Secondary Interactions in Crystals of all Ten Isomers of Di(bromomethyl)naphthalene

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The packing of all ten isomers of di(bromomethyl)naphthalene is analysed; nine of the structures were determined here, one (the 1,8-isomer) was already known. The 1,5- and 2,6-isomers display crystallographic inversion symmetry and the 2,7-isomer mirror symmetry through the central bond. For the 1,2-, 1,7- and 2,7-isomers, the bromomethyl groups point to the same side of the ring system, and for all other isomers to opposite sides. As expected, the molecules are linked into aggregates by various types of interactions: weak hydrogen bonds CH···Br, Br···Br interactions, CH···π contacts, π···π stacking and Br···π contacts. The weak hydrogen bonds tend to be numerous but relatively long, and do not combine to form readily recognisable patterns; a more readily assimilated view of the packing is based on the Br···Br interactions, which are observed for all isomers except 1,7 and 2,3, and in some cases lead to aggregation to form quadrilaterals or chains. With decreasing frequency, the interactions π···π, C–H···π and Br···π are observed, but the latter are rare (just two examples) and very asymmetric, with contacts to only one or two carbons.

Key words: Di(bromomethyl)naphthalenes, Solid-state Structure, Weak Hydrogen Bonds, Bromine-Bromine Contacts