

Table S11 The selected second order perturbation energy (E^2 in kcal mol^{-1}) for compound **2** at cation environment.

Donor NBO (i)	Acceptor NBO (j)	E^2	Donor NBO (i)	Acceptor NBO (j)	E^2
Phenyl Ring 1 (atoms 1-11)			**Imidazole ring (atoms 12,13,25,51-53)**		
BD (2) C 5 - C 7	BD*(2) C 9 - C 11	64.34	BD (1) C 13 - N 53	BD*(1) C 14 - C 15	56.72
BD (1) C 5 - H 6	BD*(2) C 5 - C 7	53.66	BD (1) C 13 - N 53	BD*(1) C 15 - H 16	23.53
BD (1) C 7 - C 9	BD*(2) C 5 - C 7	43.01	BD (1) C 13 - C 14	BD*(1) C 14 - C 15	21.98
BD (1) C 5 - H 6	BD*(1) C 7 - H 8	32.52	BD (1) C 25 - C 26	BD*(1) C 26 - C 27	11.00
BD (2) C 9 - C 11	BD*(2) C 5 - C 7	27.05	BD (1) C 12 - N 51	BD*(1) C 13 - C 14	4.07
BD (2) C 5 - C 7	BD*(2) C 9 - C 11	22.72	BD (1) C 12 - N 51	BD*(1) C 47 - H 48	4.05
BD (2) C 1 - C 3	BD*(2) C 9 - C 11	20.68	**Phenylacrylnitrile moiety**		
BD (1) C 5 - H 6	BD*(1) C 3 - H 4	22.34	BD (1) C 43 - C 45	BD*(1) C 47 - H 48	188.44
BD (2) C 1 - C 3	BD*(2) C 5 - C 7	22.30	BD (1) C 47 - C 49	BD*(1) C 47 - H 48	141.89
Phenyl Ring 2 (atoms 14-21)			BD (2) C 36 - C 38	BD*(2) C 31 - C 32	87.93
BD (1) C 21 - H 22	BD*(1) C 14 - C 15	108.26	BD (1) C 40 - C 49	BD*(1) C 47 - H 48	35.39
BD (1) C 21 - H 22	BD*(1) C 21 - C 23	95.71	BD (1) C 39 - N 54	BD*(1) C 45 - H 46	25.60
BD (1) C 21 - H 22	BD*(2) C 21 - C 23	89.40	BD (3) C 39 - N 54	BD*(2) C 31 - C 32	25.58
BD (1) C 21 - H 22	BD*(1) C 15 - H 16	56.20	BD (1) C 39 - N 54	BD*(3) C 39 - N 54	15.01
BD (1) C 21 - H 22	BD*(1) C 17 - C 19	47.61			
BD (1) C 14 - C 23	BD*(2) C 27 - C 29	30.98	**Lone pair electrons in nitrogen atoms**		
BD (1) C 19 - C 21	BD*(1) C 21 - C 23	31.41	LP (1) N 51	LP*(1) C 25	130.25
BD (1) C 19 - C 21	BD*(2) C 21 - C 23	15.48	LP (1) N 51	LP*(1) C 25	129.56
BD (1) C 19 - C 21	BD*(1) C 26 - C 27	14.13	LP (1) N 53	D*(2) C 31 - C 32	43.11
Phenyl Ring 3 (atoms 26-35)			LP (1) N 51	BD*(2) C 12 - C 13	28.32
BD (2) C 27 - C 29	BD*(2) C 31 - C 32	173.41	LP (1) N 53	BD*(2) C 12 - C 13	26.46
BD (2) C 26 - C 34	BD*(2) C 31 - C 32	83.29			
BD (2) C 31 - C 32	BD*(2) C 26 - C 34	41.35			
BD (2) C 27 - C 29	BD*(2) C 26 - C 34	29.84			
BD (1) C 25 - C 26	BD*(2) C 27 - C 29	23.24			
BD (2) C 31 - C 32	D*(2) C 36 - C 38	15.26			
BD (1) C 26 - C 34	BD*(1) C 26 - C 27	8.70			

Table S12 The selected second order perturbation energy (E^2 in kcal mol^{-1}) for title compound at anion environment.

Donor NBO (i)	Acceptor NBO (j)	E^2	Donor NBO (i)	Acceptor NBO (j)	E^2
Phenyl Ring 1 (atoms 1-11)					
BD (2) C 7 - C 9	BD*(2) C 1 - C 11	24.61	Im and Ph ring 1-2	mring3:12,13,25,51-53	
BD (2) C 1 - C 11	BD*(2) C 3 - C 5	23.39	BD (2) C 39 - N 53	BD*(3) C 39 – N53	522.44
BD (2) C 3 - C 5	BD*(2) C 7 - C 9	20.86	BD (1) C 41 - H 42	BD*(3) C 39 - N 53	322.59
BD (2) C 3 - C 5	BD*(2) C 1 - C 11	20.72	BD (3) C 39 - N 53	BD*(1) C 43 - C 45	173.45
BD (2) C 14 - C 23	BD*(2) C 19 - C 21	23.68	BD (1) C 40 - C 41	BD*(3) C 39 - N 53	168.06
BD (2) C 15 - C 17	BD*(2) C 19 - C 21	19.87	BD (2) C 39 - N 53	BD*(1) C 40 - C 41	145.19
BD (2) C 19 - C 21	BD*(2) C 15 - C 17	19.56	BD (2) C 39 - N 53	BD*(2) C 39 - N 53	134.48
BD (2) C 7 - C 9	BD*(2) C 3 - C 5	19.51	BD (1) C 41 - H 42	BD*(1) C 40 - C 41	113.22
BD (2) C 1 - C 11	BD*(2) C 7 - C 9	18.25	BD (1) C 41 - H 42	BD*(2) C 39 - N 53	81.53
BD (2) C 19 - C 21	BD*(2) C 14 - C 23	17.97	BD (1) C 40 - C 41	BD*(1) C 40 - C 41	47.62
			BD (1) C 41 - C 43	BD*(3) C 39 - N 53	43.59
Phenyl Ring 3 (atoms 26-35)			BD (1) C 39 - N 53	BD*(2) C 47 - C 49	37.17
BD (2) C 26 - C 34	BD*(2) C 31 - C 32	28.82	BD (1) C 38 - C 40	BD*(2) C 39 - N 53	35.77
BD (2) C 26 - C 34	BD*(2) C 25 - N 51	19.06	BD (1) C 31 - C 36	BD*(3) C 39 - N 53	33.58
BD (2) C 27 - C 29	BD*(2) C 26 - C 34	18.53	BD (1) C 40 - C 41	BD*(2) C 39 - N 53	33.42
BD (2) C 27 - C 29	BD*(2) C 31 - C 32	16.29	BD (1) C 38 - C 39	BD*(3) C 39 - N 53	30.16
BD (1) C 27 - C 29	BD*(1) C 40 - C 41	15.63	BD (1) C 41 - C 43	BD*(1) C 40 - C 41	28.41
BD (2) C 26 - C 34	BD*(2) C 27 - C 29	15.55	BD (3) C 39 - N 53	BD*(1) C 45 - H 46	26.41
Imidazole ring (atoms 12,13,25,51-53)			BD (2) C 43 - C 45	BD*(2) C 40 - C 41	18.92
BD (2) C 25 - N 51	LP (2) N 52	34.86	BD (2) C 47 - C 49	BD*(2) C 40 - C 41	18.98
BD (2) C 25 - N 51	BD*(2) C 12 - C 13	24.07			
BD (2) C 14 - C 23	BD*(2) C 15 - C 17	19.32	**Lone pair electrons in nitrogen atoms**		
BD (2) C 12 - C 13	BD*(2) C 25 - N 51	15.56	LP (2) N 52	BD*(2) C 12 - C 13	63.88
BD (2) C 25 - N 51	BD*(2) C 26 - C 34	14.50	LP (2) N 52	BD*(2) C 25 - N 51	83.33
BD (2) C 12 - C 13	BD*(2) C 1 - C 11	14.17			
BD (2) C 12 - C 13	BD*(2) C 14 - C 23	12.74			
BD (2) C 14 - C 23	BD*(2) C 12 - C 13	10.53			

SCXRD

Crystallographic data (excluding structure factors) reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1888014 Copies of available material can be obtained, free of charge, on application to the CCDC, 12 Union Road. Cambridge CB2 IEZ, UK, (fax: +44-(0)1223-336033 or e-mail: deposit@ccdc.cam.ac.uk).

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