Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Information

for

The Crystal Structures and Melting Point Properties of Isonicotinamide Cocrystals with Alkanediacids $HO_2C(CH_2)_{n-2}CO_2H$ n=7-9

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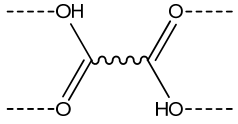
Melting point, density and packing fractions for the pure alkanediacids, 1:1 and 2:1 isonicotinamide:alkanediacid cocrystals discussed in this paper.

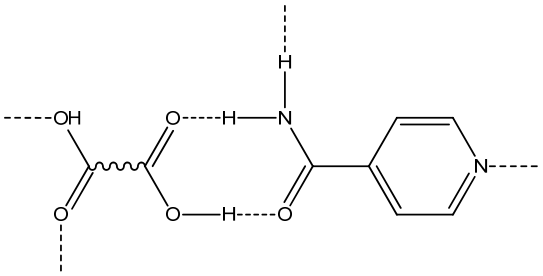
An indicator of relative intermolecular hydrogen-bond strength in each material is given by the total H…A and average H…A distance quantified by the hydrogen bonds indicated within each supramolecular building block as shown below. This information has only been provided for materials that are isostructural as indicated by the isostructural groups a) to e) below:

a) pure even alkanediacids: succinic, adipic, suberic & sebacic acid
b) pure odd alkanediacids: glutaric, pimelic & azelaic acid
c) 1:1 isonicotinamide cocrystals with even diacids - adipic & suberic acid
d) 1:1 isonicotinamide cocrystals with odd diacids - pimelic & azelaic acid
e) 2:1 isonicotinamide cocrystals with even diacids - oxalic, succinic & adipic acid

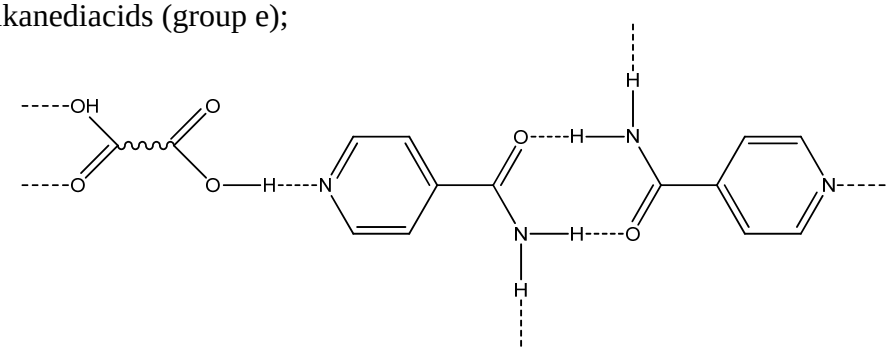
Scheme 1: The supramolecular building block within the chains of both odd and even pure alkanediacids (groups a and b); 4 hydrogen bonds.



Scheme 2: The supramolecular building block within the chains of 1:1 isonicotinamide cocrystals with both odd and even pure alkanediacids (groups c and d); 6 hydrogen bonds.



Scheme 3: The supramolecular building block within the chains of 2:1 isonicotinamide cocrystals with even pure alkanediacids (group e); 9 hydrogen bonds.



	Pure alkanediacid						1:1 isonicotinamide:alkanediacid cocrystal						2:1 isonicotinamide:alkanediacid cocrystal					
	Melting point ˚C	Density Mg/m^3	Packing fraction	No. H bonds	Total H..A Distance (Å)	Average H..A Distance (Å)	Melting point ˚C	Density Mg/m^3	Packing fraction	No. H bonds	Total H..A Distance (Å)	Average H..A Distance (Å)	Melting point ˚C	Density Mg/m^3	Packing fraction	No. H bonds	Total H..A Distance Å	Average H..A Distance Å
Oxalic	189.5	1.948	0.802										243	1.584	77.1	9	16.573	1.841
Malonic	135.6	1.669	0.749										170	1.490	73.1			
Succinic	188	1.624	0.777	4	6.924	1.731							206	1.480	74.1	9	17.186	1.910
Glutaric	99	1.484	0.741	4	6.832	1.708	134	1.399	70.3				149	1.420	71.8			
Adipic	153	1.398	0.726	4	6.728	1.685	163	1.395	71.6	6	11.048	1.841	178	1.425	73.0	9	17.495	1.944
Pimelic	106	1.372	0.727	4	6.853	1.713	112	1.331	69	6	11.566	1.928						
Suberic	144	1.319	0.714	4	6.676	1.669	165	1.369	72	6	11.698	1.950						
Azelaic	106.5	1.303	0.720	4	6.816	1.704	142	1.283	68.3	6	11.483	1.914						
Sebacic	134.5	1.257	0.704	4	6.616	1.654												