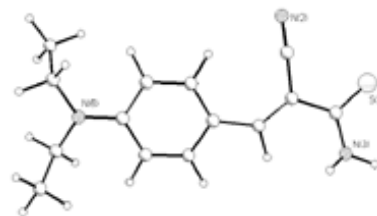


W0238

Theoretical Modeling of Crystal Structures of Three Polymorphs of (2E)-2-cyano-3-[4-(diethylamino)phenyl]prop-2-enethioamide. Tiffany Kinnibrugh, Tatiana Timofeeva, Dept. of Natural Science, New Mexico Highlands Univ., Las Vegas NM, 87701.

X-ray study of (2E)-2-cyano-3-[4-(diethylamino)phenyl]prop-2-enethioamide revealed the formation of three polymorphs that differ by both the space group *P*-1 (**I**), *P*2₁/*n* (**II**) [1], *P*2₁/*n* (**III**) and the molecular structure: orientation of the sulfur atom with respect to the cyano group and the conformation of the N(Et)₂ group (figure below).

Crystalization of one compound, in three polymorphs, with three distinct molecule conformations make this compound a perfect model for testing of predictability of these structures using method of atom-atom potentials. Polymorph Predictor module from Cerius2 program package was used throughout the calculation. After testing of more than twenty different force fields included in the Cerius2 program package, the Dreiding force field was used for these calculations because of better agreement between calculated and experimental data obtained with this force field.



General structure of molecule.

The predicted and experimental crystal structures for polymorph **I** show excellent agreement. For polymorph **II**, slightly worse agreement was obtained while third polymorph (**III**) was not predicted at all. The detailed discussion on the results obtained will be given in our presentation.

Reference 1. Brunskill, J.S.; De, A.; Ewing, D.F.; Welch, A.J. *Acta Cryst.*, **1984**, C40, 493.