Poster

The untold story of the world's most common crystal structure

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The YLID crystal (Fig. 1) has been shipped to users and employed as test crystal for adjusting and calibrating single-crystal X-ray diffractometers by the leading companies since 1969. Therefore, tens of thousands of YLID crystal structures must have been determined under various conditions and setups everywhere around the world over the past half a century. Guzei et al. have analysed lattice constants for a total of 223 measurements, but those were obtained via private communication [1]. In fact, only 8 different structure factors sets are available in the literature. Presently, new quantum crystallographic techniques are mostly validated against data of oxalic acid for which the record number of 14 independent structure factor data sets are publicly available. What if instead of these low numbers we could base method validation on tens of thousands of repeated measurements if all existing YLID structures had been deposited?

We want to motivate that every YLID measurement will be followed by a quick but accurate quantum-crystallographic refinement, and we want to motivate that the results will always be deposited in the Cambridge Structural Database together with the corresponding structure factors in the future as a community effort.

For the reliable and meaningful evaluation of the data quality that an X-ray diffractometer produces in a given setup, only a comparison of intensities (R_{int}/R_{merge}) and a check of the R-value after a routine ShelxL-type refinement (IAM = Independent Atom Model) is not enough [2]. Therefore, here we suggest a quantum crystallographic protocol using Hirshfeld Atom Refinement (HAR) based on room-temperature and low-resolution data sets of the spherical YLID test crystal that is fast and easy to do (Fig. 1). This protocol is, of course, valid in the same way for any other measurement for which the data quality is sufficient. Therefore, as a second example, we will present the case of irbesartan, a medication used to treat high blood pressure, heart failure, and diabetic kidney disease.

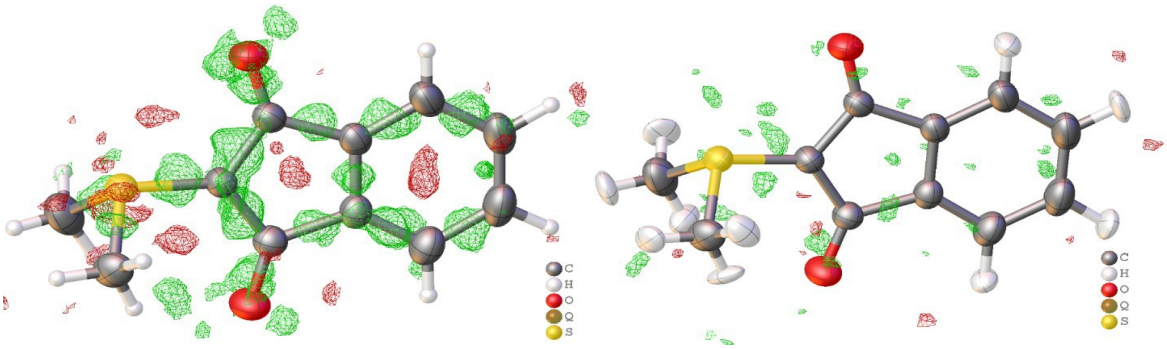

Figure 1. Residual electron density maps of the YLID test crystal after IAM modelling (left, R-value: 2.80%) and after HAR modelling (right, R-value: 1.64%). Hydrogen atom ADPs freely refined during HAR (right).

The yellow YLID test crystal is orthorhombic, and it is chiral as helicity is induced by the crystal packing. All so far published forms are of P(+) helicity, so here we present the first determination of the M(-) form. We measured 25 different YLID data sets under different conditions, so we discuss how HAR improves the precision and reliability of chirality descriptors as well as of the refined anomalous dispersion parameters of the sulfur atom [3]. The helicity of the crystal packing induces a twist in the molecular structure, so we compare the orthorhombic to the monoclinic polymorph which has planar YLID molecules. We further discuss if and how external pressure or chemical pressure can make the molecule planar, starting from the orthorhombic polymorph.

[1] Guzei, I. A., Bikzhanova, G. A., Spencer, L. C., Timofeeva, T. V., Kinnibrugh, T. L., & Campana, C. F. (2008). *Cryst. Growth Des.* **8**, 2411.

[2] Graw, N., Ruth, P. N., Ernemann, T., Herbst-Irmer, R., & Stalke, D. (2023). *J. Appl. Crystallogr.* **56**, 1315.

[3] Meurer, F., Dolomanov, O. V., Hennig, C., Peyerimhoff, N., Kleemiss, F., Puschmann, H. & Bodensteiner, M. (2022). *IUCrJ.* **9**, 604.