MS20-04 | Orientional Disorder in Monomethyl-Quinacridone Investigated by Rietveld Refinement, Pair-Distribution Function Analysis and Lattice-Energy Minimisations

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The crystal structure of the poorly crystalline, organic red pigment 2-monomethyl-quinacridone ($C_{21}H_{14}N_2O_2$) was solved from X-ray powder diffraction data. The structure solution led to a crystal structure in *P*-1 with *Z* = 1, with a molecule on the inversion centre. Correspondingly, the molecule, which itself has no inversion symmetry, must be orientionally disordered on two orientations, with a disorder of CH_3 versus H. The disorder and the local structure were investigated using various ordered structural models in *P*1 and *P*-1, *Z* = 1, 2, and 4. All models were analysed by three approaches: Rietveld refinement, fit to the pair-distribution function (PDF), and lattice-energy minimisation.

All Rietveld refinements with *TOPAS V4* [1] converged with acceptable *R*-values. All fits to the PDF using *TOPAS V6* [2] were quite reasonable. The lattice-energies of the optimised structures using the *DREIDING* [3] force field were within a range of 6 kJ mol^{-1}. In all methods there were small, but significant differences between the various structural models. In conclusion, all methods favour a statistical orientational disorder with a preferred antiparallel orientation of molecules in neighbouring chains. [4]

[1] Coelho A. A., TOPAS-*Academic* 4.1, Coelho Software, **2007**, Brisbane.
[2] Coelho A. A. *J. Appl. Cryst.* **2018**, 51, 210-218.
[3] Mayo S. L., Olafson B. D., Goddard III W. A., *J. Phys. Chem.,* **1990**, 94, 8897.
[4] Schlesinger, C., Hammer, S. M., Schmidt, M. U., submitted.