MS34-P2 **Stacking disorder in Pigment Red 170 explained by lattice-energy minimizations** Jaroslav Teteruk[a], Martin U. Schmidt [a], Tatiana Gorelik [b], Anthony Linden [c]
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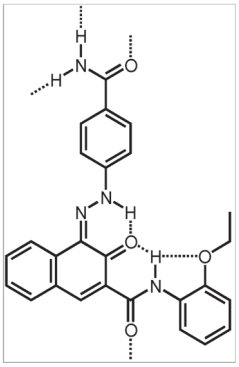
Lattice-energy minimizations were used to explain the stacking disorder in Pigment Red 170. In X-ray and electron diffraction experiments the compound shows strong diffuse scattering in parallel rods perpendicular to the monoclinic axis, pointing to a layer structure with a stacking disorder. Within each layer the molecules form a rigid hydrogen-bridged network. Neighbouring layers are held together by van der Waals interactions. Subsequent layers may be shifted laterally in different directions.



Extensive lattice-energy minimizations were performed on ordered models (including models with new cell metrics and larger supercells [1]) with various stacking sequences derived from a combinatorial approach and from further local symmetry elements. Large supercell models were optimized using customized force-field methods [2] with the Materials Studio software [3]. The lattice-energy minimizations revealed lattice energies, structural correlations and local structure variations. Boltzmann statistics were used to obtain preferred arrangements and sequence probabilities, which provide a much more detailed picture of the structure than the averaged results from the X-ray structure determination. These results were used to set up large structures with 100 layers. The simulated diffraction patterns of such structures were quite similar to the experimental diffraction patterns; the diffuse scattering was too reproduced well. This shows the possibility to calculate and explain organic structures with stacking disorder and diffuse scattering using lattice-energy minimisations.

[1] Schmidt, M.U., Glinnemann, J. (2012). *Z. Krist.,* submitted.
[2] Mayo, S.L., Olafson, B.D., Goddard III, W.A. (1990). *J. Phys. Chem.* **94**, 8897-8909.
[3] Accelrys Software Inc., San Diego (2008). Materials Studio Release Notes, Release 4.4, *Accelrys Software Inc.*, San Diego.

Keywords: disordered molecular crystals, stacking faults, lattice energy calculations

MS34-P3 **The average structure of disordered β-Pigment Red 170** Rangana Warshamanage,[a] Anthony Linden,[a] Hans Beat Bürgi,[a,b] [a]*Institute of Organic Chemistry, University of Zürich (Switzerland).* [b]*Department of Chemistry and Biochemistry, University of Bern (Switzerland)*
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The crystal structure of Pigment Red 170 (PR 170) is important for understanding the photo-assisted fading of its colour [1]. A single crystal X-ray diffraction study of the β-polymorph using synchrotron radiation revealed Bragg reflections superimposed by rods of strong diffuse scattering, which suggests the presence of layer stacking faults of the planar molecule. The analysis of the diffraction patterns led us to choose a non-conventional *B*-centered Bragg lattice in the monoclinic crystal system, which conveniently places the diffuse streaks parallel to the **c*** axis. The average structure was solved and refined in the (non-standard) space group $B2_1/d$ to $R1 \sim 8\%$. The structure consists of stacks of nearly planar molecular layers with (non-crystallographic) symmetry *pgg*. There are two molecules in the asymmetric unit, both of which are disordered with a roughly 90:10 ratio of alternate positions. This model confirms the presence of displacive disorder leading to faulted stacking along **c**. Our intention is to use the diffuse scattering to model the local structure of β-PR 170.

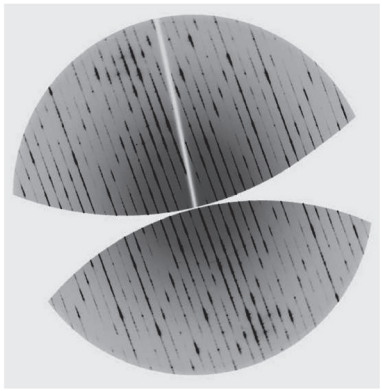

Fig. 1. The *h2l* reciprocal lattice plane from the b- phase of PR 170 collected on the BM01A beamline at the SNBL (ESRF)

[1] M. U. Schmidt, D. W. M. Hofmann, C. Buchsbaum, H. J. Metz, *Angew. Chem. Int. Ed.* **2006**, *45*, 1313-1317.

Keywords: disorder; diffuse_scattering; pigment