Structural Variety in Tris(5-acetyl-3-thienyl)methane (TATM) Inclusion Compounds

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Tripodal host molecules form a versatile class of supramolecular materials which include triphenylmethane and analogues such as TATM. TATM host-guest inclusion compounds display a wide variety of stoichiometry and structural motifs and they have demonstrated a propensity for polymorphism. Indeed we have obtained five different forms of the 2:1 host guest compound of TATM / 1,3 dichloropropane. Four of the five polymorphs can be described as polytypes that share both a similar layer motif and a similar conformation of the TATM's thienyl rings. Over the past several years we have examined the structure of more than 20 TATM inclusion compounds. In all but one example the host TATM molecules adopt one of two distinct conformations as first discussed by Herbstein [1]. The TATM frameworks that share a similar conformation may be described as polytypes composed of common layer motifs. Differences in the layer stacking leads to a variety of space groups.

In the TATM frameworks the host molecules interact through π-π and C-H••O interactions to form layers. In all the studies the host and guest interact very weakly through van der Waals forces. The disordered guest molecules are dynamic and located in channels or cages within or between the framework layers. The long-chain guests span more than one layer. Some of the frameworks appear stable upon removal of up to 90% of the guest species.

[1] Herbstein F.H., *Acta Cryst.*, 1997, **B53**, 168.

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