505a Crystal Packing Simulations - the Impact of Torsion Angles on Polymorph Formations

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Using the compound, 5-methyl-2-[(2-nitrophenyl)-amino]-3-thiophenecarbonitrile (ROY), that is known to have seven polymorphs, we have developed a computational procedure that relate polymorph existence to the two torsion angles of the molecular structure of ROY. One of the problems associated with current crystal structure predictors is that these predictors generate many possible crystal structures without having clear selection criteria for choosing the most likely crystal structures. Currently, the crystal structures with the lowest total energies or the highest packing densities are chosen as the most likely crystal structures. Total energy and packing density, however, are often not good enough to allow one to either pick out the correct space group for the molecule being simulated or to determine whether polymorphs exist in the same space group. In this presentation, we will discuss computational procedures and selection criteria used to obtain reasonable molecular conformations and space groups for crystal packing simulation. In addition, we will also discuss further refinements of the predicted crystal structures after polymorph prediction.