Electronic Supplementary Material for CrystEngComm

Supplementary Information

1. Molecular geometry

Table S1. XPac comparison of the *molecular* geometries present in forms **I-V** of sulfathiazole at 150 K (see Table 1). An average deviation δ_{mol} (in °) in corresponding internal coordinates (angles) is generated from 16 non-hydrogen positions. The very low deviations occurring in the group of **III-V** (underlined entries), indicate a high degree of similarity.

Form → ↓	Mol. → ↓	**I** 1	**I** 2	**II** 1	**II** 2	**III** 1	**III** 2	**IV**	**V**
I	1		2.0	5.0	3.6	4.6	4.0	4.4	4.2
I	2			5.9	3.9	4.4	3.9	4.1	4.0
II	1				2.9	3.9	3.6	3.7	3.7
II	2					2.2	1.9	2.0	1.9
III	1						*0.9*	*0.5*	*0.6*
III	2							*0.5*	*0.4*
IV									*0.3*
V									

2. Crystal packing

Table S2. The XPac dissimilarity index Δ (°) was computed according to Eq. 4 of ref. 5 on the basis of 16 non-hydrogen positions as corresponding points. Table entries are coloured according to which SC (Fig. 6) they refer to, dimer (Fig. 5), monolayer (Fig. 1a), bilayer A (Fig. 1b) or bilayer B (Fig. 1d). Note that the Z' = 2 form **II** has two independent dimers, while the Z' = 2 polymorph **III** has just one. The monolayer and bilayer SCs of **III-V** exhibit a very high degree of similarity (Δ < 1°) with corresponding low δ_{mol} values between 0.3° and 0.6° (Table S1). Δ results from packing differences in addition to any conformational differences (δ_{mol}).

Using an analogous procedure, the *internal* dissimilarity index Δ_{int} = 1.3° was computed for **III** as a measure of the imperfectness of the non-crystallographic symmetry elements present in the monolayer SC (see Figs. 1a, f). The corresponding δ_{mol} value in Table S1 is 0.9°.

Form → ↓	Mol. ↓	**III**	**IV**	**V**
II	1	4.3	4.5	4.1
II	2	2.6	2.5	2.3
III			0.8	0.8
IV				0.6