

Application of a quantum crystallographic protocol to YLID, the world's most common crystal structure

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Streszczenie

2-Dimethylsulfuranylidene-1,3-indanedione (YLID) is the most common crystal structure in the world not because of its chemical or physical properties, but because of its use as a test crystal for commercial diffractometers by nearly all vendors for more than 50 years. We will use it as an example here to showcase how the application of modern quantum-crystallographic refinement techniques and new experiments can unravel a so-far hidden story, which puts the emphasis back on the interesting chemical and physical properties of this crystal structure. We present a new chiral form of orthorhombic YLID (the left-handed *LS* form) and describe the complicated relationship between helical crystal packing and molecular planar chirality. We investigate polymorphs of YLID with twisted and planar molecular configuration as a function of temperature (100 to 292 K) and external pressure (0 to 4 GPa). However, finally only chemical pressure, namely the insertion of water into the crystal structure, can transform the twisted into the planar structure. A combination of quantum crystallography and repeated measurements of the orthorhombic test crystal gives access to an estimate of reproducibility and reliability of refining both anomalous dispersion and Flack parameters. It appears that the chemical environment of covalently bonded atoms has an influence on the anomalous dispersion parameters.

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