Electronic Supplementary Material (ESI) for CrystEngComm

Crystalline adducts of some substituted salicylic acids with 4-aminopyridine, including hydrates and solvates: contact and separated ionic complexes with diverse supramolecular synthons.

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Electronic Supporting Informations

Crystallizations.

Table ESI 1. Summary of the crystallization experiments in different solvents for the various 4-aminopyridinium-n-R salicylate. Conditions yielding single crystals are indicated as √ followed by the suffix anh, hyd or py according to phase obtained (anhydrous, hydrate or pyridine solvate). (●) indicates an unsuccessful experiment.

Derivative	Solvent						
	CH_3OH	CH_3OH/ H_2O	CH_3CH_2OH/ H_2O	CH_3CN	CH_3NO_2	DMSO	Py
5-Cl	√ (anh)	●	√ (hyd)	-	●	-	●
4-Cl	●	-	●	●	-	-	-
5-I	√ (anh)	√ (hyd)	-	-	√ (hyd)	-	√ (py)
5-Br	√ (hyd)	-	-	-	●	-	●
6-F	●	●	-	●	-	-	√ (anh)
5-F	√ (anh)	-	-	√ (anh)	●	-	●
4-F	●	●	●	-	-	-	●
5-NH_2	-	-	-	-	-	●	√ (py)
4-NH_2	-	-	-	-	-	●	●
3-NH_2	-	-	-	-	-	●	●
5-ACM	-	-	-	-	-	-	√ (anh)
4-ACM	-	-	-	-	-	-	●
6-MeO	●	-		●	●	-	●
5-MeO	√ (hyd)	-	●	-	●	●	-
4-MeO	●	-	-	●	-	●	●
3-MeO	●	-	-	-	-	●	●
5-Me	√ (anh)	-	●	√ (anh)	●	-	●
4-Me	●	-	-	-	-	-	●
3-Me	●	-	-	-	-	-	●
5-NO_2	√ (anh)	-	●	-	●	●	●
3-NO_2	●	-	-	-	-	-	√ (anh)

XPac Analysis

Table ESI 2. Supramolecular Construct descriptions. SC = Supramolecular Construct; D = dimensionality; Description, '>' = is related by; # = Number of structures in which construct occurs; Base = base vector of SC (see Table ESI 4); Dependencies show lower dimensionality SCs present in given SC.

SC	D	Description	Figs	#	Base	Dependencies
M0	0	Hydrogen bonded pyridinium-carboxylate	-	10	-	-
D01	0	Dimer of M0 > inversion	5.22	6	-	M0 → D0
M11	0	Stack of M0 > translation	5.14	4	t1	M0→ M11
M12	1	Pair of M11 > 2_1 screw axes	5.16	3	t1	M11 → M12
M13	1	Zig-zag chain of M0 > translation	5.18	4	t2	M0 → M13
S1	1	stacks of single molecules>translation		6	t6	S1 → M11
M2	2	Stacks of M13 > translation	5.21	2	t1, t3	M11·M13 → M2
D2	2	Tape of stacks of D01> translation, 2_1 screw axes	5.24	4	t4, t5	D01→D2
Isostructural		**5-Cl, 5-F; 5-I Hyd, 5-Cl Hyd; SA, 6-F**				

Table ESI 3. Translation vectors with lengths (Å) and angles δ (°).

	t1	**d1**	***t2***	**d2**	***t3***	**d3**	***t4***	**d4**	***t5***	**d5**	***t6***	**d6**	***δ t1, t3***	**δ *t4, t5***
5-Cl			*-1-10*	14.386			*00-1*	12.484	*0-10*	7.963				90
5-F			*110*	13.756			*00-1*	12.150	*0-10*	8.541				90
5-I							*00-1*	12.443	*010*	8.101				90
5-I Py							*00-1*	10.929	*0-10*	8.666				90
5-I Hyd	*-100*	4.400									*-100*	4.400		
5-Cl Hyd	*100*	4.457									*100*	4.457		
5-Br Hyd											*010*	*3.850*		
5-NH_2 Py														
5-ACM	*010*	4.667									*010*	4.667		
5-MeO Hyd	*00-1*	3.992									*00-1*	3.992		
5-Me														
5-NO_2	*-100*	3.778	*-210*	14.691	*1-10*	13.153					*-100*	3.778	106.691	
3-NO_2	*0-10*	4.575	*1-20*	14.288	*-110*	11.889					*0-10*	4.575	112.632	
6-F														
SA														