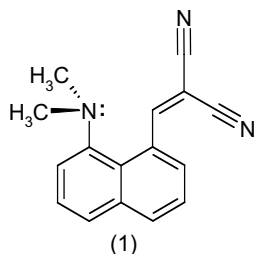


W0219

**Multipole Refinement of High-Resolution X-Ray Diffraction Data: Characterizing a Weak Through-Space Interaction in a *Peri*-Substituted Naphthalene.** C. S. Frampton, L. Straver, Bruker Nonius B.V., Oostsingel 209, 2600AV Delft, The Netherlands; J.D. Wallis, Dept. of Chemistry & Physics, Nottingham Trent Univ., Clifton Lane, Nottingham, NG11 8NS, U.K.; S. Coles, School of Chemistry, Univ. of Southampton, Highfield, Southampton, SO17 8BJ, U.K.

Multipole refinement of high-resolution X-ray diffraction data is an important and powerful methodology that is frequently employed to characterize the experimental charge density distribution in molecular crystals.

The results from a multipole refinement of high resolution, (0.44Å), X-ray diffraction data for 2-(8-Dimethylamino-naphthalen-1-ylmethylene)-malonitrile, (1), at 100 K are presented. This study was undertaken to explore further the nature and topology of the electronic charge distribution of this strained system, [1,2]. From three-dimensional maps of the Laplacian, ( $\nabla^2\rho$ ), a clear directional preference for the Me<sub>2</sub>N: lone pair of electrons can be seen and this is supported also by the observation of a large hole in the valence shell of the C(sp<sup>2</sup>) of the malonitrile which is itself directed towards the lone pair.



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