On the (Non)-Planarity of 1,2,4,5-Tetramethoxybenzene

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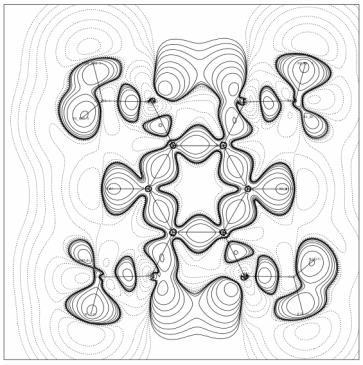
The conformation of methoxy groups on phenyl rings is a long-standing problem that has been tackled in the past with a variety of structure determination techniques and at different levels of quantum chemical calculations.

1,2,4,5-tetramethoxybenzene has two sets of *ortho*-dimethoxy moieties and displays a nearly planar structure in the crystal. We obtained a high quality data set at 150 K which was suitable for multipole refinement. The charge density maps and electronic properties in the bond critical points are compared with values from high-level quantum chemical calculations. The latter reveal a large number of energy minima on the potential energy surface.



The reason for the planarity of the molecule is not evident from the experimental structure, but the calculated bond orders in the molecule indicate that the stabilizing factor off-setting the repulsion between the free electron pairs of oxygen is the participation of the latter in the π-electron system of the ring.

Keywords: ab initio calculations, charge density, conformational studies