Electronic Supplementary Material (ESI) for CrystEngComm.

Crystal Growth and Physical Properties of the Organic Salt: Benzimidazolium 3-Nitrophthalate

R. Mekala[a], Rajaboopathi Mani[b,c], Ivo B Rietveld[d], P. Jagdish[e], R. Mathammal[a*], Huaidong Jiang [c].

[a]Department of Physics, Sri Sarada College for Women, Salem- 636 016, Tamilnadu, India

[b]Department of Physics, Periyar University, Salem-636 011, Tamilnadu, India

[c]State Key Laboratory of Crystal Materials, Shandong University, Jinan- 250 100, China

[d]Laboratoire de Chimie Physique (CAMMAT), Faculté de Pharmacie, Université Paris Descartes, 75006 Paris, France

[e]Department of Physics, Government Arts College, Dharmapuri- 636 705, Tamilnadu, India

Supporting Information

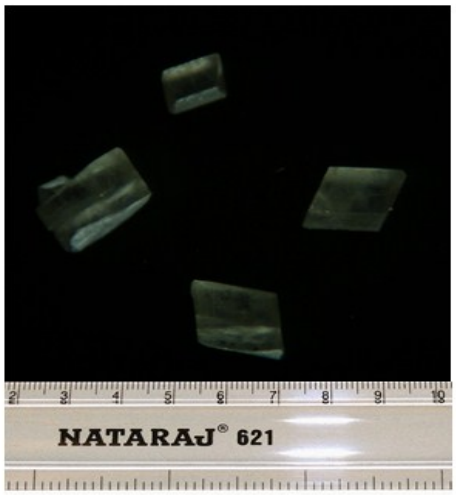

Figure S1. Photograph of as grown $BZD^{+}\cdot m NPA^{-}$ crystals.

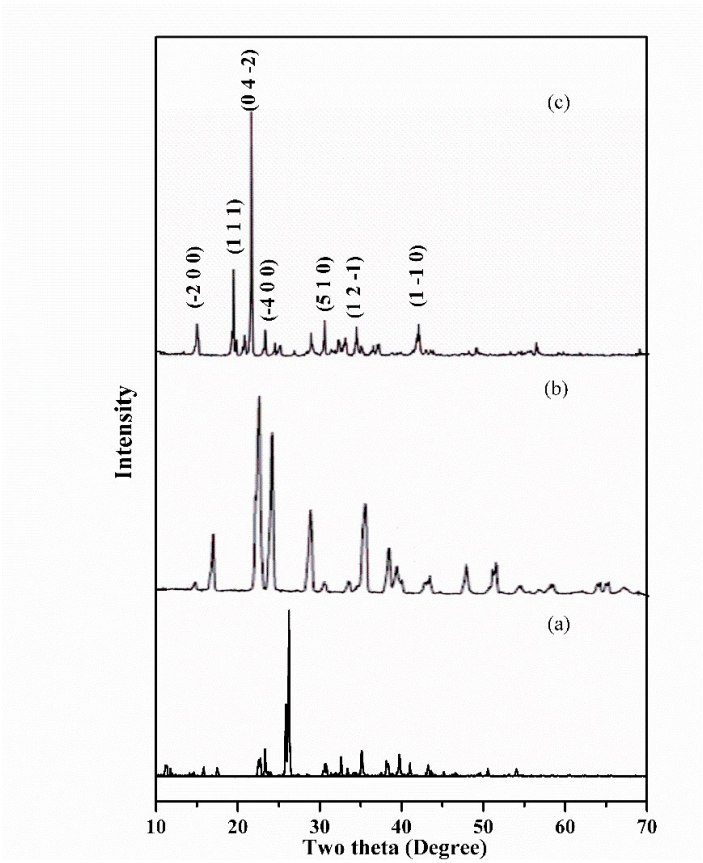

Figure S2. Powder XRD spectra of a) 3-Nitrophthalic acid b) Benzimidazole c) BZD^{+}·*m*NPA^{-} compounds.

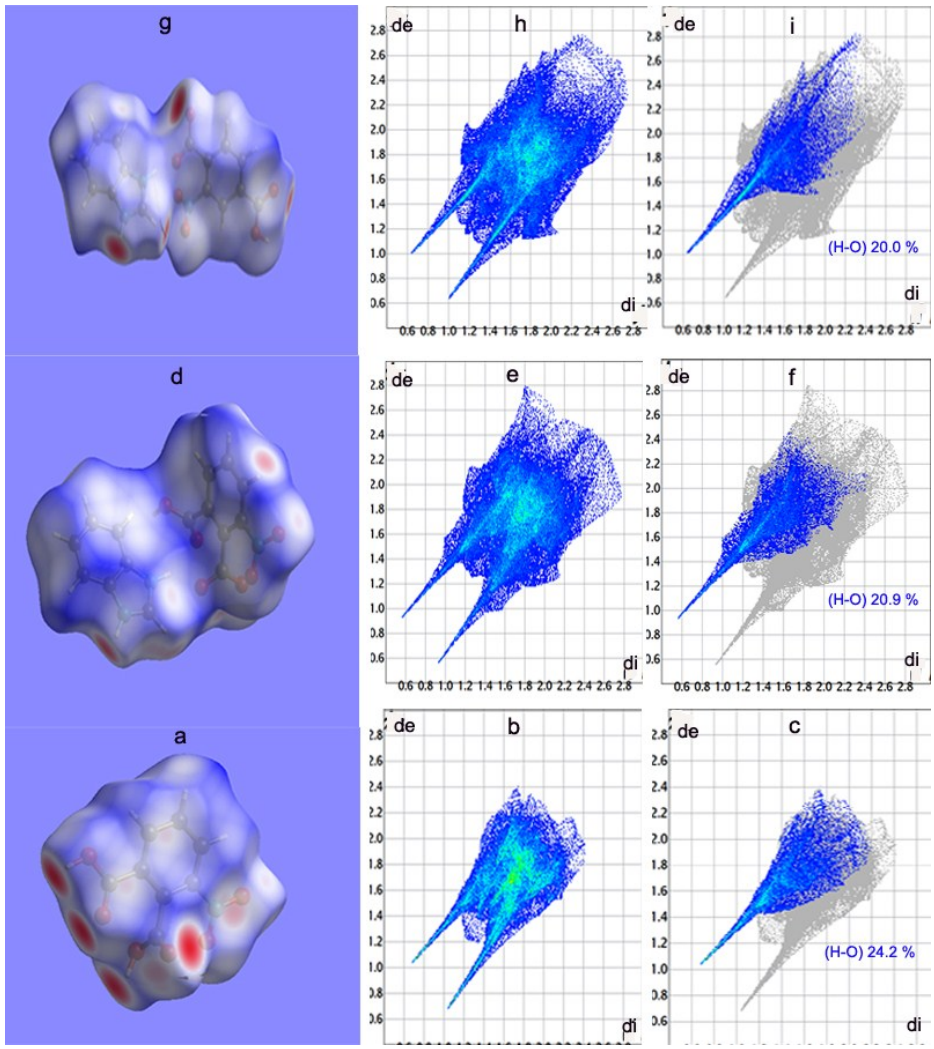

Figure S3. Hirshfeld surfaces and 2D fingerprint plots (de vs di) of 3-nitrophthalic acid (*m*NPA), benzimidazolium nitroterephthalate ($BZD^{+}\cdot NTPh^{-}$) and benzimidazolium 3-nitrophthalate ($BZD^{+}\cdot mNPA^{-}$). (a) Hirshfeld surface, (b) fingerprint plot involving all of the atoms and (c) the distances between the hydrogen atoms and the oxygen atoms on the surrounding molecules of *m*NPA. Similarly, (d-f) is for $BZD^{+}\cdot NTPh^{-}$ and (g-i) is for $BZD^{+}\cdot mNPA^{-}$. The percentages in comparison to all interactions (distances) have been provided.

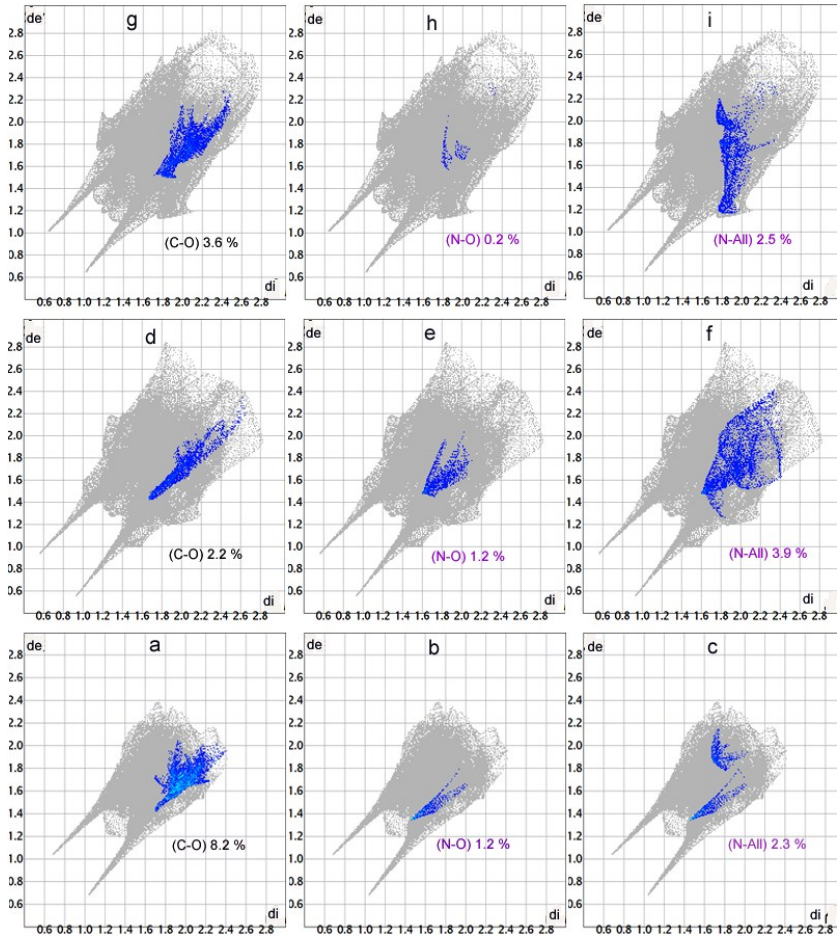

Figure S4. Fingerprint plots of *m*-nitrophthalic acid (*m*NPA), benzimidazolium nitroterephthalate ($BZD^{+}\cdot NTPh^{-}$) and benzimidazolium *m*-nitrophthalate ($BZD^{+}\cdot mNPA^{-}$.(a) Interaction between the carbon atoms and oxygen atoms on the surrounding, (b) interaction between nitrogen atom and oxygen atom on the surrounding, (c) interaction between nitrogen atom and all the atoms on the surrounding for *m*NPA. Similarly, (d-f) is for $BZD^{+}\cdot mNPA^{-}$ and (g-i) is for $BZD^{+}\cdot NTPh^{-}$. The percentages in comparison to all interactions (distances) have been provided.

Table S1. Bond lengths [Å] and angles [°] of BZD^{+}·*m*NPA^{-}.

Bond length [Å]	
C(1)-C(2)	1.373(3)
C(1)-C(6)	1.385(2)
C(1)-H(1)	0.9300
C(2)-C(3)	1.393(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.371(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.387(2)
C(4)-H(4)	0.9300
C(5)-N(2)	1.383(2)
C(5)-C(6)	1.391(2)
C(6)-N(1)	1.390(2)
C(7)-N(2)	1.316(2)
C(7)-N(1)	1.320(2)
C(7)-H(7)	0.9300
C(8)-C(9)	1.392(2)
C(8)-C(13)	1.397(2)
C(8)-C(15)	1.514(2)
C(9)-C(10)	1.382(2)
C(9)-N(3)	1.471(2)

C(10)-C(11)	1.373(2)
C(10)-H(10)	0.9300
C(11)-C(12)	1.378(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.390(2)
C(12)-H(12)	0.9300
C(13)-C(14)	1.503(2)
C(14)-O(2)	1.2190(19)
C(14)-O(1)	1.2820(18)
C(15)-O(3)	1.2278(18)
C(15)-O(4)	1.2782(18)
N(1)-H(1B)	00.91(2)
N(2)-H(2A)	0.89(2)
N(3)-O(6)	1.2188(18)
N(3)-O(5)	1.2203(18)
O(1)-H(1A)	0.8200
Bond angles [°]	
C(2)-C(1)-C(6)	116.22(18)
C(2)-C(1)-H(1)	121.9
C(6)-C(1)-H(1)	121.9
C(1)-C(2)-C(3)	122.29(18)
C(1)-C(2)-H(2)	118.9
C(3)-C(2)-H(2)	118.9

C(4)-C(3)-C(2)	121.67(18)
C(4)-C(3)-H(3)	119.2
C(2)-C(3)-H(3)	119.2
C(3)-C(4)-C(5)	116.49(18)
C(3)-C(4)-H(4)	121.8
C(5)-C(4)-H(4)	121.8
N(2)-C(5)-C(4)	131.83(16)
N(2)-C(5)-C(6)	106.47(14)
C(4)-C(5)-C(6)	121.70(16)
C(1)-C(6)-N(1)	132.70(16)
C(1)-C(6)-C(5)	121.62(16)
N(1)-C(6)-C(5)	105.68(14)
N(2)-C(7)-N(1)	109.96(16)
N(2)-C(7)-H(7)	125.0
N(1)-C(7)-H(7)	125.0
C(9)-C(8)-C(13	116.86(13)
C(9)-C(8)-C(15)	124.02(13)
C(13)-C(8)-C(15)	119.12(12)
C(10)-C(9)-C(8)	123.04(14)
C(10)-C(9)-N(3)	117.19(13)
C(8)-C(9)-N(3)	119.77(13)
C(11)-C(10)-C(9)	118.77(14)
C(11)-C(10)-H(10)	120.6

C(9)-C(10)-H(10)	120.6
C(10)-C(11)-C(12)	120.11(15)
C(10)-C(11)-H(11)	119.9
C(12)-C(11)-H(11)	119.9
C(11)-C(12)-C(13)	120.77(15)
C(11)-C(12)-H(12)	119.6
C(13)-C(12)-H(12)	119.6
C(12)-C(13)-C(8)	120.40(14)
C(12)-C(13)-C(14)	119.54(14)
C(8)-C(13)-C(14)	120.04(13)
O(2)-C(14)-O(1)	125.19(14)
O(2)-C(14)-C(13)	121.16(13)
O(1)-C(14)-C(13)	113.65(13)
O(3)-C(15)-O(4)	124.09(14)
O(3)-C(15)-C(8)	118.57(13)
O(4)-C(15)-C(8)	117.34(12)
C(7)-N(1)-C(6)	108.97(15)
C(7)-N(1)-H(1B)	121.4(15)
C(6)-N(1)-H(1B)	129.5(15)
C(7)-N(2)-C(5)	108.93(15)
C(7)-N(2)-H(2A)	126.2(15)
C(5)-N(2)-H(2A)	124.5(14)
O(6)-N(3)-O(5)	123.72(15)

O(6)-N(3)-C(9)	117.94(15)
O(5)-N(3)-C(9)	118.33(13)
C(14)-O(1)-H(1A)	109.5