

## **ESTIMATION OF EXTENT OF DISORDER IN CSD ENTRIES**

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Cambridge Structural Database (CSD) Version 5.28 has 75,459 disordered structures out of 390081. Calculating powder diffraction patterns using these disordered structures is cumbersome as CSD does not store site occupation factors in their atomic coordinate list. It is important to select disordered structures for the calculation based on their impact on the calculated intensity. This poster presents the employed criteria in assessing the extent of disorder while choosing disordered structures for the calculation. Analysis of the extent of the disorder in commercially important compounds will be presented in detail.