

Electronic Supporting Information

Engineering the Solid-State Luminescence of Organic Crystals and Cocrystals

Aijaz A. Dar,^{a*} Shaista H. Lone^a, Ishtiyaq Ahmad^a, Arshid A. Ganie^a, Cherumannil Femina^b

^aCrystal Engineering Laboratory, Department of Chemistry, University of Kashmir, Hazratbal, Srinagar-190006, Jammu & Kashmir, India

^bDepartment of Chemistry, Farook College P.O, Kozhikode 673632 Kerala India

Figure ESI-1: FT-IR Spectrum of 1.

Figure ESI-2: FT-IR Spectrum of 2.

Figure ESI-3: FT-IR Spectrum of 3.

Figure ESI-4: PXRD and its simulated spectrum of 2.

Figure ESI-5: PXRD and its simulated spectrum of 3.

Figure ESI-6: Kubelka-Munk plots of reactants and product 1.

Figure ESI-7: Kubelka-Munk plots of reactants and product 2.

Figure ESI-8: Kubelka-Munk plots of reactants and product 3.

Figure ESI-9: Tauc plots of 1.

Figure ESI-10: Tauc plots of 2.

Figure ESI-11: Tauc plots of 3.

Figure ESI-12: Solid State Emission of 1a.

Figure ESI-13: Solid State Emission of 2a.

Figure ESI-14: Solid State Emission of 3a.

Figure ESI-15: Solid State Emission of 5-SSA .

Figure ESI-16: Solid State Emission of Product 1

Figure ESI-17: Solid State Emission of Product 2

Figure ESI-18: Solid State Emission of Product 3

Figure ESI-19: AIE in 1.

Figure ESI-20: AIE in 2.

Figure ESI-21: AIE in 3.

Figure ESI-22: DLS of 1.

Figure ESI-23: DLS of 2.

Figure ESI-24: DLS of 3.

Figure ESI-25: Picture of AIEgens in visible and UV light.

Figure ESI-26: 2-D hydrogen bonded network in 1.

Figure ESI-27: 3-D packing fragment of 2.

Figure ESI-28: Centrosymmetric $R_2^2(10)$ synthon observed in 2.

Figure ESI-29: 3-Dimensional packing fragment of 3.

Figure ESI-30: Contribution of individual intermolecular interaction to overall packing of 1, 2, and 3 and their respective 1a, 2a and 3a Schiff bases.

Figure ESI-31: Hirshfeld surface b) Shape index c) Curvedness of 1.

Figure ESI-32: Total and individual fingerprint plots of 1.

Figure ESI-33: Hirshfeld surface b) Shape index c) Curvedness of 2.

Figure ESI-34: Total and individual fingerprint plots of 2.

Figure ESI-35: Hirshfeld surface b) Shape index c) Curvedness of 3.

Figure ESI-36: Total and individual fingerprint plots of 3.

Table ESI-1: Crystallographic table of 1-3.

Table ESI-2. Comparative parameters of solution and solid-state emission of 1a-3a and 1-3.

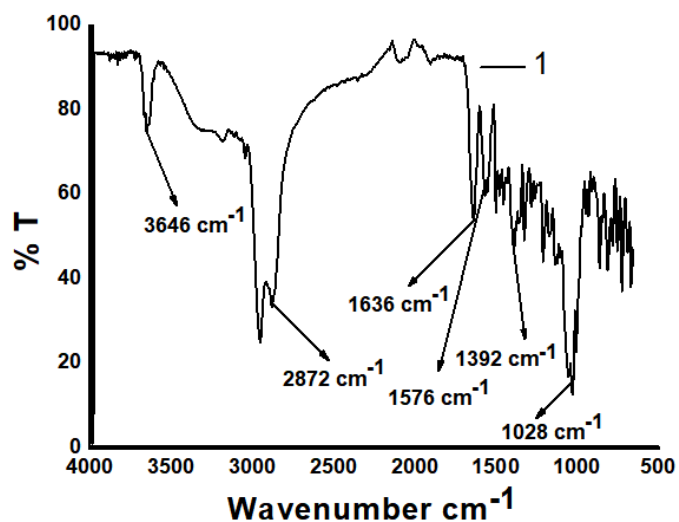


Figure ESI-1: FT-IR Spectrum of 1.

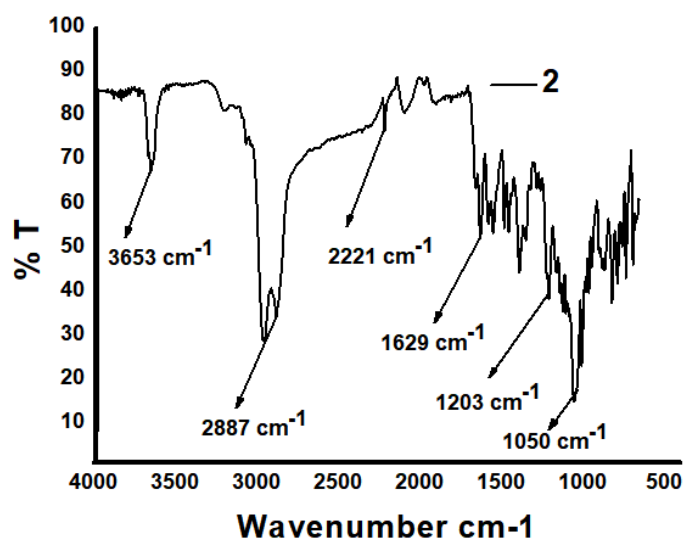


Figure ESI-2: FT-IR Spectrum of 2.

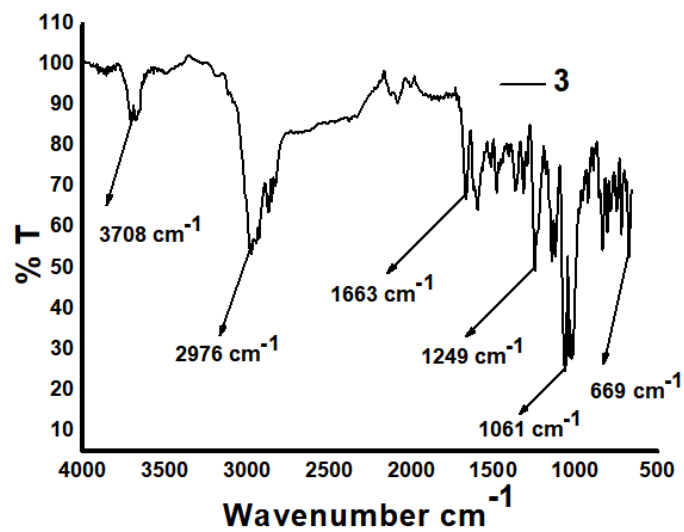


Figure ESI-3: FT-IR Spectrum of 3.

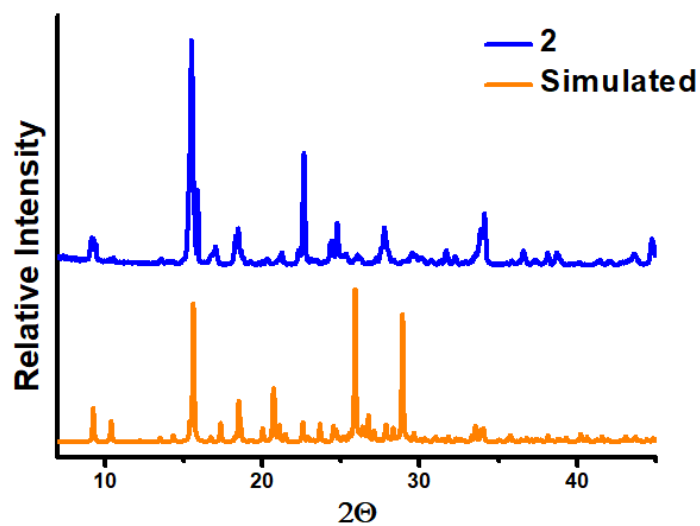


Figure ESI-4: PXRD and its simulated spectrum of 2

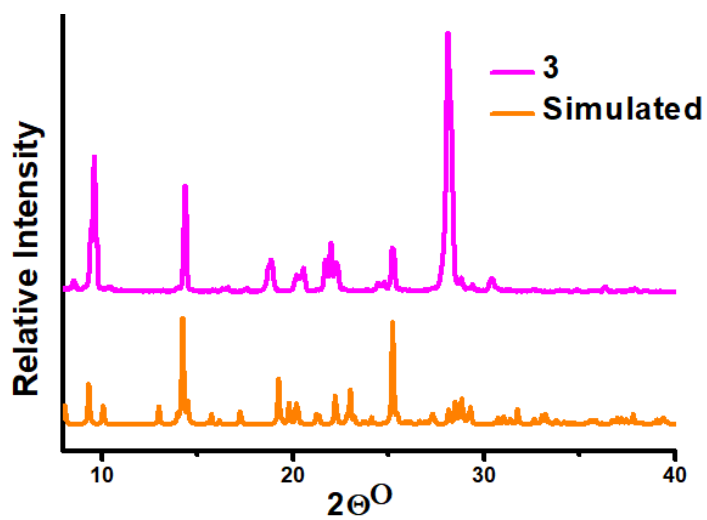


Figure ESI-5: PXRD and its simulated spectrum of 3.

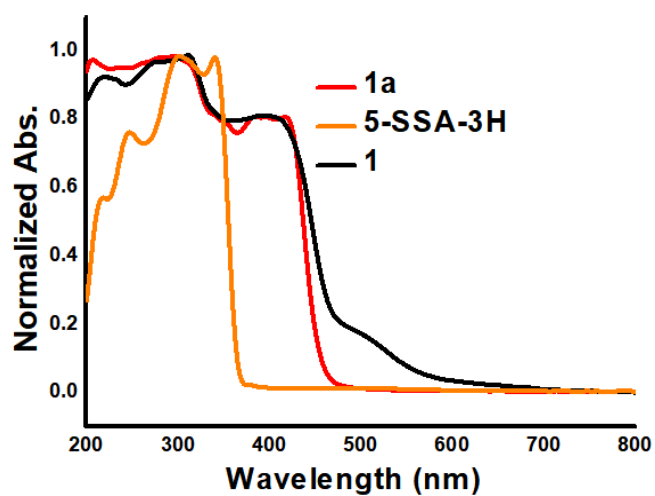


Figure ESI-6: Kubelka-Munk plots of reactants and product 1.

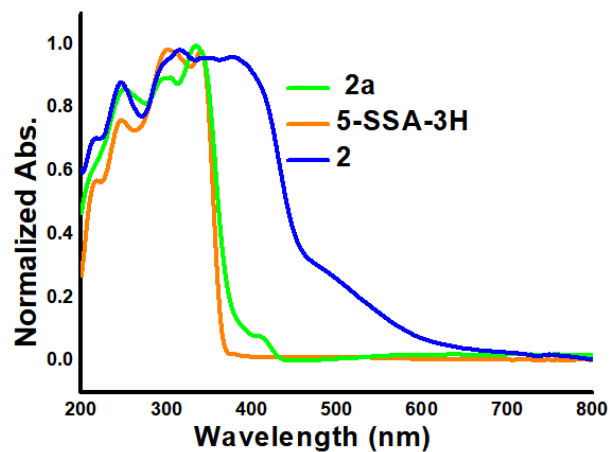


Figure ESI-7: Kubelka-Munk plots of reactants and product 2.

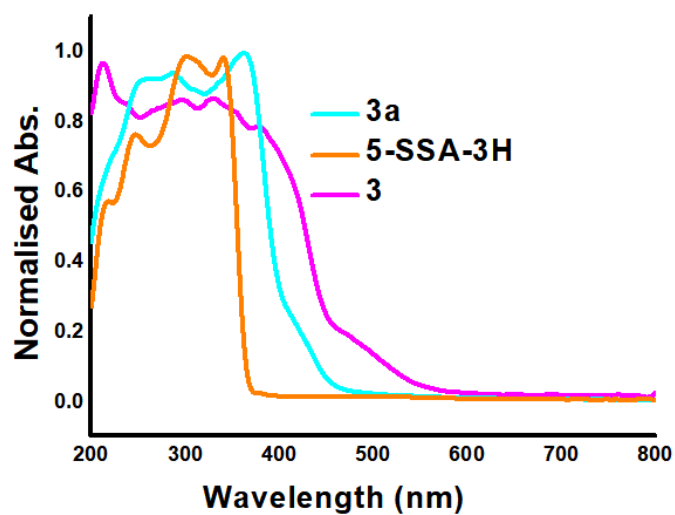


Figure ESI-8: Kubelka-Munk plots of reactants and product 3.

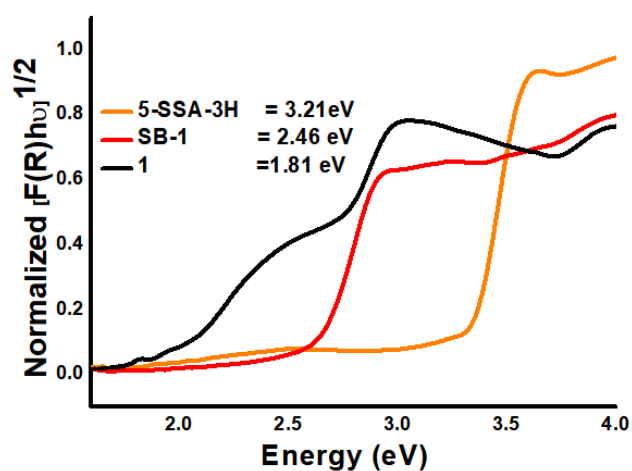


Figure ESI-9: Tauc plots of 1

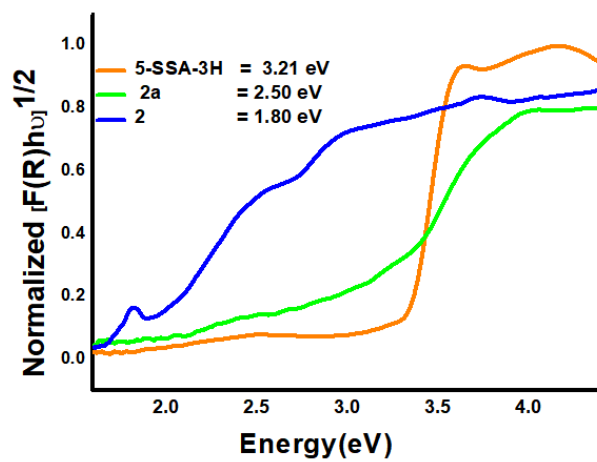


Figure ESI-10:Tauc plots of 2

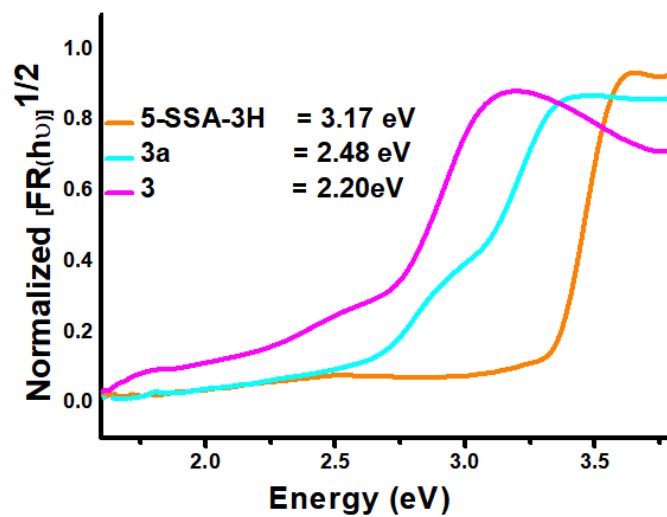


Figure ESI-11:- Tauc plots of 3

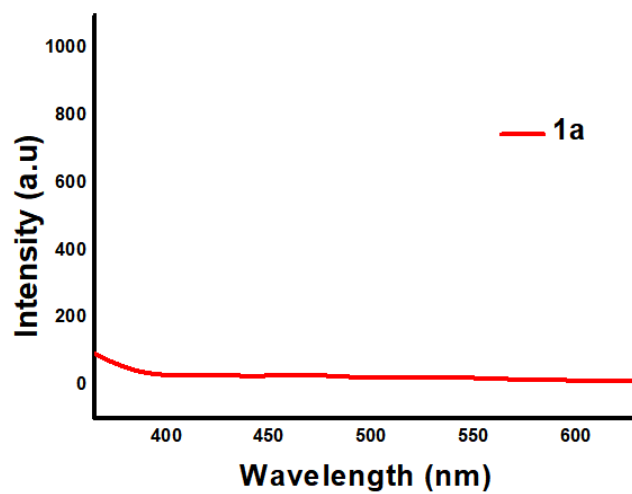


Figure ESI-12: Solid State Emission of 1a.

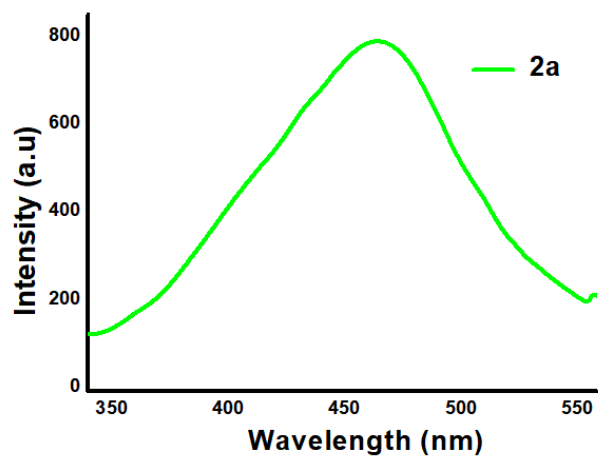


Figure ESI-13: Solid State Emission of 2a

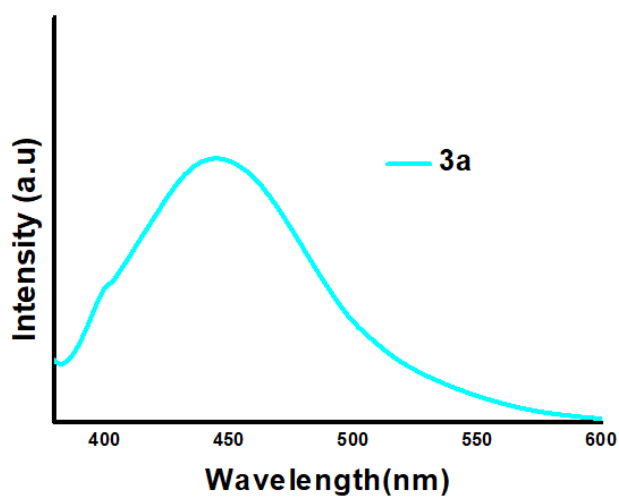


Figure ESI-14: Solid State Emission of 3a.

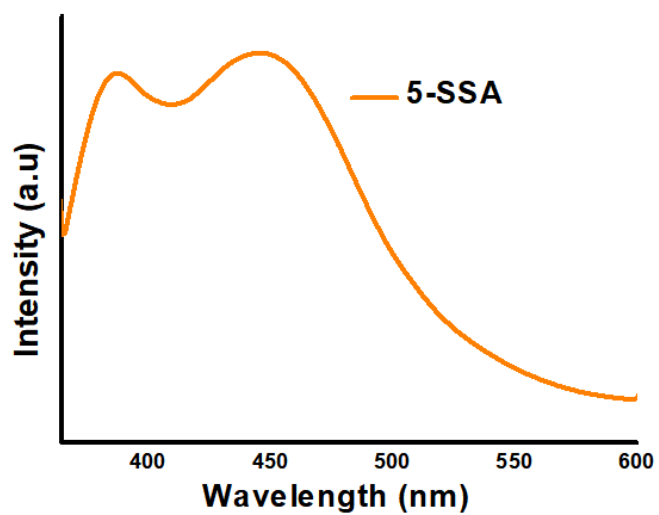


Figure ESI-15: Solid State Emission of 5-SSA

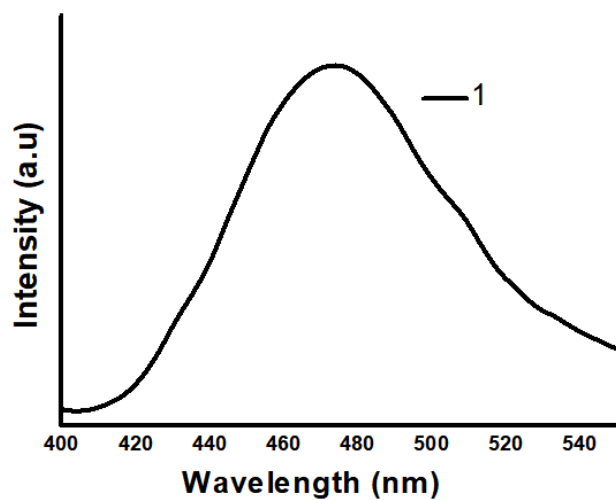


Figure ESI-16: Solid State Emission of Product 1

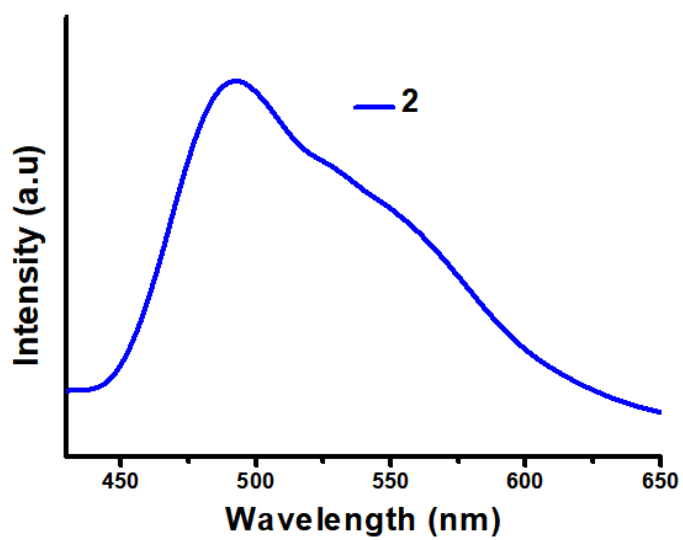


Figure ESI-21: Solid State Emission of product 2

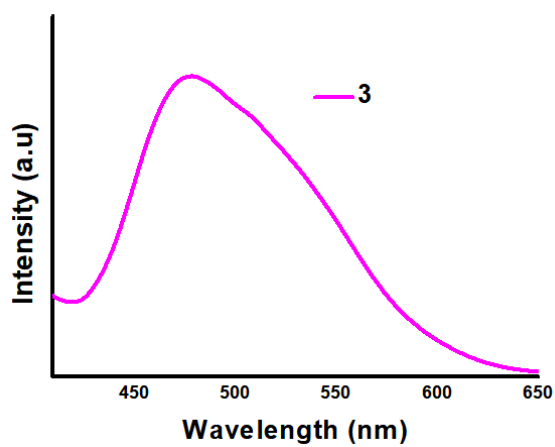


Figure ESI-18: Solid State Emission of Product

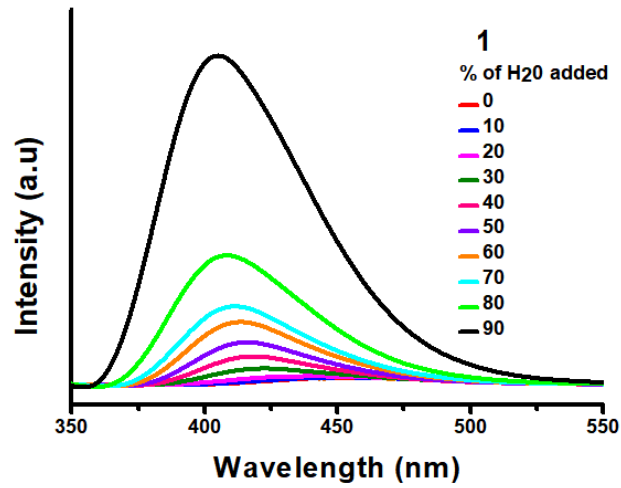


Figure ESI-19: AIE in 1.

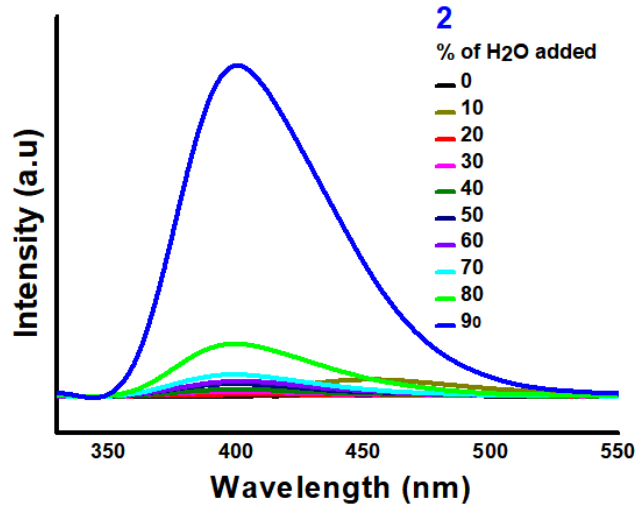


Figure ESI-20: AIE in 2.

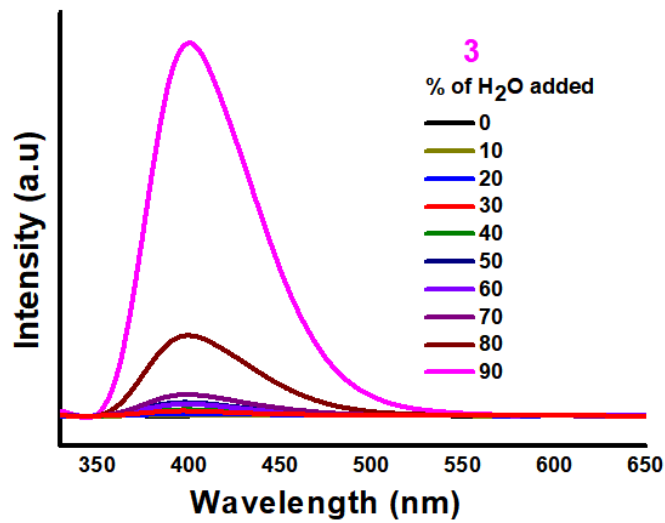


Figure ESI-21: AIE in 3.

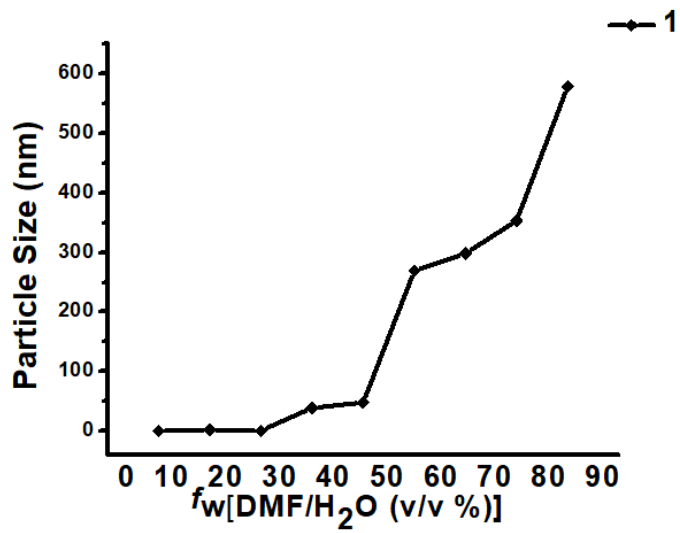


Figure ESI-22: DLS of 1

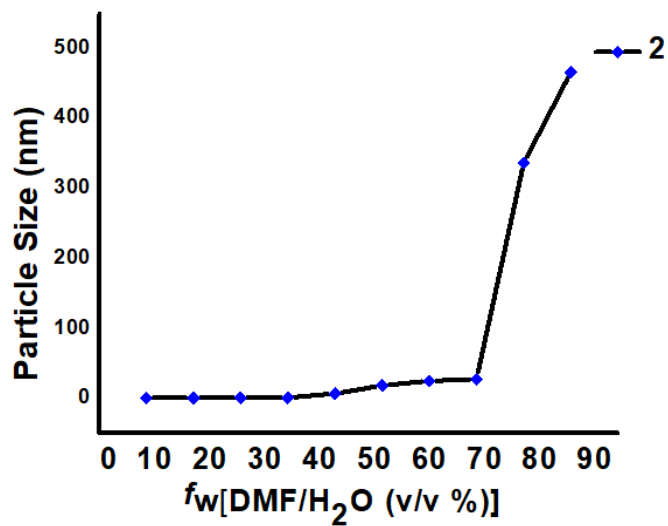


Figure ESI-23: DLS of 2

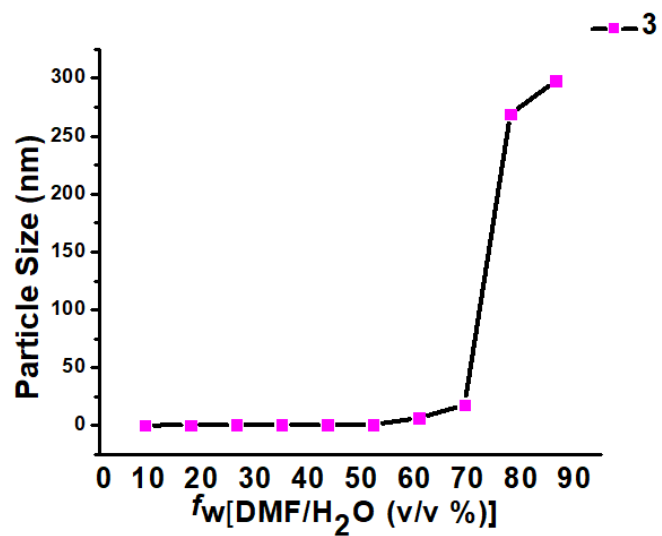


Figure ESI-24: DLS of 3

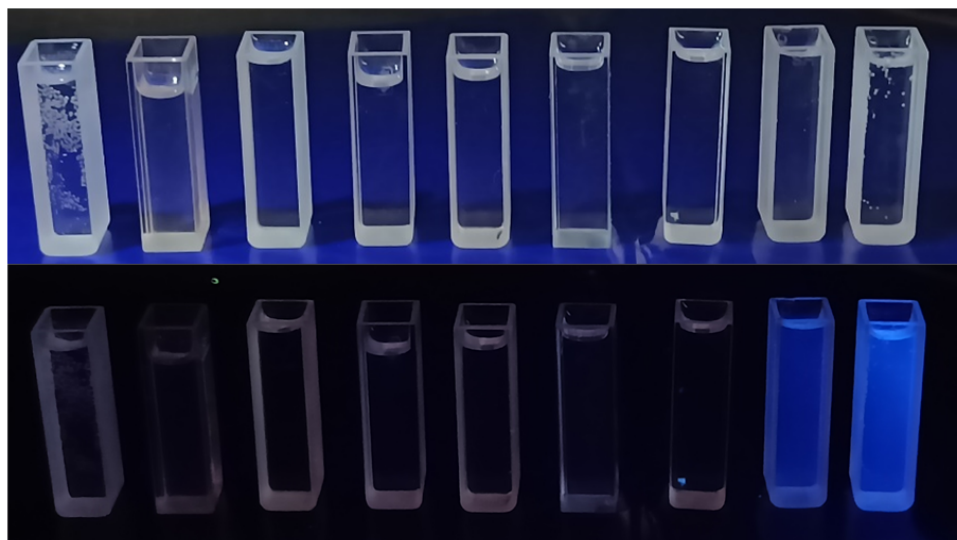


Figure ESI-25: Picture of AIEgens in visible and UVlight

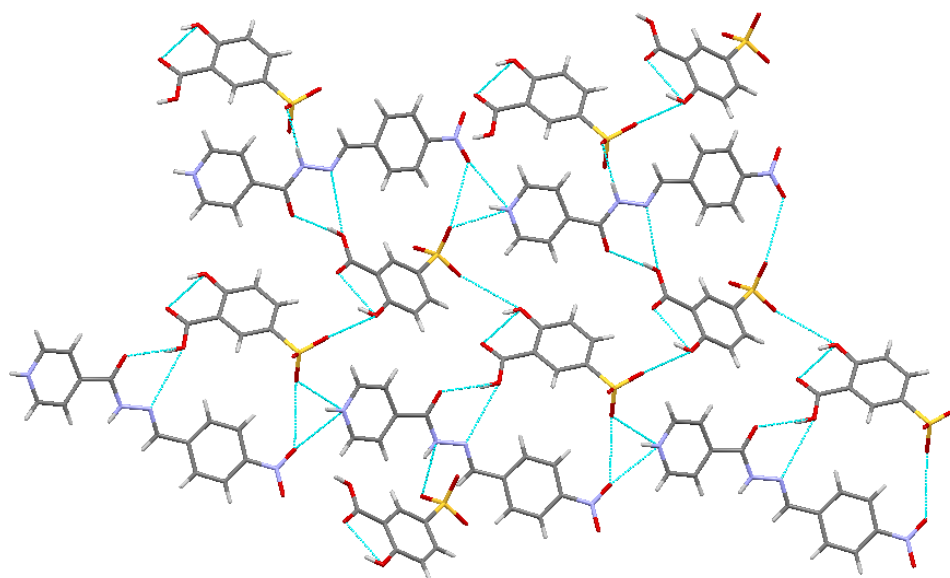


Figure ESI-26: 2-D hydrogen bonded network in 1.

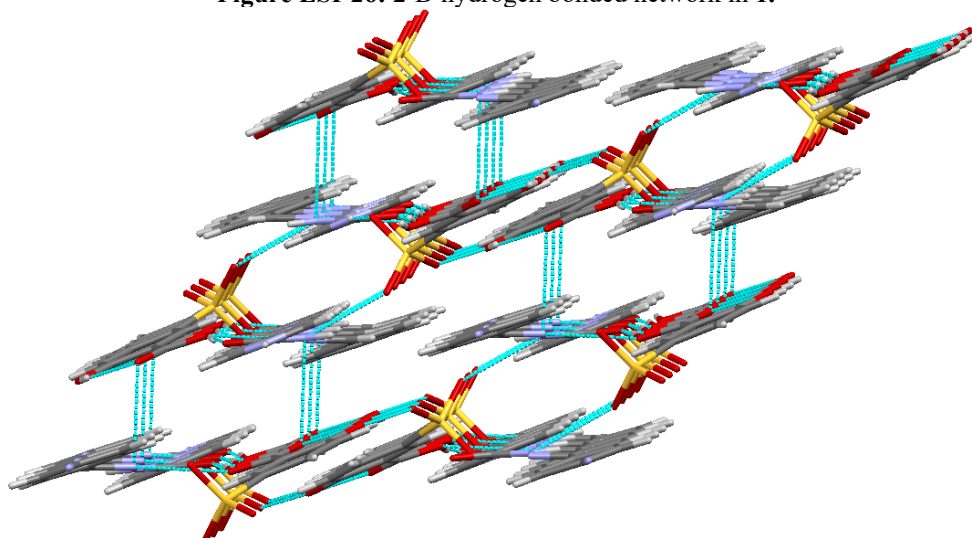


Figure ESI-27: 3-D packing fragment of 2.

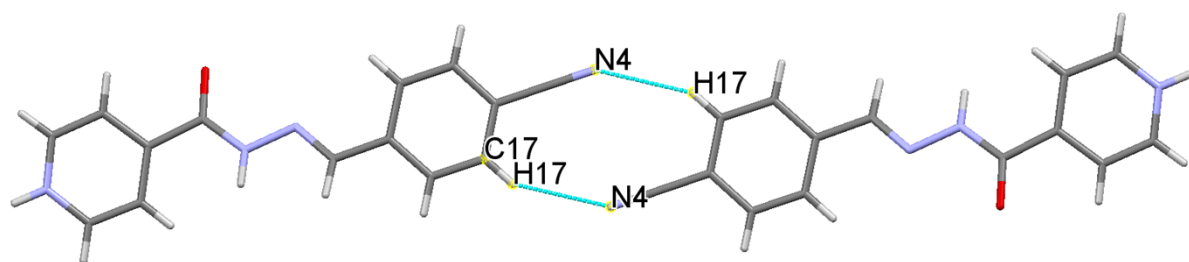


Figure ESI-28: Centrosymmetric $R_2^2(10)$ synthon observed in **2**.

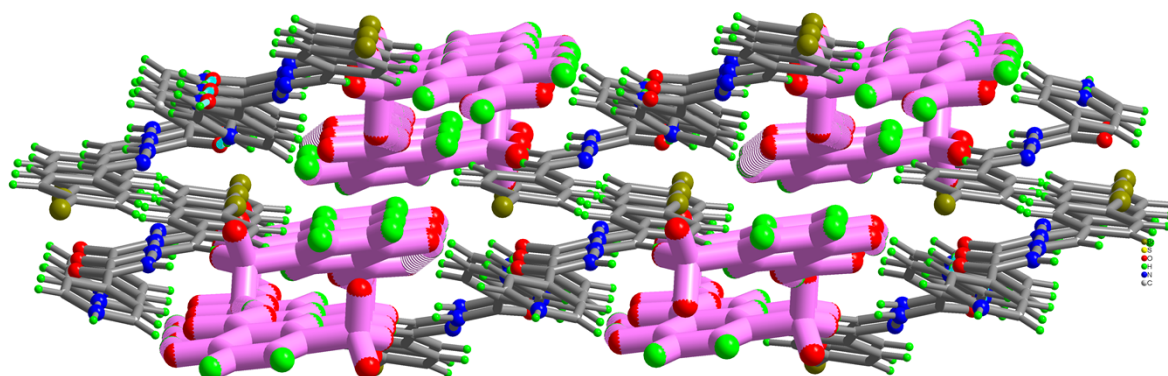


Figure ESI-29: 3-Dimensional packing fragment of **3**.

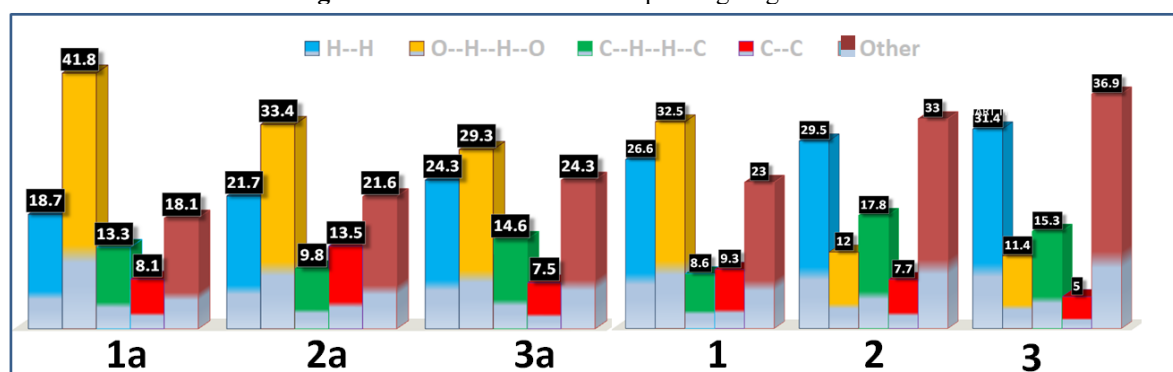


Figure ESI-30: Contribution of individual intermolecular interaction to overall packing of **1**, **2**, and **3** and their respective **1a**, **2a** and **3a** Schiff bases.

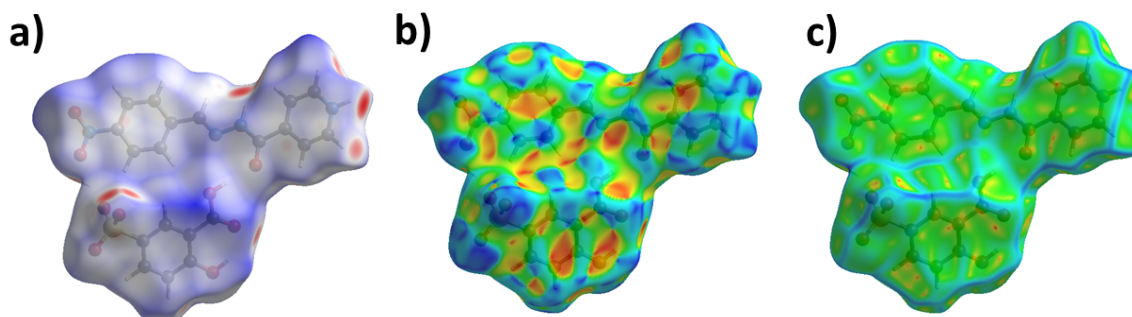


Figure ESI-31: Hirshfeld surface b) Shape index c) Curvedness of 1.

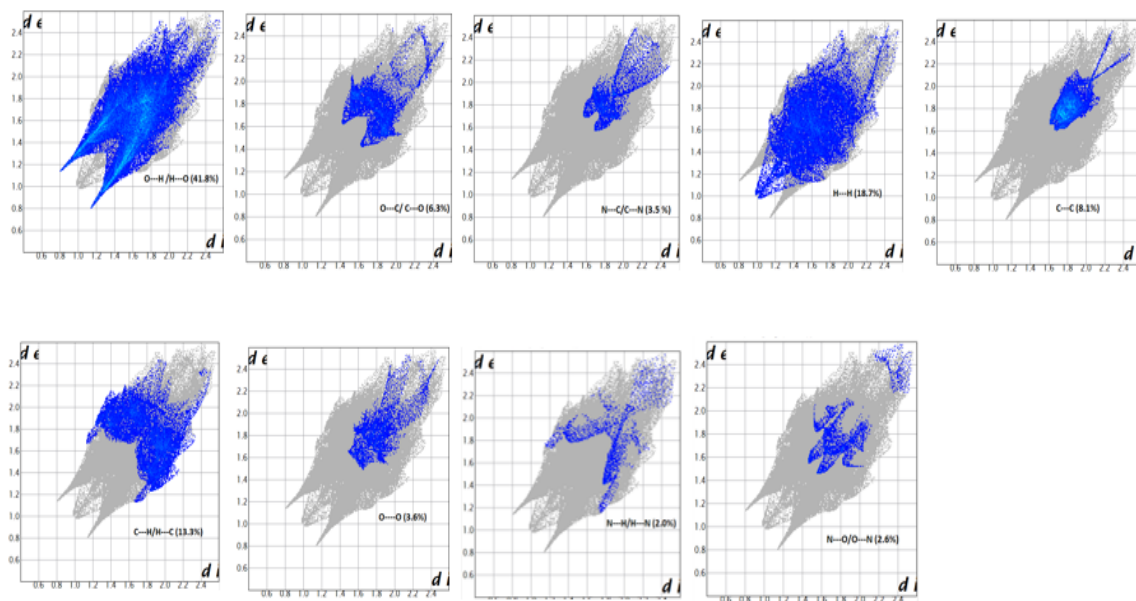


Figure ESI-32: Total and individual fingerprint plots of 1

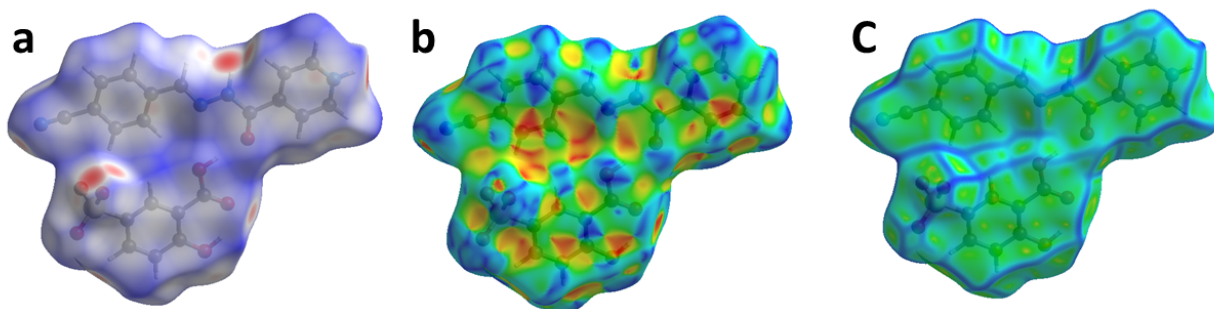


Figure ESI-33: Hirshfeld surface b) Shape index c) Curvedness of 2.

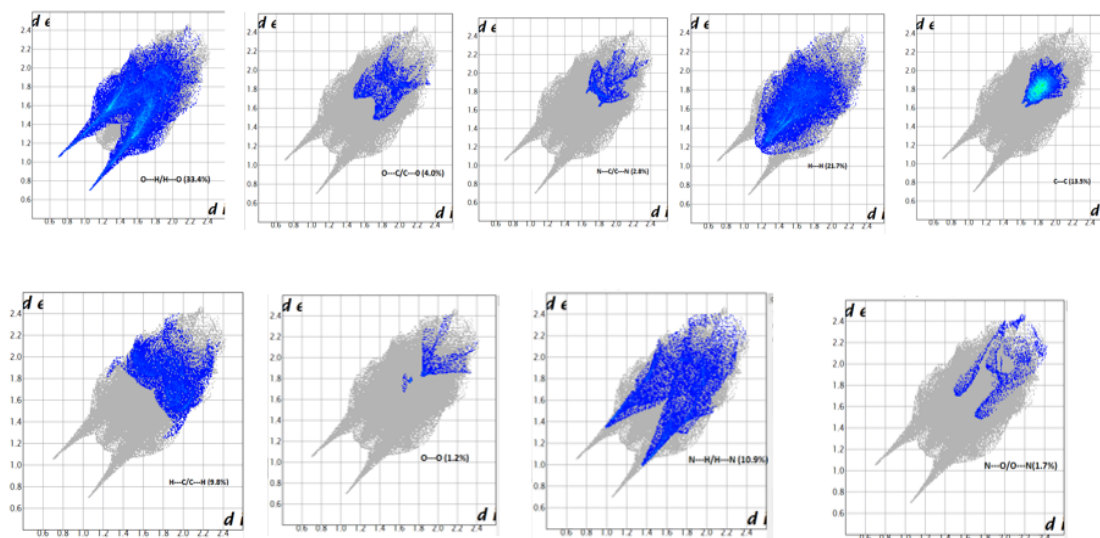


Figure ESI-34: Total and individual fingerprint plots of 2.

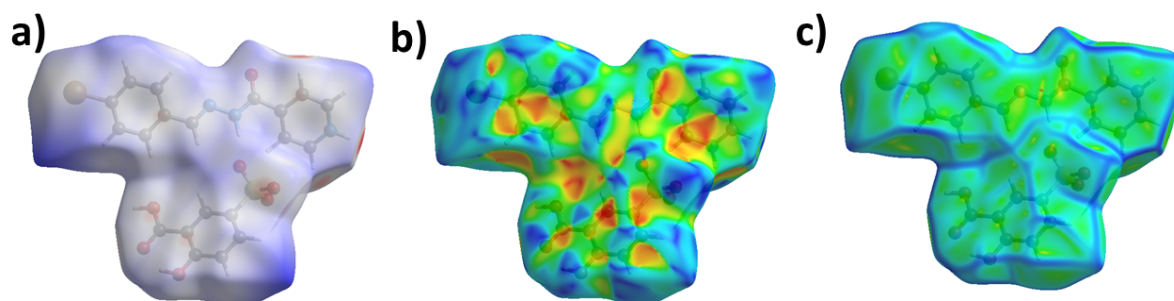


Figure ESI-35: Hirshfeld surface b) Shape index c) Curvedness of 3

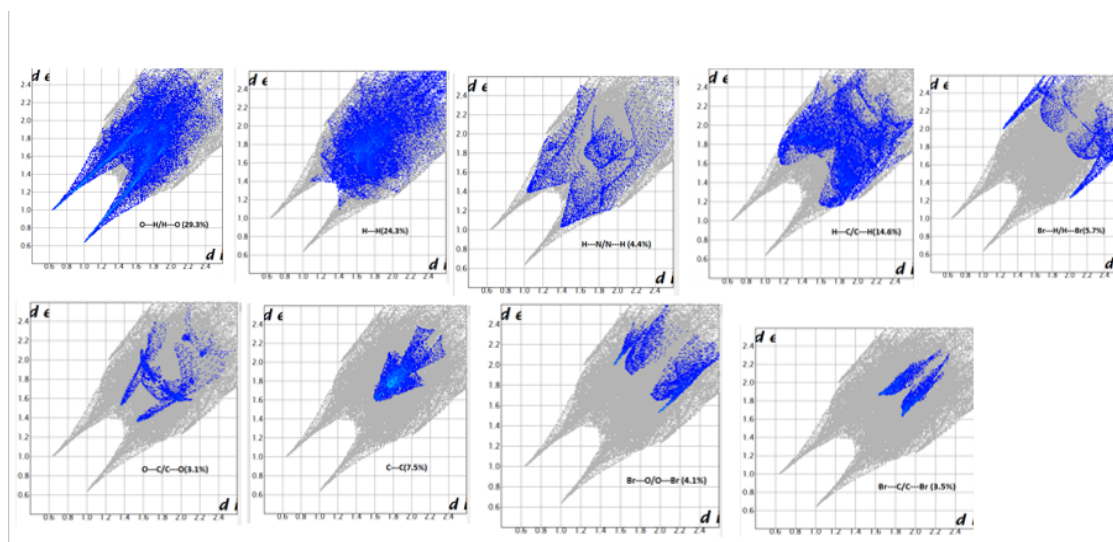


Figure ESI-36: Total and individual fingerprint plots of 3..

Table ESI-1: Crystallographic table of 1-3.

Compound	1	2	3
Reaction Number	SHL-09	SHL-10	SHL-31
CCDC no.	2255995	2255996	2255997
Empirical formula	C ₂₀ H ₁₆ N ₄ O ₉ S	C ₂₁ H ₁₆ N ₄ O ₇ S	C ₂₀ H ₁₆ N ₄ O ₉ S
fw	488.43	468.44	522.32
Temp [K]	293	293	293
Crystal system	Orthorhombic	Monoclinic	Monoclinic

Space group	P 21 21 21	P 21/n	P 21/c
a, [Å]	10.7818(7)	10.3934(6)	12.189(2)
b, [Å]	12.1565(11)	15.5510(5)	14.7571(12)
c, [Å]	15.1497(10)	12.4041(4)	13.783(3)
α , [deg]	90.00	90.00	90.00
β , [deg]	90.00	99.762(4)	115.79(2)
γ , [deg]	90.00	90.00	90.00
V, [Å ³]	1985.7(3)	1975.82(15)	2232.3(7)
Z	4	4	4
D(calcd) [Mg/cm ³]	1.634	1.575	1.554
μ [mm ⁻¹]	0.230	0.221	1.982
Θ range [°]	24.991	24.999	66.727
Reflns collected	3125	3461	3008
Indep. reflns	2802	3461	2562
GOF	1.062	1.072	1.451
R1 (I0 > 2 σ (I0))	0.0642	0.0472	0.1003
wR2 (all data)	0.1749	0.1340	0.3290

Table ESI-2. Comparative parameters of solution and solid-state emission of 1a-3a and 1-3.

Compound	Solution phase				Solid phase			
	λ_{abs} [nm]	λ_{ex} [nm]	λ_{em} [nm]	Φ (%)	λ_{abs} [nm]	λ_{ex} [nm]	λ_{em} [nm]	Φ (%)
1a	320	300	380	18.11	490		0.00	0.00
2a	300	300	400	10.21	380	320	464	0.10
3a	305	300	470	36.31	410	320	442	0.07
1	295	300	420	81.22	470	320	467	0.14
2	304	300	425	60.14	430	320	472	0.13
3	302	300	418	53.42	405	320	484	0.12