Exploring possibilities for RMC modelling for single crystal diffuse scattering in molecular materials

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Reverse Monte Carlo (RMC) methods have been previously used to model single crystal diffuse scattering in materials with a limited number of atoms in the unit cell, i.e. less than about 15 (see [1] for a systematic investigation). Due to the complexity and large number of atoms in the unit cell so far RMC methods have not been applied to model diffuse scattering in molecular materials. Treating molecules or molecular components as rigid bodies significantly simplifies the diffuse scattering calculation, as the intensity variations due to molecular form facto effects can be effectively decoupled form the pure disorder diffuse scattering [2]. Constraining the molecules as rigid bodies, we explore the possibility to use RMC to model single crystal diffuse scattering from molecular materials. We compare the calculation times using both FFT based scattering calculations [3] and direct Fourier transform calculations that employ the method of sub-boxes [4].
RMC fits are performed to model simulated single crystal diffuse scattering data from disordered molecular structures obtained via direct MC using DISCUS [4] and results from mean field calculations [5].

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