# Quantum crystallographic evaluation of the YLID crystal structure; reconsidering data quality

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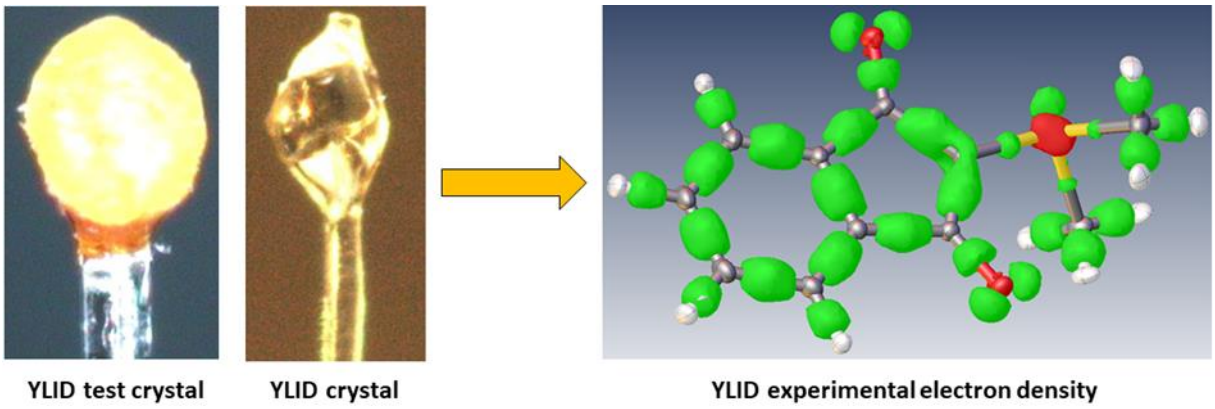
Since 1969, YLID (2-dimethylsufuranylidene-l,3-indanedione) crystals have been routinely used as test crystals for X-ray diffractometers. YLID is stable at room temperature, crystals could easily be ground to spheres, its small unit cell (ca. 1000 Å$^3$), and orthorhombic symmetry are advantageous properties for an off-the-shelf test system. Therefore, the crystal structure has been determined innumerable times.[1] Despite that, no charge density evaluation has been performed for this test system. It is certainly more meaningful if we compare, e.g.,hydrogen anisotropic displacement parameters and the residual density distribution instead of average intensities or internal R-values to evaluate if our diffractometer and experimental setup provide high-quality data.




Quantum crystallographic analysis of YLID test crystal

In this study, the crystal structure of the YLID test crystal for X-ray diffractometers is studied under different conditions. The data for the study were collected using three different wavelengths (Cu=1.54184 Å, Mo=0.71073Å, Ag=0.56087Å) and three different temperatures (272K, 150K, 100K). The YLID experimental electron density was obtained using multipole refinement[2] and X-ray wavefunction refinement[3].

Our results demonstrate that for data quality evaluation of an X-ray diffractometer, quantum crystallographic procedures are most helpful. Also, we analyze the axial chirality of the YLID molecule and the chiral packing in the orthorhombic polymorph of this compound.

[1] Guzei, Ilia A., et al. "Polymorphism and History of 2-Dimethylsufuranylidene-1, 3-indanedione (YLID)." Crystal Growth and Design 8.7 (2008): 2411-2418.

[2] Koritsanszky, Tibor S., and Philip Coppens. "Chemical applications of X-ray charge-density analysis." Chemical Reviews 101.6 (2001): 1583-1628.

[3] Woińska, Magdalena, et al. "Validation of X-ray Wavefunction Refinement." ChemPhysChem 18.23 (2017): 3334-3351.