

## **X-Ray Diffraction and Computational Studies of a Series of Aryl Amides: Comparisons Between Molecular Structure in the Crystal State and in Isolation**

Synthesis of aryl amides by copper-catalyzed amidation of aryl chlorides using a concurrent tandem catalytic methodology has been a focus of our research group. X-Ray structures for a series of aryl amides have been determined at 173 K. R(F) values range from 3.8 – 6.3 %. Torsion angles involving groups attached to the amide linkages were found to vary from a relatively flat 5.3(1) degrees to a considerable twist of 46.2(1) degrees. The wide range of twist angles prompted our investigation into the origins of these observations. The contribution of inherent molecular structure and crystal packing, principally pi stacking in the unit cell, will be discussed. Variable temperature X-Ray studies were performed to examine the correlation between unit cell dimensions and torsion angles. Computational studies with density functional theory (DFT) methods were performed to gain insight about the preferred molecular structures of the amides in isolation. Comparisons between experimental and calculated structures were then used to obtain an estimate of the energies involved in crystal packing.

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