

**W0090**

**Polymorphism in Tris (5-acetyl-3-thienyl) methane (TATM) Inclusion Compounds with 1,3-dichloropropane Guest.** Gary Enright, Paul Sidhu, John Ripmeester, Steacie Institute for Molecular Sciences, National Research Council, Ottawa, Ont., K1A 0R6, Canada.

TATM has been shown to form 2:1 host:guest clathrates with a wide variety of organic compounds. As part of a study of the guest binding strength in these compounds a series of halogenated propane solvents were incorporated as guests. As polymorphism has occasionally been reported in such compounds the single-crystal structure was checked against the powder diffraction pattern of the bulk product prior to thermal analysis. Remarkably for the 1,3 dichloropropane inclusion compound five distinct polymorphs have been encountered and characterized by single-crystal structural analysis. As with all such compounds the guest is disordered with a conformation that is dependent on the inclusion geometry. It appears that minor changes in synthetic procedures can have a profound effect on the structure of the resulting 2:1 inclusion compounds. Three of the five polymorphs could be synthesized with reasonably high purity (as determined by PXRD) and characterized with thermal gravimetric analysis and differential scanning calorimetry (DSC). As would be expected the rate of guest loss upon heating is correlated with the decomposition enthalpy (as determined by DSC). On the other hand the melting temperatures (DSC) showed no such correlation.