Improved Quantitative Crystal-Structure Comparison Using Powder Diffractograms via Anisotropic Volume Correction

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Crystal structure prediction (CSP) aims to predict the crystal structure(s) of a molecule given only its 2D molecular diagram. While CSP studies remain very expensive computationally, they are becoming an increasingly common accompaniment to experimental development of novel materials and pharmaceuticals. The ability to match putative structures generated via CSP to known experimental structures is critical in both benchmarking new CSP methods, and assessing the polymorphic risk of these new crystalline solids. Two common quantitative methods that assess similarity are measurement of the root-mean-squared-difference (RMSD) in the atomic positions and comparison of simulated powder diffractograms. The generality of powder diffractogram comparison is enticing, but is complicated by the fact that the peak positions shift significantly with small changes in the unit cell lengths, as arise from thermal expansion. Normalization of the unit cell volume is a natural approach to correct for this and powder diffractogram comparisons typically use an isotropic volume correction [1]. However, this approach is less successful for structures that undergo significant anisotropic volume changes with temperature. A new method for powder diffractogram comparison has been developed that features automated unit cell reduction and an anisotropic volume correction. The method has been applied to targets of the 6th CSP blind test to demonstrate its ability to identify the target experimental structure within lists of putative, static-lattice structures submitted by contributors. The importance of using an anisotropic volume correction for the quantitative comparison of crystal structures is demonstrated by comparison with currently available methods, including RMSD measurements.

[1] van der Streek and Motherwell, *Acta. Cryst. B*, **61**, 504-510, (2005)