Supplementary Material (ESI) for Chemical Communications

Structural basis for bending of organic crystals

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Table 1. Details of the bending crystals

S.No	Compound Name	Melting Point/ K (±1)	Crystallographic Short Axis	CSD Refcode
1	2-(Methylthio)nicotinic acid	488	3.9834(10)	[a]
2	Pyrazine-2-carboxamide	463	3.750(10)	PYRZIN14
3	Hexachlorobenzene	491	3.8861(1)	HCLBEN11
4	Hexabromobenzene	598	4.007(1)	HBRBEN, HBRBEN01
5	3,4-Dichlorophenol	339	3.859(5)	DCLPHM
6	Venlafaxine hydrochloride	484	5.797(6)	WOBMUV01
7	1,3,5-Trichlorobenzene	336	3.921(1)	TCHLBZ
8	1,3,5-Tribromobenzene	394	4.080(10)	TBRMBZ
9	1,3,5-Trifluoro-2,4,6-triiodobenzene	425	4.7931(20)	CCDC 261303
10	4-Fluorobenzonitrile	308	3.869(1)	PFBZCY
11	4-Chlorobenzonitrile	364	4.038(1)	CLBZNT02
12	6-Chloro-2,4-dinitroaniline	432	3.6646(8)	CCDC 250456
13	1,3-Dinitrobenzene	361	3.677(1)	DNBENZ11
14	2-Nitrobenzaldehyde	316	3.960	NIBZAL
15	3,4,5-Trimethoxybenzaldehyde	346	4.6649(12)	RAJKOC

[a] S. Basavoju, C. M. Reddy and G. R. Desiraju, *Acta Crystallogr., Sect. E: Struct. Rep. Online,* 2005, **61**, o822.