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Disorder in mixed crystals of cis/trans-perinone explained by d-DFT calculations.

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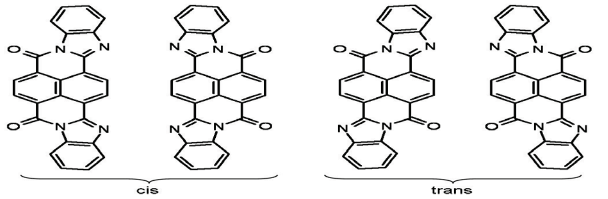
Lattice-energy minimisations using dispersion-corrected density-functional theory (d-DFT) calculations [1] were used to explain the disorder in a mixed crystal, which is formed in the industrial synthesis of perinone, and contains nearly equal amounts of the *cis*-isomer (Pigment Red 194) and the *trans*-isomer (Pigment Orange 43) of perinone. The space group of the mixed crystal is $P2_1/c$, $Z = 2$. The molecules are situated on crystallographic inversion centres. Each *cis*- or *trans*-molecule can be situated in two different orientations, leading to a fourfold disorder.



In the single-crystal X-ray structure determination, the central part of the molecule is ordered, but the terminal groups are found in at least 3 different positions.

Extensive lattice-energy minimisations were performed on various ordered models (including models with much larger supercells) using the program *GRACE* [2], which uses *VASP* [3-5] for single-point DFT calculations. The lattice-energy minimisations reveal local structures and lattice energies, from which the preferred arrangements and the neighbourhood probabilities for all neighbouring molecules were derived, as well as spatial structural correlations. The results provide a much more detailed picture of the structure than the averaged results from the X-ray structure determination.

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Organic thin film layer investigation with pair distribution function technique.

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Organic semiconducting materials allow new optoelectronic devices which combine the excellent optical properties of organic dyes with semiconductor behavior. Organic Light Emitting Diodes (OLED) and Organic Solar Cells (OSC) are successful examples in this field [1, 2]. Organic devices contain several layers with different molecules and often show an amorphous morphology, especially in the case of mixed layers (more than one type of molecule per layer). The electro-optical properties of such a device depend dramatically on the morphology at a sub-nm scale. Molecules show a strongly anisotropic behavior in the transport and in the optical properties [3]. A way to get information about the short range order of such an amorphous system is the pair distribution function (PDF) technique received from X-ray diffraction (XRD) measurements. We produced Buckminsterfullerene C60 and oligothiophene thin film samples via vacuum deposition on glass substrates and measured the diffraction pattern under grazing incidence condition. After removing the contribution of the substrate in the diffraction pattern, the PDF of the organic layer can be calculated and being compared to powder measurements. Comparison to partial crystalline thin film samples shows good results for estimated molecule distances with the PDF. C60 thin film deposited on a glass-substrate at room temperature contains a large amount of amorphous C60. The mean distance between two C60 molecules in a 50 nm thin film is 10.19 Å in contrast to 10.04 Å in a powder sample. Surprisingly, the orientation between the C60 molecules in the powder shows a higher degree of disorder in comparison to the C60 molecules in the thin film. Oligothiophene thin film samples show a stronger tendency to crystallization with preferred orientation, also at room temperature.

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