MS29-03 | Structure Specific Restraints for Least-Squares Refinement from Tight Binding Quantum Chemistry

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Disordered crystal structures [1] can cause problems in a statistical post analysis as performed as part of solid-form selection in the pharmaceutical industry [2]. Underlying challenges posed by disorder are inaccurate atomic positions in a crystal structure. Their determination is especially difficult when atoms with disordered split sites are closer to each other than the resolution of a single-crystal diffraction experiment. While non-hydrogen atom positions can usually be resolved, the situation is even more difficult for hydrogen-atom positions due to their scattering power [3], especially when these are rotationally disordered. This asks for a "quantum-chemical aide" [4]. We have therefore extended the functionality of the program Baerlauch [5] to read/write input/output files of the dispersion-corrected tight-binding program XTB [6]. The output of Baerlauch cluster computations then (among other results) provides bond distance and bond angle restraints for use in classical independent-atom model refinements e.g. with SHELXL. Results of this generally applicable workflow to optimize crystal structures (or only their hydrogen atoms) are presented.

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