MS29-P05 | Comparison of X-ray Wavefunction Refinement and Multipole Refinement Based on the Energetic Analysis of the Crystal Structures of 2-Hydroxo-8-X-Quinoline Derivatives (X = Cl, Br, I, S-Ph)

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This study compares two methods of high-resolution X-ray data refinement – multipole refinement (MM) and X-ray wavefunction refinement (XWR) – applied to data sets collected for crystals of four quinoline derivatives substituted by Cl, Br, I atoms and the -S-Ph group. Problems such as refinement of hydrogen positions (unrestrained vs restrained to average neutron distances) and ADPs (unrestrained vs estimated with SHADE2), anharmonic thermal motion refinement and the influence of rejection of weak reflections for data of varying quality are investigated. Bond lengths and angles are verified against the values obtained in the course of dispersion-corrected periodic DFT geometry optimization. Hydrogen ADPs are compared, based on the similarity index (Spackman), whereas for the anharmonic refinement, the number of non-zero Gram-Charlier coefficients and probability density function are analysed. Another aspect of the presented study are energetic investigations, comprising dimer interactions, cohesive and geometrical relaxation energy. Formation of similar crystal structures of the Cl and Br derivatives is governed by halogen bonds and the N-H…O hydrogen bonds, the latter also present in the -S-Ph derivative. For the crystal lattice of the I compound, in which molecules interacting via halogen bonds are arranged in slabs, interlayer interaction energies were calculated. To extend the analysis of dimer interactions and investigate the contribution of electrostatic and dispersive terms, energy frameworks were generated. The results show superiority of XWR over MM in terms of refinement of hydrogen positions, comparable performance in the energetic aspect and the importance of refinement based on the full set of reflections.