

Modelling Disorder in 3,3'-dimethoxybenzil, C₁₆H₁₄O₄

T.R. Welberry, D.J. Goossens, A.P. Heerdegen, *Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia*. E-mail: welberry@rsc.anu.edu.au

This work is part of an extended study of benzil (C₁₄H₁₀O₂) and derivatives which aims to understand the role that molecular flexibility plays in determining crystal packing and polymorphism [1,2]. In this study diffuse X-ray scattering is used to probe both the inter- and intra-molecular correlated motions of a series of similar compounds in order to gain insight into how molecular motion influences crystal packing. In future studies it is hoped to apply the methodology to compounds of pharmaceutical interest which display polymorphism. In the present paper we present results for the compound 3,3'-dimethoxybenzil, C₁₆H₁₄O₄, 33'DMOB. For this molecule the molecular flexibility is afforded by rotations about three C–C and two C–O single bonds, defined by the dihedral angles, ϕ_1 – ϕ_5 . Other molecular groups are considered rigid. Diffuse scattering arises from differences between the local structure of a crystal and the underlying *average* structure. Such differences (termed disorder) may be either static or dynamic in origin. The disorder in 33'DMOB is purely thermal, and conventional crystal structure determination using Bragg scattering yields a perfectly normal average structure with no anomalous atomic displacement patterns. Nevertheless all studies have observed strong and highly structured thermal diffuse scattering.

[1] Welberry T. R., Goossens D. J., Edwards A. J., David W. I. F., *Acta Cryst.*, 2001, **A57**, 101–109. [2] Welberry T. R., Heerdegen A. P., *Acta Cryst.*, 2003, **B59**, 760–769.

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