Electronic Supplementary Material for CrystEngComm

Competition between hydrogen bonding and arene-perfluoroarene stacking. X-ray diffraction and molecular simulation on 5,6,7,8-tetrafluoro-2-naphthoic acid and 5,6,7,8-tetrafluoro-2-naphthamide crystals.†

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SUPPLEMENTARY MATERIAL

Table S1 Cell parameters as a function of temperature. Å and degree units.

tetrafluoronaphthoic acid, $P2_1/c$ Z=4

T, K	*a*	*b*	*c*	*β*	*V*
93	4.943(2)	5.902(2)	30.706(12)	90.88(2)	895.7(6)
143	4.966(3)	5.903(5)	30.80(2)	91.31(2)	902.4(13)
193	5.002(5)	5.908(6)	30.94(3)	91.75(2)	913.9(16)
243	5.022(4)	5.893(5)	30.98(3)	92.27(2)	916.2(14)
295	5.053(2)	5.884(24)	31.085(12)	92.83(1)	923.1(6)

tetrafluoronaphthamide, P1-, Z=2

T, K	*a*	*b*	*c*	*α*	*β*	*γ*	*V*
93	4.9386(14)	7.250(2)	13.210(4)	97.63(1)	96.44(1)	100.47(1)	456.5(2)
143	4.942(3)	7.278(5)	13.284(9)	97.41(2)	96.66(2)	100.60(2)	460.9(12)
193	4.946(4)	7.295(5)	13.345(9)	97.08(2)	96.90(2)	100.67(2)	464.5(13)
223	4.948(6)	7.3018(8)	13.384(15)	96.90(2)	97.05(2)	100.71(2)	466(2)
295	4.9553(10	7.3353(15)	13.504(3)	96.42(1)	97.36(1)	100.81(1)	473.5(3)

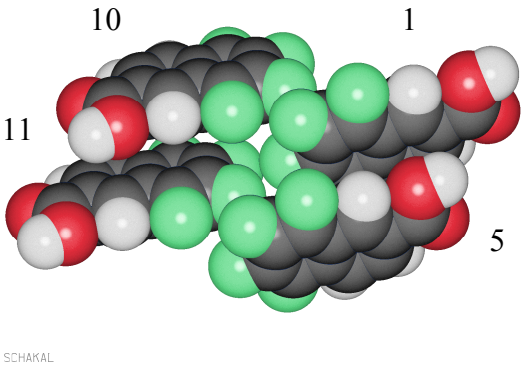

Figure S1 . Tetrafluoronaphthoic acid: the screw-supported molecular engagement at the fluorine segregation region. Shortest F...F distances are 3.4 and 3.7 Å. See the corresponding cohesion energy in Table 1.

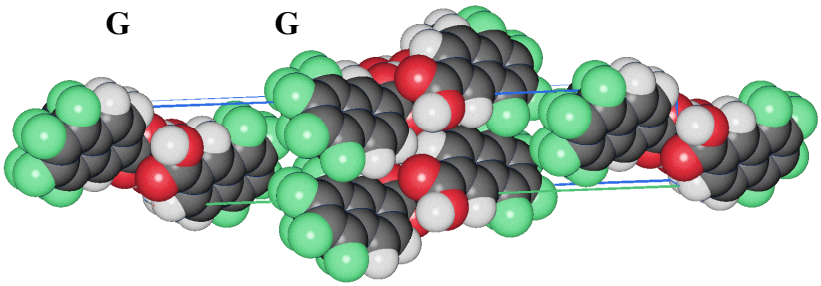

Figure S2. The overall crystal packing of tetrafluoronaphthoic acid. The *c* cell translation is horizontal. The fluorine segregation zones are visible at 1/4 and 3/4 of the cell length. Glide-related molecules (G...G) are second-neighbours too far away to interact significantly.

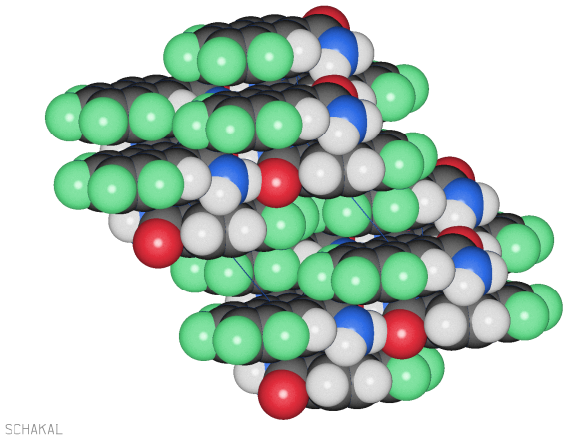

Figure S3. Overall packing view of the.tetrafluoronaphthamide crystal. Cyclic H-bonds are in the layers, interlayer H-bonds are as in Figure 5.