Determination of 'Experimental' Wavefunctions from X-ray Diffraction Data

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Wavefunction fitting experiments aim to build an 'experimental' wavefunction by combining traditional quantum mechanical calculations with experimental measurements according to some well defined procedure. One such approach developed by Jayatilaka [1] and implemented in the program Tonto, attempts to minimise a function based on the sum of the quantum mechanical energy and a weighted chi-squared function, in order to determine the wavefunction.

Using Tonto, experimental wavefunctions and related properties have been determined for a series of organic NLO materials [2] using high resolution X-ray diffraction data. The results of which have been compared with those derived from Charge Density analyses of high resolution, low temperature X-ray data collected at Durham University.

[1] Jayatilaka D., Grimwood D.J., *Acta Cryst.*, 2001, **A57**, 76. [2] Cole J.M., Howard J.A.K.H, McIntyre G.J., Copley R.C.B., Goeta A.E., Szablewski M., Cross G.H., *Acta Cryst.*, 1996, **A52**, C-349.

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