Obtaining Anisotropic Atomic Displacements from NMR Methods

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Crystal structures for certain molecules can now be derived solely from NMR methods. One limitation in all NMR derived structures is the inability to provide errors in atom positions due to thermal disorder (i.e. thermal ellipsoids). In this poster, an NMR approach is presented for estimating errors in COOH hydrogen positions in four polymorphs of palmitic acid. A Monte Carlo sampling procedure is employed to sample positions and feasible candidates are selected based on agreement between experimental and DFT computed ^{13}COOH chemical shift tensors. Overall, two types of structures are found involving localized COOH hydrogens and those having dynamically disordered protons. Uncertainties in hydrogen positions are further evaluated by comparing to single crystal x-ray and neutron diffraction data.