Modulation and structural disorder in the solid phase of the 4,4'-azoxydiphenetole

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Weak hydrogen bonds are known to have repulsive and destabilizing character implying that, for short distances, they can transit into the positive energy region because the energy bond itself is of this order. They are electrostatic but this characteristic can be modified by variable dispersive and charge-transfer components that depend substantially on the nature of the donor and acceptor group [1]. A great variety of these bonds are found in the solid state but very few structural experimental studies highlighting the strength and the packing role of these interactions have been reported so far. When crystallized below 356 K, the molecular compound 4,4'-azoxydiphenetole shows a stable disordered modulated phase [2,3]. This phase is characterized by the presence of satellite reflections and diffuse scattering rods in the reciprocal space. Structural refinements indicate a high correlation between the shifts of the molecules (modulation) and the probability of finding them in different configurations (disorder). The interplay between disorder and modulation can be explained by a local competition between destabilizing and/or repulsive $CH_3...O$, $C_{ar}H...\pi$ and $CH_3...\pi$ weak hydrogen bonds constrained by the strong $C_{ar}H...O$ bonds connecting the 4,4'-Azoxydiphenetole molecules in the same layer.

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