Supporting Information

Proton-transfer Supramolecular Salts Resulted from 3,5-Dinitrobenzoic Acid and Aminomethyl Pyridine

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Table 1. Crystallographic data for the complex of **1**−**3**

Compounds	**1**	**2**	**3**
Formula	$C_{13}H_{12}N_4O_6$	$C_{13}H_{12}N_4O_6$	$C_{26}H_{24}N_8O_{12}$
Formula weight	320.27	320.27	640.53
Crystal system	monoclinic	orthorhombic	triclinic
Space group	$P2_1/n$	$P2_12_12_1$	$P-1$
a (Å)	6.5494 (13)	6.8770 (14)	7.4234 (15)
b (Å)	9.1960 (18)	9.2116 (18)	11.738 (2)
c (Å)	23.512 (5)	22.056 (4)	17.698 (4)

α (°)	90°	90°	102.99 (3)°
β (°)	90.39 (3)°	90°	100.52 (3)°
γ (°)	90°	90°	101.26 (3)°
V (Å^3)	1416.0 (5)	1397.2 (5)	1431.8 (5)
D_x (Mg m^{-3})	1.502	1.522	1.486
μ (mm^{-1})	0.12	0.12	0.12
Z	4	4	2
T (K)	293	293	293
F (000)	664	664	664
θ range for data collection (°)	3.2−27.5	3.1−27.5	3.0−27.5
Index ranges	−8 ≤ h ≤ 8, −11 ≤ k ≤ 11, −30 ≤ l ≤ 30	−8 ≤ h ≤ 8, −11 ≤ k ≤ 11, −28 ≤ l ≤ 28	−9 ≤ h ≤ 9, −15 ≤ k ≤ 15, −22 ≤ l ≤ 22
Measured reflections	14201	14505	14831
Independent reflections	3246	3190	6511
Data/restraints/parameters	3246/0/208	3190/0/208	6511/0/416
R_{int}	0.045	0.041	0.063
Reflections with $I > 2\sigma(I)$	2348	2831	3674
R_1 [$I > 2\sigma(I)$]	0.055	0.039	0.062
wR_2 (all data)	0.148	0.092	0.167
S	1.09	1.08	1.03

Table 2. Hydrogen Bond Distances and Parameters for the complex of **1**−**3** (Å, °)

D–H···A	D–H	H···A	D···A	D–H···A
		Compound **1**		
N4–H4A···O2^{i}	0.89	1.93	2.810(2)	172
N4–H4B···O1^{ii}	0.89	2.52	3.374(2)	162
N4–H4B···O2^{ii}	0.89	2.15	2.908(2)	142

N4–H4C···O1^{iii}	0.89	1.93	2.776(2)	157
C9–H9A···O3^{iv}	0.93	2.57	3.149(3)	121
		Compound **2**		
N4–H4A···O2^{iv}	0.89	1.98	2.7635(19)	146
N4–H4B···O1^{v}	0.89	1.93	2.8028(19)	167
N4–H4C···O1	0.89	1.95	2.8323(19)	170
C13–H13B···O4^{vi}	0.97	2.57	3.236(2)	126
		Compound **3**		
N6–H6A···N7^{iv}	0.89	2.02	2.900	171
N6–H6B···O1	0.89	1.80	2.668	166
N6–H6C···O5^{vii}	0.89	2.59	3.080	116
N6–H6C···N5^{viii}	0.89	2.51	3.139	129
N8–H8C···O7^{ix}	0.89	2.48	2.973	115
N8–H8C···O8^{ix}	0.89	2.04	2.921	169
N8–H8A···O7	0.89	1.88	2.750	167
N8–H8B···O2	0.89	1.95	2.757	151
C15–H15A···O1^{viii}	0.93	2.58	3.419	150
C22–H22A···O11^{x}	0.93	2.55	3.282	136
C26–H26B···O7^{ix}	0.97	2.57	3.168	120

Symmetry codes: (i) x−1, y+1, z; (ii) −x+1, −y+1, −z; (iii) x, y+1, z; (iv) x−1, y, z; (v) x−1/2, −y+3/2, −z+1; (vi) −x, y−1/2, −z+3/2; (vii) x−1, y−1, z; (viii) −x+1, −y, −z+1; (ix) −x, −y, −z; (x) x, y−1, z.

Table 3. Summary of Mass (m/g) and Moles (n/mmol) Used of Acid and Amine for the Synthesis and Elemental analyses results of Compounds **1-3**

Compound	Amine (m, n)	Acid (m, n)	Elemental analyses results
1	2-aminomethyl pyridine (0.029, 0.24)	3,5-dinitrobenzoic acid (0.047, 0.22)	Anal. Calc. For $C_{13}H_{12}N_4O_6$: C, 48.75; H, 3.78; N, 17.49. Found: C, 48.90; H, 4.00; N, 17.27 %.
2	3-aminomethyl pyridine (0.013, 0.11)	3,5-dinitrobenzoic acid (0.025, 0.12)	Anal. Calc. For $C_{13}H_{12}N_4O_6$: C, 48.75; H, 3.78; N, 17.49. Found: C, 48.92; H, 3.88; N, 17.37 %.
3	4-aminomethyl pyridine (0.038, 0.32)	3,5-dinitrobenzoic acid (0.064, 0.30)	Anal. Calc. For $C_{13}H_{12}N_4O_6$: C, 48.75; H, 3.78; N, 17.49. Found: C, 48.60; H, 4.01; N, 17.40 %.