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Stacking interactions in homomolecular crystals formed by organic compounds containing s-tetrazine moiety

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Abstract

Thirty two crystal structures formed by organic compounds containing *s*-tetrazine moiety are considered. Crystal motifs formed by stacking-interactions and orthogonal contacts of *s*-tetrazine aromatic systems are extracted and quantitatively described. It is observed that an introduction of aromatic substituents in the *s*-tetrazine ring results in stack structure whereas an introduction of aliphatic substituents results in switching stack packing into orthogonal packing.