Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Isostructurality in Amino Molecular Salts of Two Dicarboxylic Acids Driven by Noncovalent Synthons

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Table S1. Cell data for **1**-**6**.

Crystal Data **CCDC Number**	**ndc-4apy (1)** **2075478**	**cca-4apy (2)** **2075479**	**ndc-2abi (3)** **2075480**	**cca-2abi (4)** **2075481**	**ndc-2apy (5)** **2075482**	**cca-2apy (6)** **2075483**
Formula	$C_{22}H_{28}N_4O_8$	$C_{20}H_{28}N_4O_8$	$C_{26}H_{24}N_6O_5$	$C_{24}H_{24}N_6O_5$	$C_{22}H_{20}N_4O_4$	$C_{20}H_{24}N_4O_6$
Mol. Wt.	476.48	452.46	500.51	476.49	404.42	416.43
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic
Sp. Gr., Z	$P2_1/c$, 2	$P2_1/c$, 2	$C2/c$, 4	Cc,* 4	$P\bar{1}$, 2	$P2_1/c$, 4
a, Å	7.2366(5)	7.0741(11)	17.7868(13)	17.637(2)	9.1101(5)	9.7799(11)
b, Å	11.3931(8)	11.0582(17)	9.9141(7)	10.0843(13)	10.3633(6)	12.2291(15)
c, Å	14.1809(10)	14.289(2)	12.5079(9)	12.2714(15)	11.2788(7)	18.194(2)
α, º	90	90	90	90	100.613(2)	90
β, º	96.390(2)	98.460(3)	100.210(2)	102.452(3)	98.629(2)	93.443(3)
γ, º	90	90	90	90	113.035(2)	90
V, Å^3	1161.91(14)	1105.6(3)	2170.7(3)	2131.2(5)	933.68(10)	2172.1(4)
D_{calc}(g/cm^3)	1.362	1.359	1.532	1.485	1.439	1.273
μ (mm^{-1})	0.105	0.106	0.109	0.107	0.102	0.095
GOOF	1.059	1.263	1.073	1.105	1.035	1.027
R_1	0.0481	0.0699	0.0538	0.0485	0.0402	0.0794
wR_2	0.1250	0.1858	0.1475	0.1380	0.1001	0.1914

* Flack parameter 0.3(6)

In **2**, **4** and **6**, cca has static disorder as shown in Fig. 1.

Table S2. The hydrogen bond table for **1**.

D-H···A	**d(D-H) / Å**	**d(H..A) / Å**	**D···A / Å**	**D-H···A / (º)**
N1-H1···O1	0.870	1.784	2.653	176.24
N2-H2A···O4$^{(a)}$	0.870	2.041	2.887	163.93
N2-H2B···O3$^{(b)}$	0.870	2.139	2.992	166.89
O3-H3A···O1	0.848	1.923	2.771	177.58
O3-H3B···O2$^{(c)}$	0.858	1.936	2.790	172.98
O4-H4A···O2$^{(d)}$	0.903	1.906	2.809	178.46
O4-H4B···O3	0.802	2.106	2.896	168.34

Symmetry code: a = [x+1, -y+1/2, z-1/2]; **b** = [-x+2, y+1/2, -z+1/2]; **c** = [-x+1, y-1/2, -z+1/2]; **d** = [-x+1, -y+1, -z+1]

Table S3. The hydrogen bond table for **2**.

D-H···A	d(D-H) / Å	d(H..A) / Å	D···A / Å	D-H···A / (º)
N1-H1···O1	0.986	1.687	2.671	175.40
N2-H2A···O4 [(a)]	0.909	2.027	2.931	172.25
N2-H2B···O3 [(b)]	0.854	2.020	2.850	163.79
O3-H3A···O4	0.851	2.018	2.863	171.58
O3-H3B···O2	0.810	1.958	2.762	172.10
O4-H4A···O2 [(c)]	0.858	1.919	2.772	172.41
O4-H4B···O1 [(d)]	0.788	1.917	2.700	172.71

Symmetry code: a = [x+1, -y+3/2, z-1/2]; **b** = [-x+2, y-1/2, -z+1/2]; **c** = [x, -y+3/2, z+1/2]; **d** = [-x+1, -y+1, -z+1]

Table S4. The hydrogen bond table for **3**.

D-H···A	d(D-H) / Å	d(H..A) / Å	D···A / Å	D-H···A / (º)
N1-H1···O1 [(a)]	0.868	1.913	2.779	175.73
N2-H2···O2	0.871	1.916	2.746	158.68
N3-H3A···O1 [(b)]	0.868	2.024	2.887	172.19
N3-H3B···O2 [(c)]	0.868	2.047	2.875	159.09
C6-H6···O3	0.950	2.556	3.448	156.43
O3-H3W···O2	0.865	2.086	2.911	159.13

Symmetry code: a = [-x+1/2, y-1/2, -z+3/2]; **b** = [-x+1/2, -y+1/2, -z+1]; **c** = [-x+1/2, y-1/2, -z+3/2]

Table S5. The hydrogen bond table for **4**.

D-H···A	d(D-H) / Å	d(H..A) / Å	D···A / Å	D-H···A / (º)
N1-H1···O4 [(a)]	0.880	1.870	2.749	177.14
N2-H2···O1	0.880	1.892	2.722	156.44
N3-H3A···O3 [(b)]	0.880	2.057	2.899	159.80
N3-H3B···O4 [(c)]	0.880	2.003	2.856	162.96
C6-H6···O1W	0.950	2.651	3.531	154.41
C13-H13···O1W	0.950	2.596	3.487	156.21
N4-H4···O2 [(d)]	0.880	1.877	2.756	177.98
N5-H5···O3 [(e)]	0.880	1.888	2.749	165.57
N6-H6A···O1 [(f)]	0.880	1.992	2.833	159.47
N6-H6B···O2 [(g)]	0.880	2.000	2.857	164.46
O1W-H1W···O3 [(h)]	0.985	2.023	2.826	137.12
O1W-H2W···O1	0.985	2.067	2.850	135.05

Symmetry code: a = [x+1/2, -y+1/2, z-1/2]; **b** = [x+1/2, -y+1/2, z-1/2]; **c** = [x+1/2, y+1/2, z]; **d** = [x-1/2, y-1/2, z]; **e** = [x, -y+1, z-1/2]; **f** = [x-1/2, y-1/2, z]; **g** = [x-1/2, -y+3/2, z-1/2]; **h** = [x, -y+1, z-1/2]

Table S6. The hydrogen bond table for **5**.

D-H···A	**d(D-H) / Å**	**d(H..A) / Å**	**D···A / Å**	**D-H···A / (º)**
N1-H1···O1	0.942(10)	1.702(10)	2.6371(13)	171.2(17)
C1-H1A···O4 [(a)]	0.95	2.34	3.2060(15)	151.9
N2-H2A···O2	0.939(10)	1.854(10)	2.7927(13)	179.0(15)
N2-H2B···O3 [(b)]	0.928(9)	2.044(12)	2.9024(13)	153.2(14)
N3-H3···O3	0.942(10)	1.715(10)	2.6524(13)	173.5(16)
N4-H4A···O4	0.931(10)	1.859(10)	2.7885(13)	176.4(15)
N4-H4B···O2 [(c)]	0.926(9)	1.917(10)	2.8392(13)	174.0(16)

Symmetry code: a = [1-x,1-y,-z]; **b** = [1-x,1-y,1-z]; **c** = [+x,+y,-1+z]

Table S7. The hydrogen bond table for **6**.

D-H···A	**d(D-H) / Å**	**d(H..A) / Å**	**D···A / Å**	**D-H···A / (º)**
N1-H1N···O2 [(a)]	0.898	1.805	2.700	174.71
N2-H21N···O1W [(b)]	0.892	1.979	2.852	165.99
N2-H22N···O1 [(c)]	0.888	1.971	2.846	168.29
N3-H3N···O4	0.901	1.717	2.612	172.47
N4-H41N···O2W [(d)]	0.888	2.104	2.915	151.52
N4-H42N···O3	0.887	2.030	2.900	166.74
C15-H15···O4 [(e)]	0.940	2.624	3.331	132.42
O1W-H11W···O1	0.847	2.040	2.873	167.64
O1W-H12W···O3 [(f)]	0.854	1.958	2.790	164.17
O2W-H21W···O1 [(g)]	0.858	2.069	2.846	150.19
O2W-H22W···O2	0.854	1.920	2.756	165.89

Symmetry code: a = [-x+1, -y+2, -z]; **b =** [x-1, y, z]; **c =** [-x+1, -y+2, -z]; **d =** [-x, -y+1, -z]; **e =** [-x+1,y+1/2,-z+1/2]; **f** = [-x+1, -y+1, -z]; **g =** [-x+1, -y+2, -z]

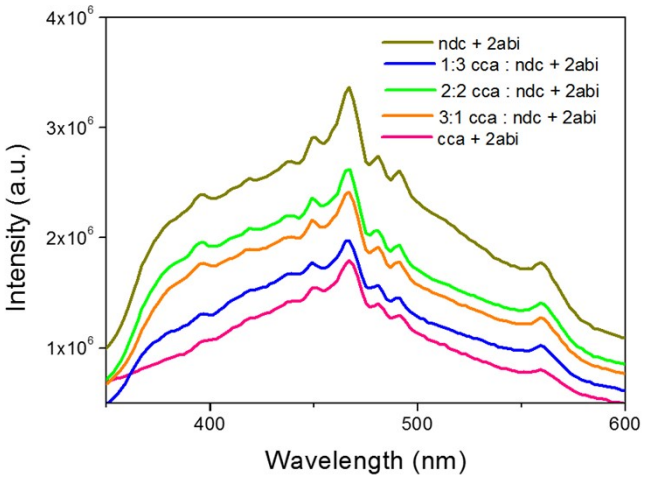

Figure S1. Photoluminescence properties of solid-solutions of molecular salts of **3** and **4**.

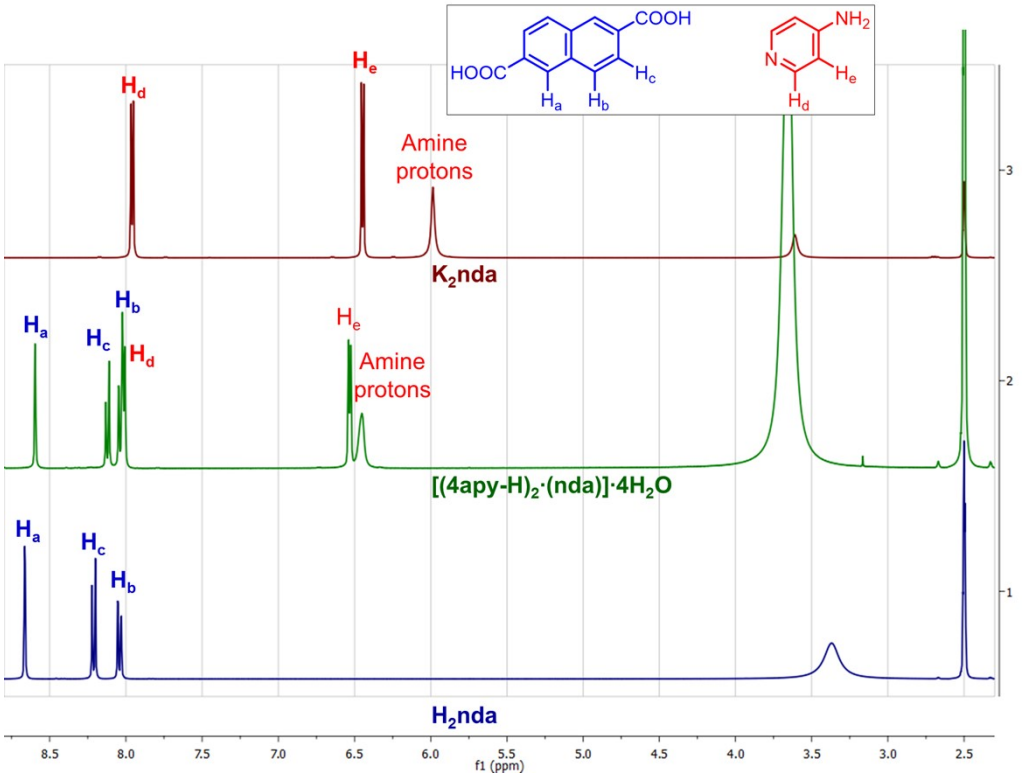

Figure S2. Shifting of ^{1}H-NMR peaks of ndc in **1** to higher field suggests the electron cloud enhancement on the ndc core.

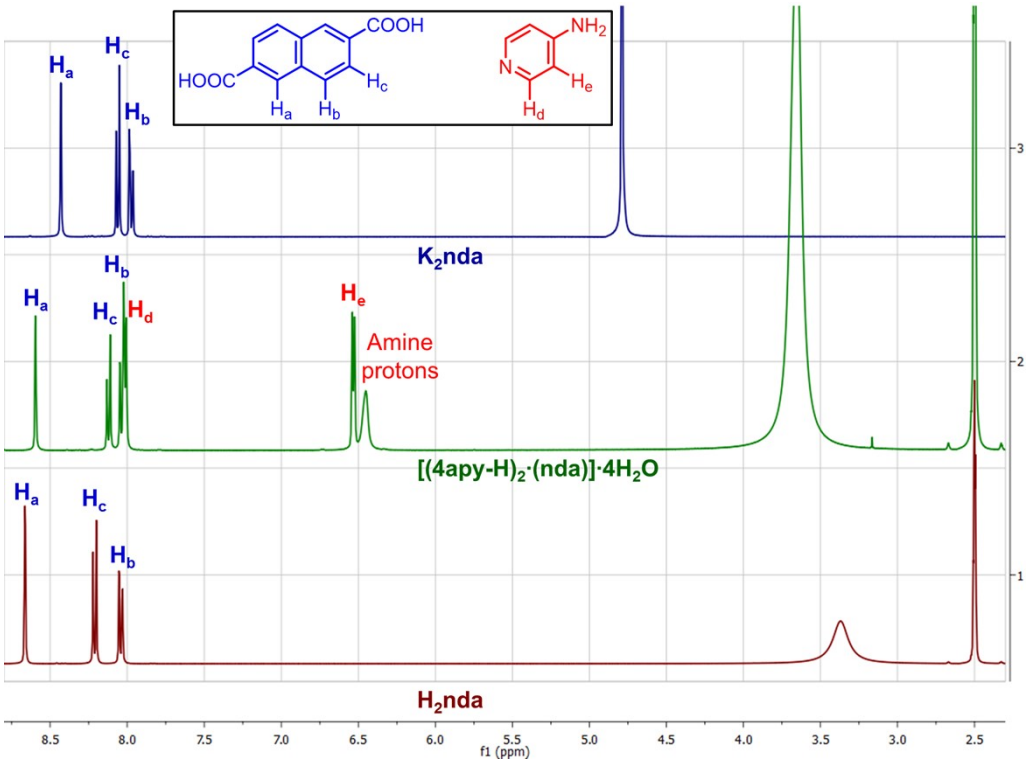

Figure S3. Shifting of ^{1}H-NMR peaks of ndc in **1** to higher field suggests the electron cloud enhancement on the ndc core.

NMR spectra were recorded on a Bruker DRX 400 at room temperature. Chemical shifts are given in parts per million (ppm) and the spectra were referenced by using the residual solvent shift as internal standards (dimethyl sulfoxide-d_6, ^{1}H-NMR δ 2.50).

The proton signals of ndc are slowly shifted to higher field from H_2ndc, **1** and K_2ndc. This suggests the slow accumulation of electron cloud on the ndc unit. In addition, ndc peaks of **1** are between H_2ndc and K_2ndc.

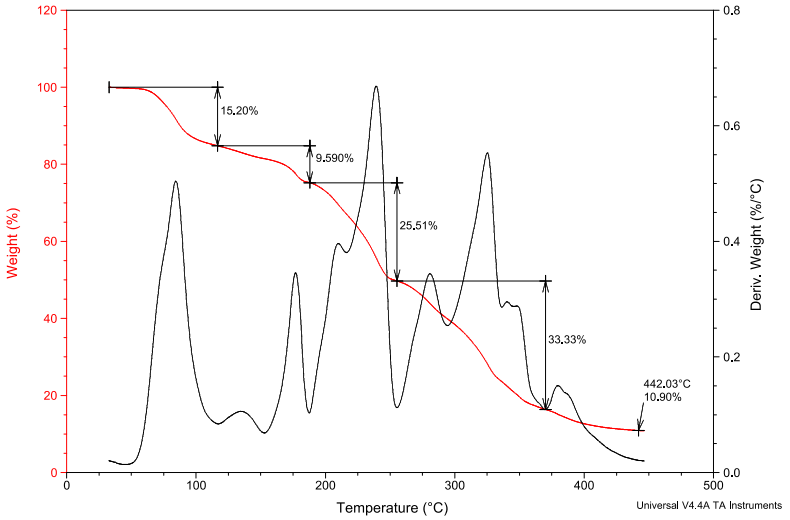

Figure S4. TGA analysis of compound **1**.

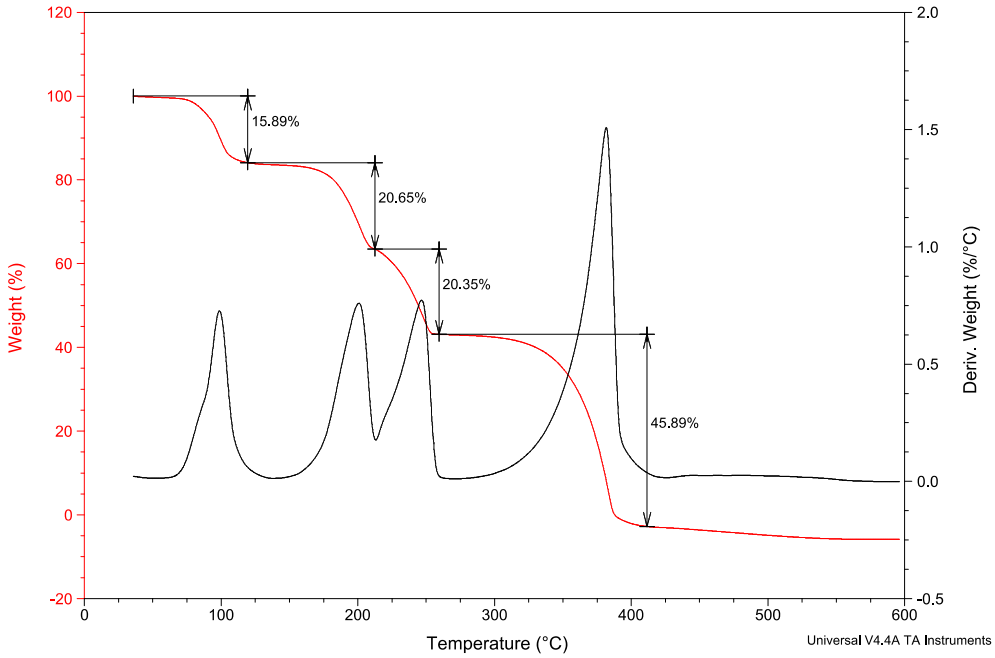

Figure S5. TGA analysis of compound **2**.

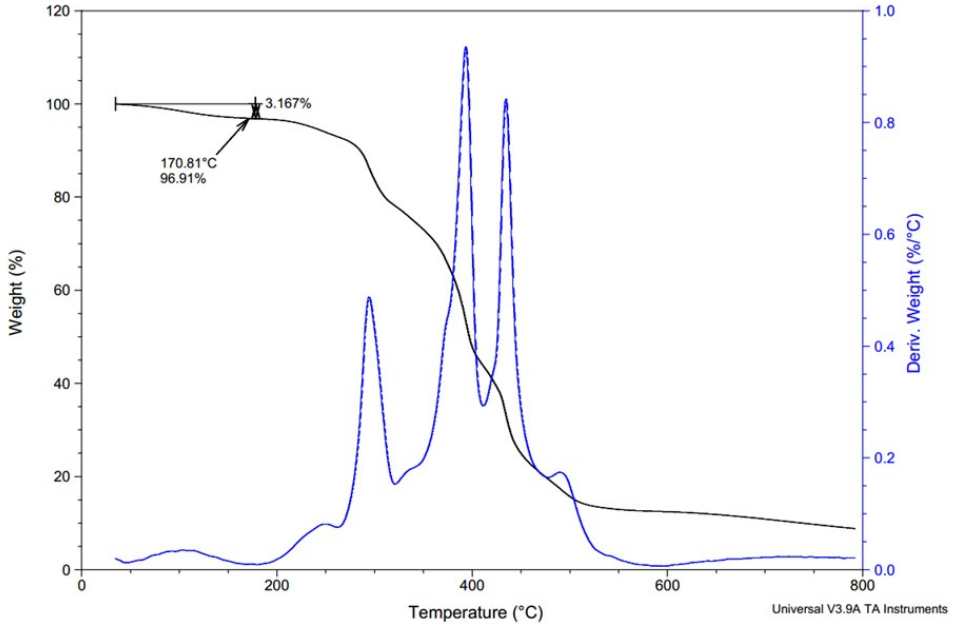

Figure S6. TGA analysis of compound **3**.

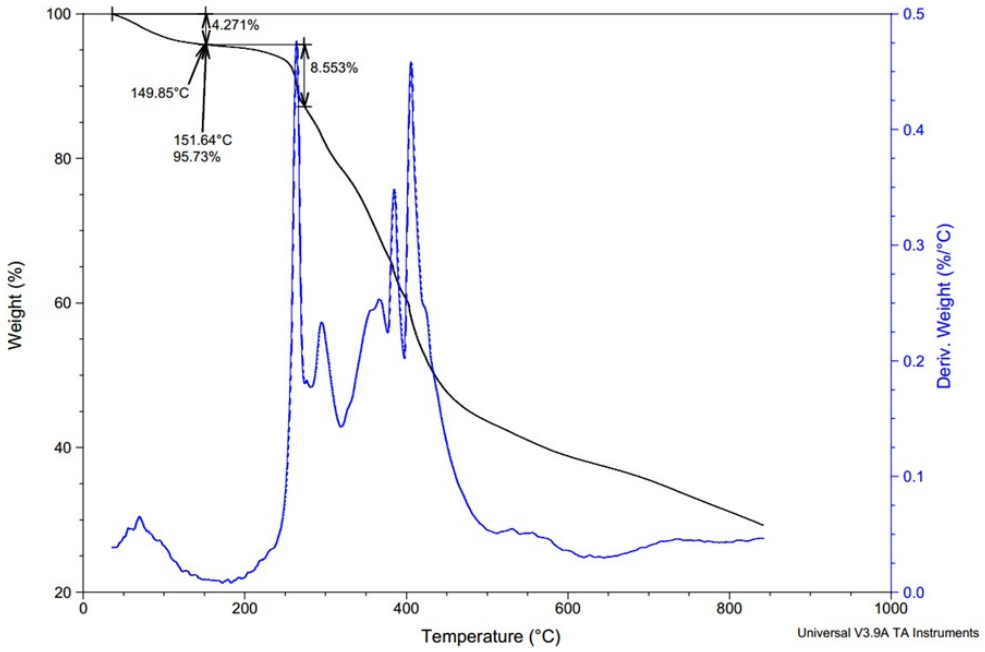

Figure S7. TGA analysis of compound **4**.