Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Anion assisted conformational guided self-assemblies of multi-component cocrystals of dioxime

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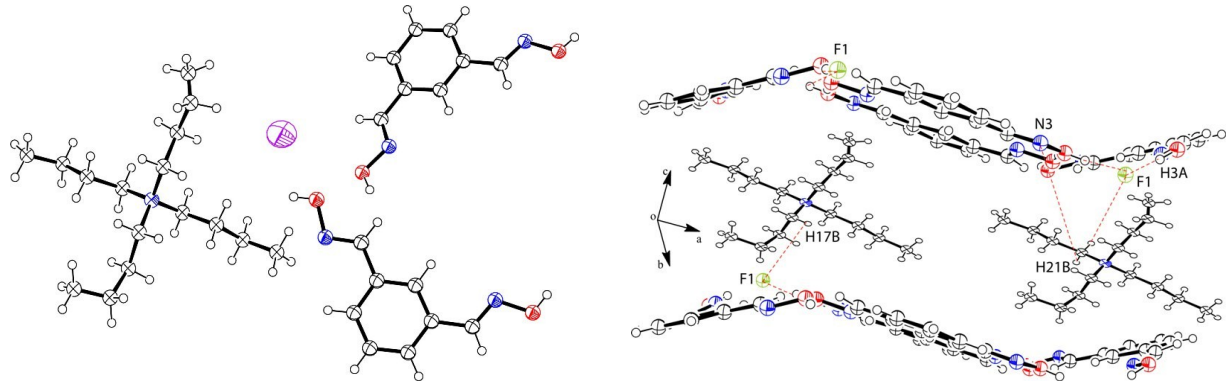
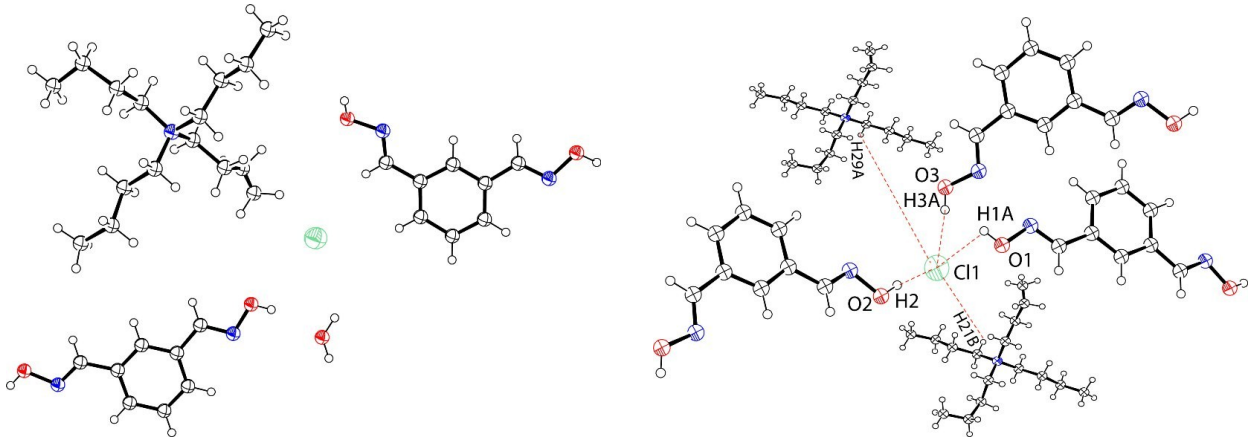
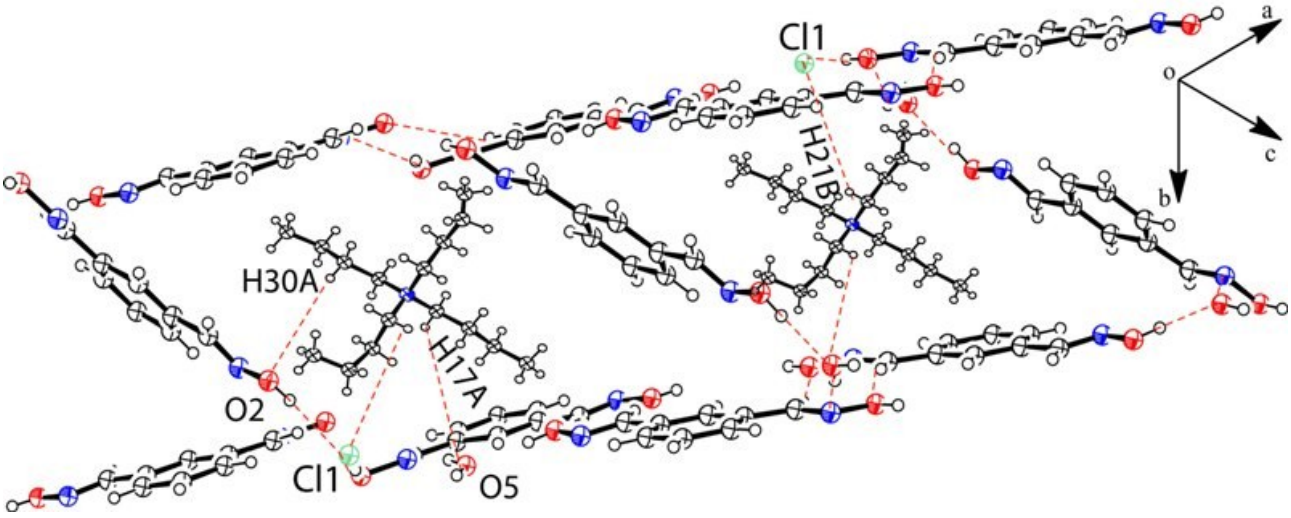


(a) (b)

Figure 1S: (a) Asymmetric unit of cocrystal **2(H_2BNAD).(TBAF)**. (b) Cation encapsulation by oxime molecules in **2(H_2BNAD).(TBAF)**.



(a) (b)



(c)

Figure 2S: (a) Asymmetric unit of cocrystal **2(H_2BNAD).(TBACl).H_2O**. (b) Coordination environment of chloride ion in cocrystal **2(H_2BNAD).(TBACl).H_2O**. (c) Cation encapsulation by oxime molecules in **2(H_2BNAD).(TBACl).H_2O**.

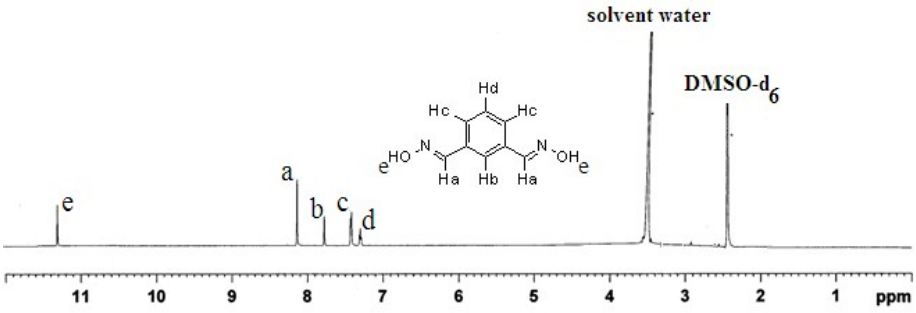


Figure 3S: ^{1}H-NMR (600 MHz, DMSO-d_6) of **H_2BNAD**.

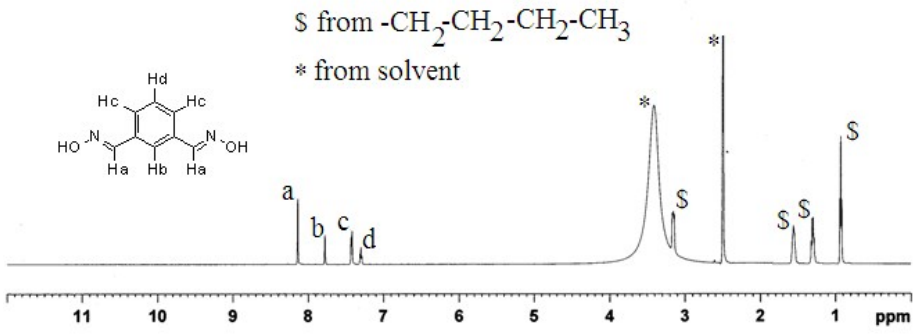


Figure 4S: ^{1}H-NMR (600 MHz, DMSO-d_6) of salt **(TBA)(HBNAD).H_2BNAD**.

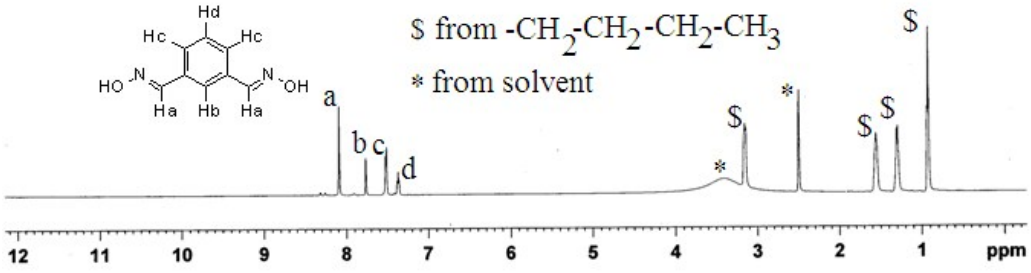


Figure 5S: ^{1}HNMR (600 MHz, DMSO-d_6) of cocrystal 2(H_2BNAD).(TBAF).

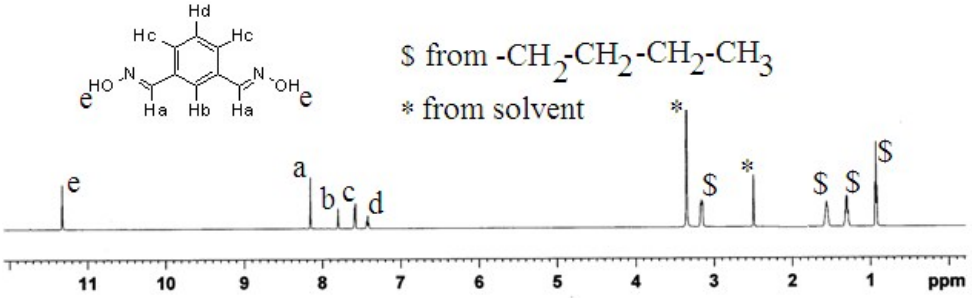


Figure 6S: ^{1}H-NMR (600 MHz, DMSO-d_6) of cocrystal 2(H_2BNAD).(TBACl).H_2O.

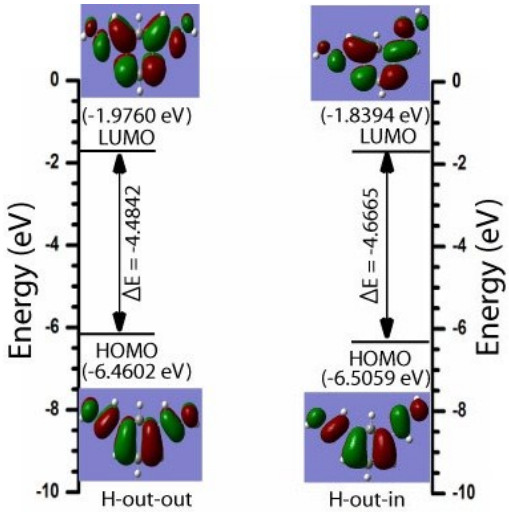


Figure 7S: HOMO and LUMO gap in two conformers of 1,3-Benzenedialdoxime calculated at by DFT using B3LYP/6-31+G (d,p) as basis set.

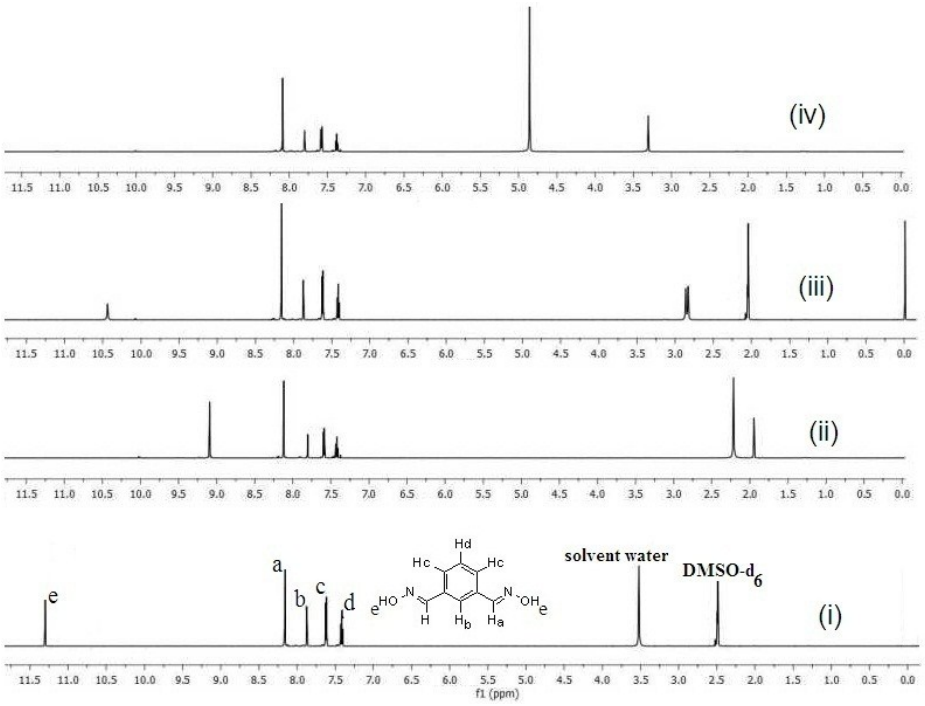


Figure 8S: Solvent dependent ^{1}H-NMR spectra of 1,3-Benzenedialdoxime **(H_2BNAD)** in (i) DMSO-d_6, (ii) Acetonitrile-d_3, (iii) Acetone-d_6 and (iv) Methanol-d_4.

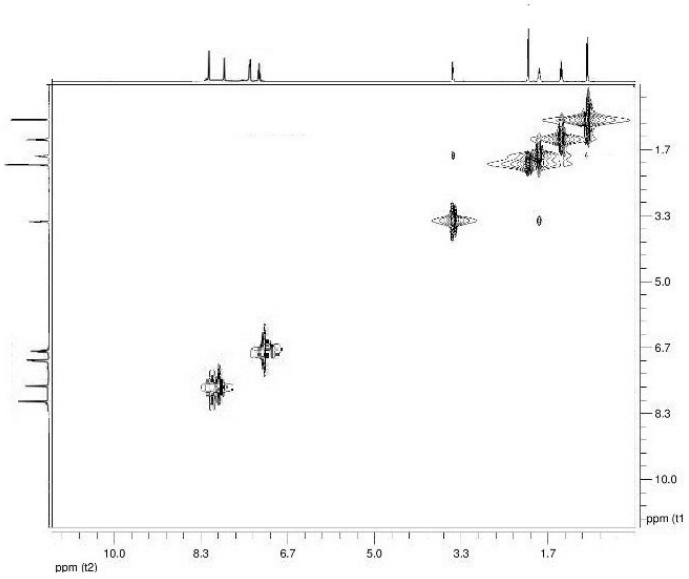


Figure 9S: ^{1}H-NOESY spectra (600MHz, Acetone-d_6) of 2(H_2BNAD).(TBAF).

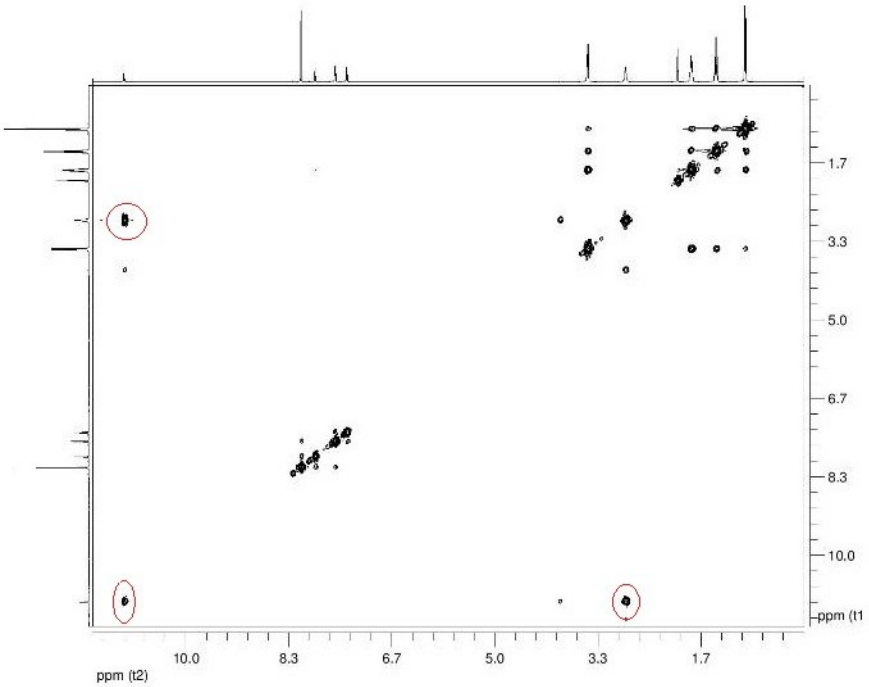


Figure 10S: ^{1}H-NOESY spectra (600MHz, Acetone-d_6) of 2(H_2BNAD). (TBACl).H_2O.

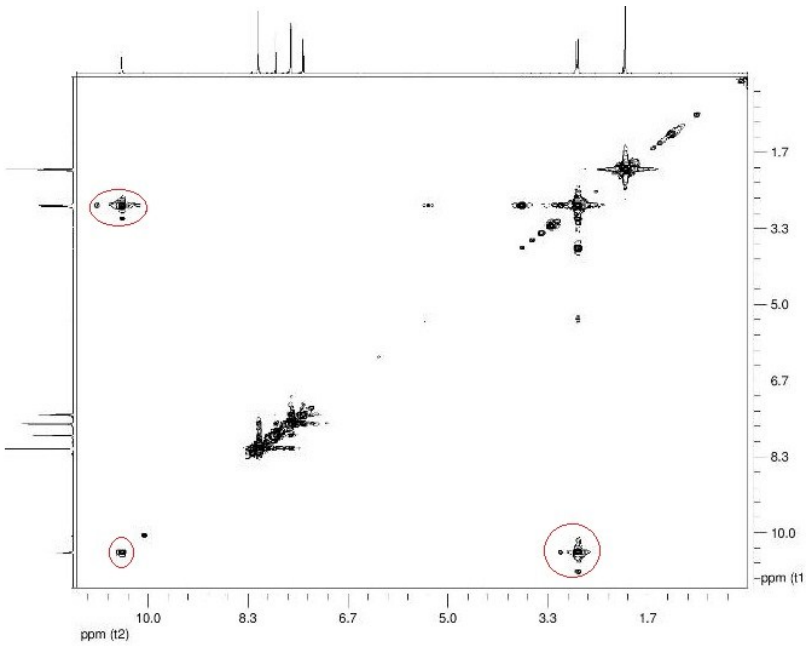


Figure 11S: ^{1}H-NOESY spectra (600MHz, Acetone-d_6) of H_2BNAD.

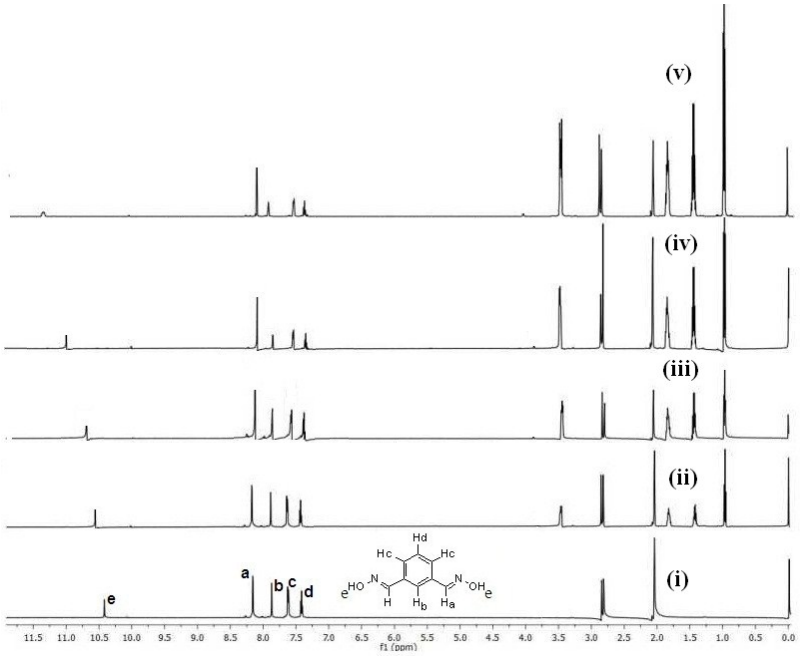


Figure 12S: ^{1}H-NMR (Acetone-d_6) spectra during titration of **(H_2BNAD)** with tetrabutyl ammonium chloride (i) 0.0, (ii) 0.5, (iii) 1 (iv) 1.5, (v) 2 equivalents.

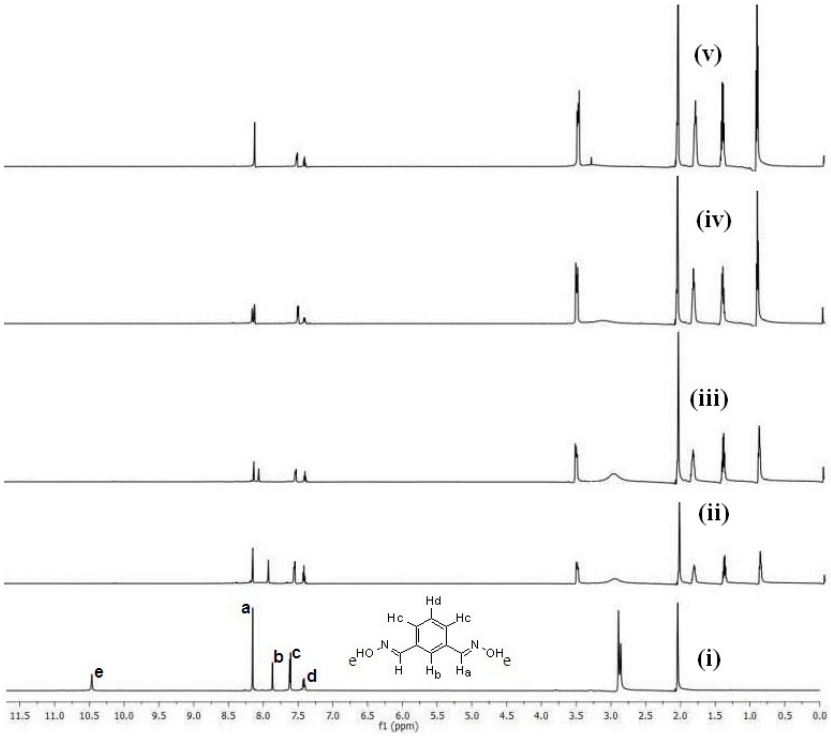


Figure 13S: ^{1}H-NMR (Acetone-d_6) spectra during titration of 1,3-Benzenedialdoxime **(H_2BNAD)** with tetrabutyl ammonium fluoride (i) 0.0, (ii) 0.5, (iii) 1 (iv) 1.5, (v) 2 equivalents.

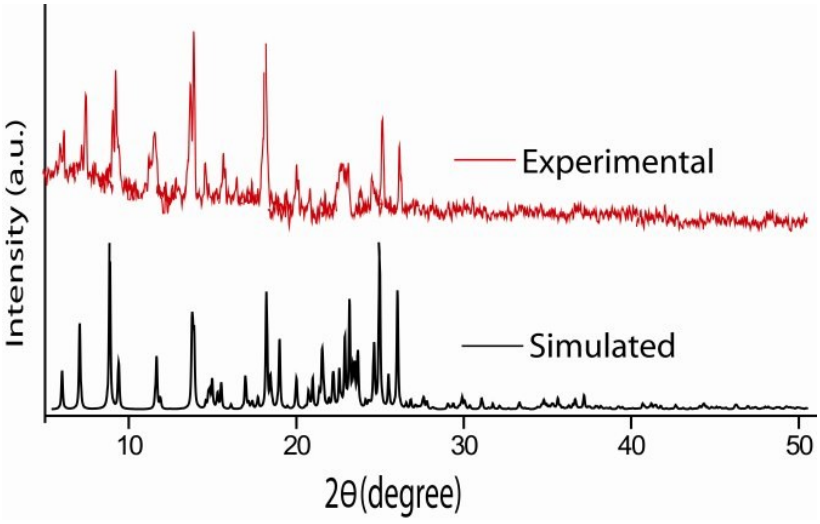


Figure 14S: PXRD of **(TBA)(HBNAD).H_2BNAD** (Red = Experimental, Black = Simulated), Simulated pattern generated from CIF file.

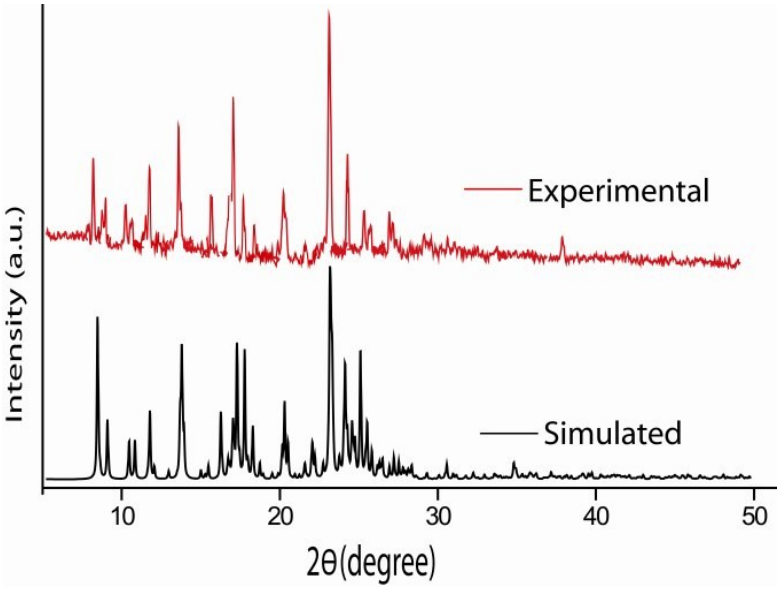


Figure 15S: PXRD of 2(H_2BNAD).(TBAF) (Red = Experimental, Black = Simulated), Simulated pattern generated from CIF file software.

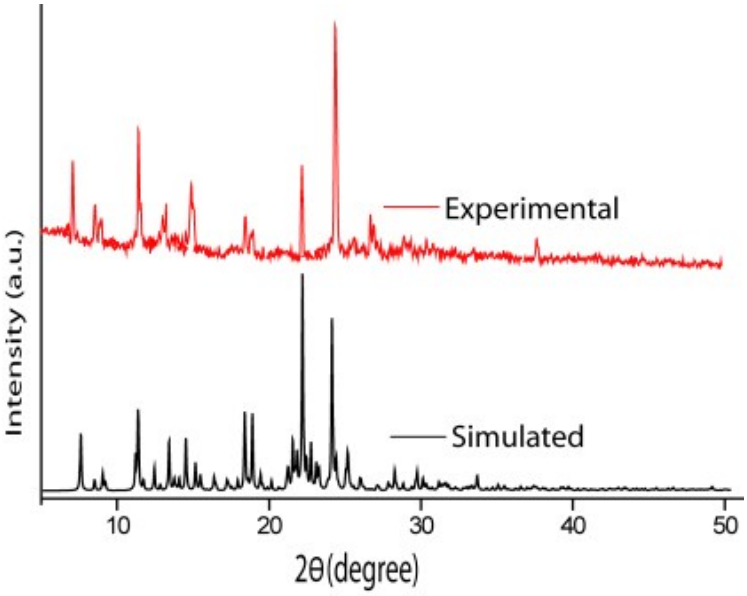


Figure 16S: PXRD of 2(H_2BNAD).(TBACl).H_2O (Red = Experimental, Black = Simulated), Simulated pattern generated from CIF file .

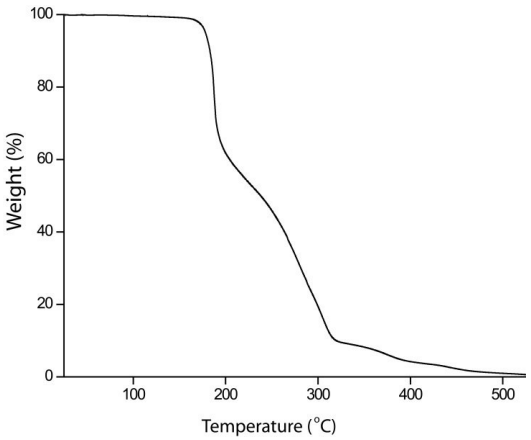


Figure 17S: TGA of Cocrystal **(TBA)(HBNAD).H_2BNAD**.

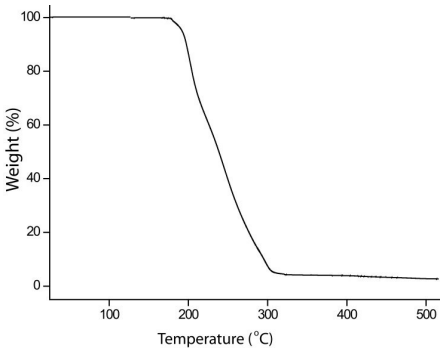


Figure 18S: TGA of cocrystal 2(H_2BNAD).(TBAF)**.**

Table 1S: Hydrogen bond parameters of the crystals

Cocrystal.	D-H ··A	d_{D-H} (Å)	$d_{H\cdots A}$ (Å)	$d_{D\cdots A}$ (Å)	∠D-H ··A (°)
	O(1)-H(1A) ··Cl(1) [1-x,-y,-z]	0.82	2.22	3.039(3)	172
	O(2)-H(2) ··Cl(1)[1-x,1/2+y,1/2-z]	0.82	2.22	3.036(3)	171
2(H_2BNAD).	O(3)-H(3A) ··Cl(1) [-x,1-y,-z]	0.82	2.28	3.078(3)	166
(TBACl).H_2O	O(4)-H(4A) ··O(5)	0.82	1.86	2.681(5)	176
	O(5)-H(5A) ··N(1) [-x,1/2+y,1/2-z]	0.89(3)	2.12(3)	2.998(7)	170(6)
	O(5)-H(5B) ··N(3) [-x,-1/2+y,1/2-z]	0.85(4)	2.31(4)	3.146(6)	171(4)
2(H_2BNAD)	O(1)-H(1A) ··F(1) [x,1/2-y,-1/2+z]	0.89(3)	1.66(3)	2.545(3)	176(3)
.(TBAF)	O(2)-H(2) ··F(1)	0.82	1.71	2.525(3)	173
	O(3)-H(3A) ··F(1) [-x,1/2+y,1/2-z]	0.82	1.64	2.460(3)	177
	O(4)-H(4A) ··O(3) [-x,1-y,-z]	0.82	2.00	2.797(3)	164
(TBA)(HBNAD).	O(1)-H(1A) ··N(3) [x,-1+y,z]	0.82	1.98	2.797(4)	171
H_2BNAD	O(2)-H(2) ··O(3) [1-x,2-y,1-z]	0.82	1.78	2.598(4)	171
	O(4)-H(4A) ··O(3) [-x,2-y,-z]	0.82	1.77	2.567(a)	165