

Different carboxylic acid homodimers in self-assemblies of adducts of 3-carboxyphenoxyacetic acid with nitrogen containing compounds

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Abstract. Different hydrogen bonded dimeric motifs of 3-carboxyphenoxyacetic acid (H2cpa) observed in the self-assemblies of salts or cocrystals of H2cpa with nitrogen containing compounds are discussed. Pyridinium salt of the H2cpa is a self-assembly of Hcpa with the pyridinium cation. The assembly is a combination of sub-assemblies of two Hcp anions with two pyridinium cations, in which the Hcpa cations are interconnected through carboxylate-carboxylic acid interactions. The cocrystals of H2cpa with isoquinoline or isonicotinamide are self-assemblies of hydrogen bonded dimers of H2cpa holding the respective guest molecule. However, the dimeric assemblies of H2cpa in these two cases are different from each other; the former cocrystal has carbonyl-hydroxyl type interactions in it whereas the latter cocrystal has unconventional dimeric sub-assemblies of H2cpa with hydroxyl-hydroxyl type hydrogen bond interactions. The cocrystal of H2cpa with theophylline has sub-assemblies of two H2cpa molecules interacting with two theophylline guest molecules, where the theophylline molecules are hydrogen bonded in two different ways.

Keywords. Dicarboxylic acid; bifurcated hydrogen bonds; self-assembly; cocrystal; homodimer; heterodimer.

1. Introduction

Seminal work of Desiraju on synthons^{1–3} and their subsequent applications in understanding supramolecular assemblies have made a big headway.^{4–12} Dunitz and Gavezzotti had suggested early examples to show the importance on understanding of the energetic of the interactions between molecules bonded by each synthon.¹³ On the other hand, Etter's rules have not only helped to provide qualitative pictures to prioritize on bond hierarchy to form a synthon but also provided a simple way to demarcate them through graph set-notations.^{14,15} Beside these, while forming supramolecular assemblies complications may arise from the competition of the constituent components forming self-assembly to form homomeric assembly or to form adduct by forming heteromeric assembly or combinations of both types of units to form self-assembly of adduct.^{16,17} For example, carboxylic acids can form neutral or partly deprotonated assembly in different ways as shown in scheme 1.¹⁸ In a latest analysis on different conformations of catemers of different carboxylic acids generated by hydroxyl-hydroxyl or carbonyl-hydroxyl type interactions (scheme 1) suggested the scope to discover new conformers in the assembly of carboxylic acids.¹⁹ Due to the directional nature of hydrogen bond, such

conformers would decide the suitability of a specific guest molecule to bind with a host carboxylic acid. Furthermore, the directional properties of weak interactions have definite roles in soft materials,^{20–23} framework structures,^{24–36} polymorphs,³⁷ and self-assemblies.^{38–48} Hence, even to use any of the existing small building blocks with multiple hydrogen bond sites require prior analysis on different possibilities to form hydrogen bonds. With these points, we have chosen to study 3-carboxyphenoxyacetic acid (**I**) abbreviated as H2cpa. H2cpa is a dicarboxylic acid having flexible and rigid arms along with an ether linkage. A close analysis on the published structure of 3-carboxyphenoxyacetic acid, has made us to realize that it forms dimeric assembly as illustrated in figure 1(a) by hydrogen bond interactions.⁴⁹ This was a curious point to start a new study, as a carboxylic acid having multiple numbers of electronegative atoms such as oxygen atoms should easily remain as discrete units keeping the electronegative atoms apart. In other words, an assembly formed by such compounds should be possible to segregate easily by solvent molecules or guest molecules to provide different packing patterns which may lead to different arrangements. If the dimeric motifs are not dislodged by guest or solvent molecules, then also there are possibilities to reorganize the dimeric motifs to closely related structural motifs such as the ones shown in

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Table 1. Crystallographic parameters of the cocrystals/salt.

Cocrystal/salt	II	III	IV	V
Formula	C ₂₃ H ₂₁ NO ₁₀	C ₂₇ H ₂₃ N O ₁₀	C ₁₅ H ₁₄ N ₂ O ₆	C ₁₆ H ₁₆ N ₄ O ₇
CCDC No.	1432461	1432462	1417584	1417583
formula weight	471.41	521.46	318.28	376.33
crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P-1	P-1	P-1	P-1
<i>a</i> (Å)	7.5510(12)	7.6699(6)	7.7934(5)	11.4675(7)
<i>b</i> (Å)	10.474(2)	8.9654(8)	8.6548(7)	12.0693(8)
<i>c</i> (Å)	13.943(3)	9.0521(8)	10.7658(8)	14.3043(9)
α (deg)	98.763(16)	76.802(8)	100.178(6)	74.990(6)
β (deg)	95.754(15)	80.215(7)	95.315(5)	66.587(6)
γ (deg)	97.518(15)	89.098(7)	92.523(6)	64.482(6)
<i>V</i> (Å ³)	1072.4(3)	597.03(9)	710.30(9)	1630.32(17)
<i>Z</i>	2	1	2	4
ρ_{calc} (g · cm ⁻³)	1.460	1.450	1.488	1.533
μ (mm ⁻¹)	0.116	0.112	0.117	0.123
<i>F</i> (000)	492	272	332	784
reflins collected	7327	3986	8581	9261
reflins unique	3879	2156	2510	5597
Ranges (h, k, l)	-8 ≤ h ≤ 9 -12 ≤ k ≤ 12 -16 ≤ l ≤ 16	-9 ≤ h ≤ 9 -10 ≤ k ≤ 10 -10 ≤ l ≤ 10	-9 ≤ h ≤ 9 -10 ≤ k ≤ 10 -12 ≤ l ≤ 12	-13 ≤ h ≤ 13 -14 ≤ k ≤ 13 -14 ≤ l ≤ 16
Completeness to 2 θ	99.7	99.5	97.4	99.7
GOF (<i>F</i> ²)	1.099	0.958	1.126	1.331
R ₁ [<i>I</i> ≥ 2 σ (<i>I</i>)]	0.0817	0.0442	0.0562	0.0485
wR ₂ [<i>I</i> ≥ 2 σ (<i>I</i>)]	0.1628	0.1057	0.1024	0.0961
R ₁ (all data)	0.1684	0.0619	0.1075	0.0717
wR ₂ (all data)	0.2049	0.1253	0.1160	0.1328
Largest diff peak/hole (e Å ⁻³)	0.580 / -0.262	0.146 / -0.211	0.373 / -0.216	0.320 / -0.326

SMART software was used for data collection and also for indexing the reflections and determining the unit cell parameters. Data reduction and cell refinement were performed using SAINT and XPREP software. Multi-scan empirical absorption corrections were carried out with the help of face-indexing. Structures were solved by direct methods using SHELXS-97 and were refined by full-matrix least-squares on *F*² using SHELXL-97. The crystallographic parameters are listed in the table 1.

3. Results and Discussion

Slow evaporation of methanol solutions of 3-carboxyphenoxyacetic acid monohydrate (I) and a guest chosen from a series of nitrogen containing compounds was carried out. From such crystallizations, crystals of the respective salt or cocrystal were obtained which are listed in table 2. The stoichiometry of each salt or cocrystal was found to be invariant of

Table 2. Dimeric assemblies in salt and cocrystals of 3-carboxyphenoxyacetic acid #.

Guest molecule (abbreviation) [pKa, (adduct type)]	Composition	Types of catemers in the assembly (conformer symmetry)	Principal cyclic motif with heterocycle
Pyridine (Py) [5.14 (Salt)]	(HPy).(HCarbophen). (H ₂ Carbophen) (II)	One end carboxyl(ate), (AS) Other end carbonyl type (AS-A)	Held by pyridinium cation
Isoquinoline (Iqn) [5.14 (Cocrystal)]	(H ₂ Carbophen) ₂ .(Iqn) (III)	Both end carbonyl type (AS-A)	Held by disordered isoquinoline molecule
Isonicotinamide (Inic)[3.61,(Cocrystal)]	(H ₂ Carbophen).(Inic) (IV)	Both end hydroxyl type (AS-A)	Held by homodimer of isonicotinamide
Theophylline (Thp) [1 and 8.81, (Cocrystal)]	[(H ₂ Carbophen).(Tph)] ₂ (V)	Both end carbonyl type (AS-A)	Held by theophylline.

@ Compounds were crystallized from solution in methanol. # pKa = 4.25 (in methanol)

the molar proportions of the two components used in their preparations. This conclusion was reached on the basis of the powder XRD patterns of each crystalline sample obtained from different solutions under different conditions and comparison with the respective PXRD pattern generated from CIF. Furthermore, the integrations of the proton signals in the respective $^1\text{H-NMR}$ spectra (provided as Supporting Information) of the salt or cocrystal was in excellent agreement with the stoichiometry given in table 2.

Structures of each cocrystal and salt were determined. The packing pattern of the crystal structure of 3-carboxyphenoxyacetic acid monohydrate⁴⁹ is comprised of a self-assembly constituted by dimers formed between two acid molecules. H2cpa molecule has two carboxylic acid groups at two different non-equivalent locations, hence the molecule is unsymmetrical, and the end of the which has the carboxylic acid directly linked to phenyl ring may be designated as head and other end of carboxylic acid attached through ether link as tail. Then each dimer formed in the assembly may be described as assembly of two molecules in head to tail manner (figure 3a). Such dimers have carbonyl-hydroxyl interactions and possess a center of inversion and each side of the dimers has AS-A conformation¹⁹ (inset of figure 3a).

Pyridinium salt **II** consists of three components comprising of an acid molecule, a mono deprotonated acid molecule and a pyridinium cation (figure 3b). The self-assembly of the salt has dimeric motifs formed by interactions between carboxylic acid and carboxylate. These motifs interact with the pyridinium cation by $\text{N-H}\cdots\text{O}$ interactions. One end of each dimer motif has a carboxyl(ate) catemer possessing AS conformer and the other side has a carbonyl type catemer comprising of AS-A conformer. These motifs are held to each other through $\text{O-H}\cdots\text{O}$ interactions. The hydrogen bond parameters are listed in table 3.

The cocrystal **III** is a self-assembly of two carboxylic acid molecules with one isoquinoline molecule. From crystallographic point of view, it is a self assembly of dimer of H2cpa flanked by two halves of an isoquinoline molecule at two ends. There is a crystallographic disorder in the isoquinoline ring which was resolved by sharing CH and N atoms at two symmetry equivalent positions as illustrated in figure 3c. Alternatively, the self-assembly may be described as an assembly of sub-assemblies of two carboxylic acid molecules holding one isoquinoline at one end. Due to such a disorder, isoquinoline nitrogen apparently bridges two neighboring dimeric assemblies of carboxylic acid molecules and forms a chain-like structure. The structure of the adduct shows short $\text{H}(4)\cdots\text{H}(4)$

contact between the carboxylic acid protons and this is due to disorder associated with hydrogen atom and can be resolved easily by sharing hydrogen atoms while solving the structure. But in X-ray crystallography, positions of the hydrogen atoms are sometimes non-realistic; hence, we have not done so and left it as obtained without sharing the electron density of hydrogen to maintain the charge balance and also it does not make significant effect on our discussion on the self-assembling process. The heterodimers present in this cocrystal has resemblance with heterodimers observed in cocrystals formed between a carboxylic acid with pyridine,^{51–54} the difference being the half occupancy of nitrogen atoms. Pyridine and isoquinoline have similar pKa value (5.14), yet they bind in different ways to the same carboxylic acid (pKa = 4.25). These two examples may be considered as exceptional examples to note as the differences of pKa between the acid and guest molecules being similar and small (~ 0.9), yet they show different behaviors towards the proton exchange process with the same acid, namely, H2cpa. However, one point is clear that due to the small difference between the respective pKa values there is uncertainty⁵⁵ in observing uniform way for both to fall in same category namely, salts or cocrystals.

Nicotinamide and isonicotinamide are well known cofomer to form cocrystals with different dicarboxylic acids.⁵⁶ Our attempts to prepare corystalline products from solution of H2cpa with nicotinamide or isonicotinamide yielded crystals of cocrystal of H2cpa with isonicotinic acid, whereas the H2cpa and nicotiamide were precipitated from the solution of the former combination without forming cocrystals. The cocrystal **IV** was formed by one H2cpa molecule interacting with one isonicotinamide molecule but in practice the crystal structure has shown that it is a self-assembly comprising of sub-assemblies of dimer formed by two carboxylic acid molecules with dimers of two isonicotinamide molecules. The dimers formed between isonicotinamide molecules act as bridge between the dimers of H2cpa through hydrogen bond interactions of carboxylic OH with pyridine nitrogen atom of isonicotinamide. The hydrogen bond patterns in the dimers formed between the two molecules of H2cpa in this cocrystal is exceptional. It possesses hydroxyl-hydroxyl interactions at both the ends with AS-A conformations. The hydroxyl-hydroxyl type dicarboxylic acid motifs are relatively less in literature but the one with AS conformer is not known.¹⁸ Hence, this hydroxyl type carboxylic acid dimer possessing AS conformers is a new finding in dicarboxylic acid. The self assemblies formed by the pair of carboxylic acids are flanked by homodimeric assemblies formed between

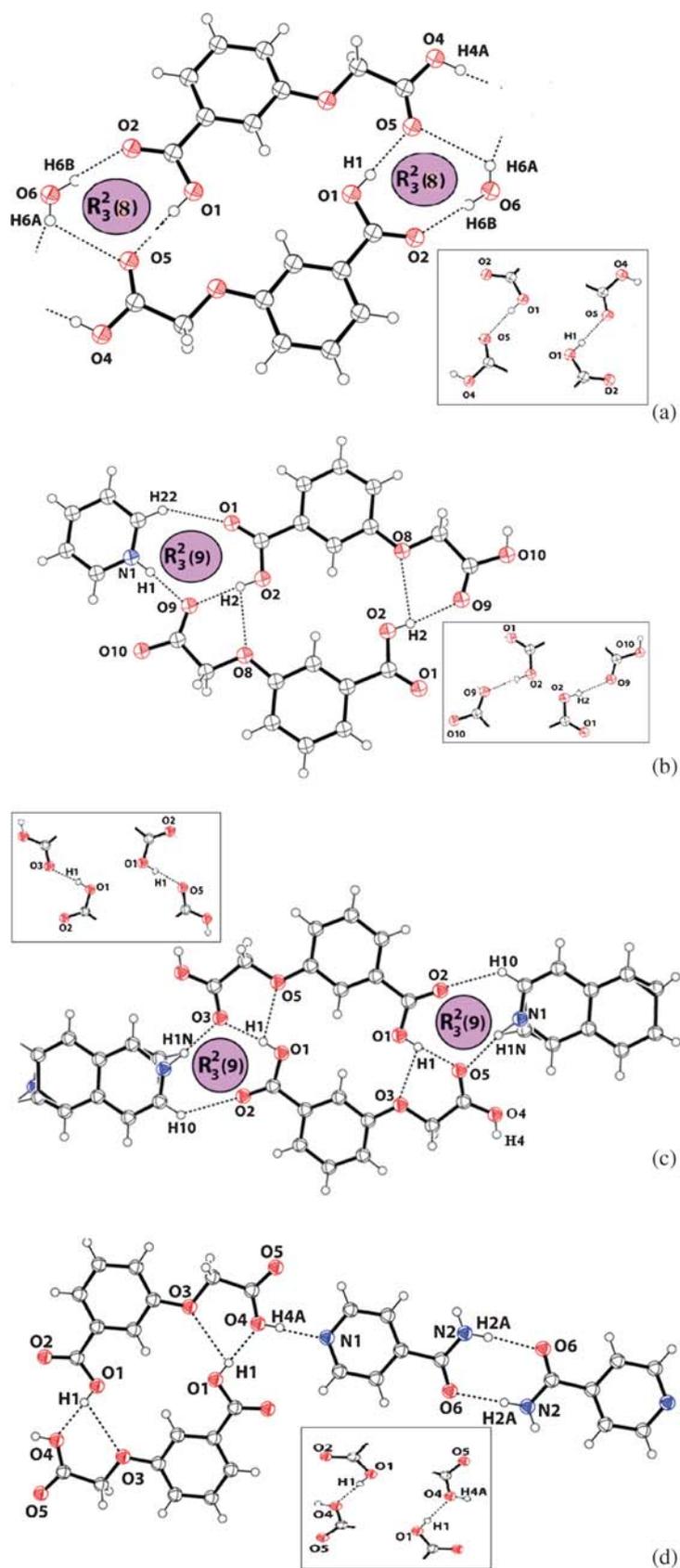


Figure 3. Self-assembly of (a) 3-carboxyphenoxyacetic acid monohydrate (I); (b) Pyridinium salt (II); (c) Cocrystal with isoquinidinium salt (III); (d) Cocrystal with isonicotinamide (IV). Insets are the two catemers of carboxylic acid/ carboxylate motifs.

Table 3. Hydrogen bond parameters of the salt and cocrystals.

Cocrystal/salt	Bond (symmetry)	$d_{DH}(\text{\AA})$	$d_{H...A}(\text{\AA})$	$d_{D...A}(\text{\AA})$	$\angle D-H...A(^{\circ})$
II	N(1)-H(1) \cdots O(9)[2-x,1-y,1-z]	0.86	1.86	2.719(6)	176
	O(2)-H(2) \cdots O(9)[x,y,-1+z]	0.82	1.86	2.673(4)	172
	C(22)-H(22) \cdots O(1)[2-x,1-y,1-z]	0.93	2.45	3.277(7)	148
III	O(1)-H(1) \cdots O(5)[-x,1-y,-z]	0.82	1.88	2.695(2)	174
	N(1)-H(1N) \cdots O(5)[-x,1-y,1-z]	0.99(4)	2.00(4)	2.981(15)	169(4)
	O(4)-H(4) \cdots O(4)[-x,2-y,1-z]	0.85(8)	1.70(8)	2.539(2)	169(8)
	C(10)-H(10) \cdots O(2)[x,y,1+z]	0.97(3)	2.45(3)	3.130(4)	127(2)
IV	O(1)-H(1) \cdots O(3)[-x,2-y,1-z]	0.82	2.55	2.09(3)	108
	O(1)-H(1) \cdots O(4)[-x,2-y,1-z]	0.82	1.85	2.671(3)	178
	N(2)-H(2A) \cdots O(6)[2-x,1-y,1-z]	0.86	2.04	2.892(3)	172
	O(4)-H(4A) \cdots N(1)[x,1+y,1+z]	0.82	1.78	2.599(3)	178
V	O1-H2 \cdots O10[x,-1+y,z]	0.82	1.99	2.802(4)	173
	O4-H4 \cdots N3[1-x,1-y,1-z]	0.82	1.83	2.654(3)	177
	O6-H7 \cdots O5[x,1+y,z]	0.82	1.94	2.755(3)	175
	O9-H9 \cdots O11[x,y,z]	0.82	1.75	2.550(3)	165
	N8-H8AB \cdots O10 [x,y,z]	1.01(4)	2.02(4)	3.007(4)	166(4)

two isonicotinamide molecules. The homodimer of the isonicotinamides comprises of $R_2^2(8)$ motifs^{14,15} having N-H \cdots O interactions as shown in the figure 3(d). Amide molecules generally form self-assemblies by forming homodimers or cocrystals with carboxylic acids by forming heterodimers.⁵⁷ The present example of cocrystal **IV** is an assembly formed by combination of such homodimers and heterodimers. The major difference in the cocrystal of H2pca with isonicotinamide with the cocrystal with isoquinoline arises from the type of donor-acceptors involved in the hydrogen bonds in their constituent dimers between the acid molecules.

Theophylline is generally a good guest molecule to form cocrystals with carboxylic acids through O-H \cdots N interactions.⁵⁸⁻⁶² Different possibilities to form heterodimers and homodimers shown in the figures 4b-e in assemblies of carboxylic acids with theophylline were illustrated by MacGillivray and his coworkers.⁶³ In this study, we find that the compound H2cpa forms easily 1:1 cocrystal (**V**) with theophylline. The crystal structure has shown that the self assembly of the cocrystal is an assembly of assemblies formed by 1:1 cocrystals. Each dimer formed by two H2cpa molecules hydrogen bonds two theophylline molecules at two ends through hydrogen bonds in different manners. The dimers formed by two molecules of H2cpa are identical to the parent compound **I**. They have carbonyl type catemers with AS-A conformations. The different ways of forming hydrogen bonds by two independent theophylline molecules with H2cpa dimer may be attributed to competition between the theophylline molecules

to form homodimer or to remain a single unit by interacting with H2cpa by forming heterodimer. It was earlier suggested that the energy of a motif can be an important factor for observing a particular synthon in a self-assembly.¹³ Accordingly, we have done DFT calculations at b3lyp/6-31++g(d,p) level to find out the difference between the two heterodimers shown in the figures 4e and 4f having $R = H$. It is found that the heterodimer shown in figure 4e is more stable by energy 6.75 kJ/mole. This energy is comparable to very weak hydrogen bond interactions. As a consequence of the small energy difference, a mild acid such as H2cpa compromises to accommodate either form (monomer or dimeric motifs) of theophylline in the lattice. Hence, one side of the dimer of the H2cpa molecule holds a theophylline through a $R_2^2(9)$ type^{14,15} synthon involving O-H \cdots O and N-H \cdots O interactions and remains as a single molecule, whereas the other end has N-H \cdots O as the major interaction to hold a dimer formed between two theophylline molecules. Hence, we find an exceptional example within a two component cocrystal to have two different synthons independently in the same cocrystal.

Theophylline and caffeine are structurally related compounds; cocrystal of 3-carboxyphenoxyacetic acid with theophylline was easily formed but not with caffeine. Attempted crystallization of cocrystals, if any, from the solutions of 3-carboxyphenoxyacetic acid and caffeine from different solvents was not successful, but such solutions yielded the crystals of the parent compounds.

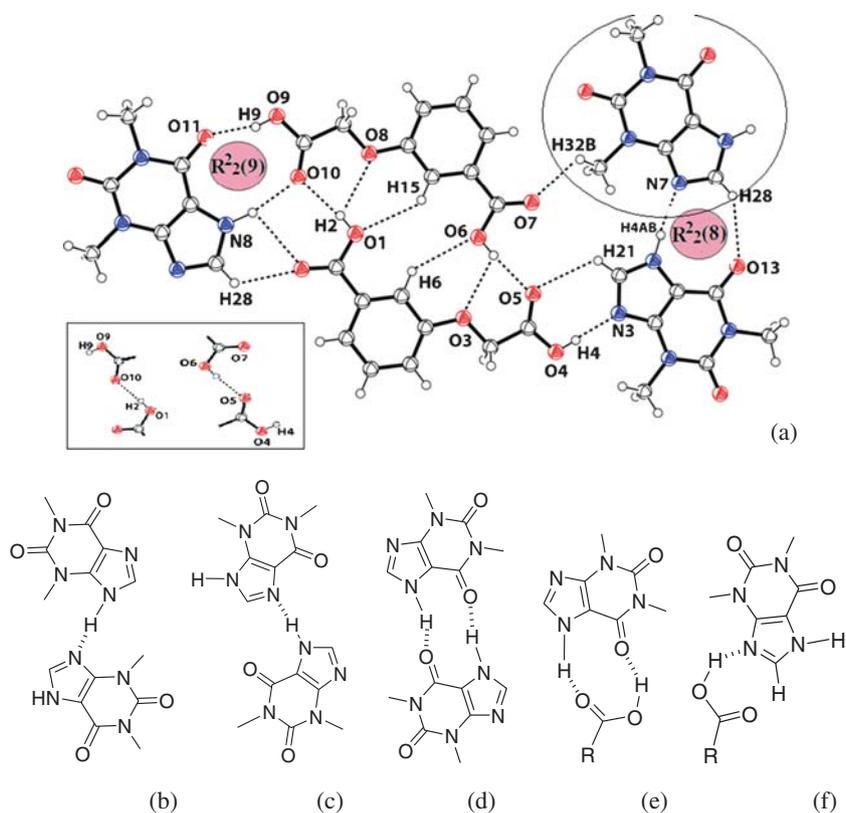


Figure 4. (a) A portion of the self-assembly of the cocrystal **V** formed between **I** with theophylline (the circled portion is from another repeat unit) (b)-(d) Generally formed homodimers of theophylline; (e)-(f) Heterodimers in cocrystals of theophylline with carboxylic acids.

4. Conclusions

In conclusion, homodimers present in the self assembly of H2cpa are adjusted in different ways by nitrogen containing guest molecules. As a result of competition to retain the dimeric self-assembly between a pair of isonicotinamide or H2cpa molecules, and to meet the packing requirements to construct a tight packed structure, slight reorganization of hydrogen bonded motif originally present in the homodimers formed between two H2cpa molecules took place. Hence, unconventional hydroxyl-hydroxyl type hydrogen bonds were observed in the cocrystal of H2cpa with isonicotinamide. On the other hand, two symmetry independent theophylline molecules held across the two ends of a dimeric assembly formed by two H2cpa molecules are attributed to the competition of theophylline molecules to retain cyclic hydrogen bonded homodimers versus formation of cyclic type hydrogen bonded heterodimers between theophylline and carboxylic acid. Thus, this study depicts examples showing the importance of inter-motif interactions beyond synthons in non-covalent synthesis.

Supplementary information (SI)

The crystallographic information files are deposited to Cambridge Crystallographic Database and have the CCDC numbers 1432461, 1432462, 1417584, 1417583 (for **II-V**) respectively. The powder XRD patterns of the salt and cocrystal **II-V** and the packing patterns and spectroscopic details are given in Supplementary Information which is available at www.ias.ac.in/chemsci.

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