

## W0375

**Whole-Molecule Disorder in Adenine Salts and Substituted Adenine Derivatives.** John Desper, Christer Aakeroy, Michelle Smith, Goran Wennerberg, Chemistry, Kansas State Univ., 304 King Hall, Manhattan, KS 66506 USA.

A pair of co-crystals containing adenine or an adenine derivative and a carboxylic acid were analyzed by single-crystal X-ray diffraction. Although both structures contained both expected components, refinement as single ordered species proved unsatisfactory. In both cases, successful refinement was achieved by incorporating two structural models, disordered over a single site, for the adenine fragment. Disorder consists of exchanging the position of the 5-membered (imidazole) and 6-membered (pyrimidine) rings. The combination of both fragments significantly improved refinement, as reflected both in statistical figures of merit and difference density maps.