

approaching the true values are derived and numerical examples are given.

[1] Haight, F. A., "Handbook of the Poisson Distribution", John Wiley & Sons, Inc., New York, 1967.

Keywords: Poisson distribution, significance, low intensity observation

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Remarks on an erroneous omission of an ellipse in the gap of the hyperbola in the dispersion curves.

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Based upon the Laue method, the biquadratic secular equation as the dispersion relation in X-ray diffraction is

$$|S_{ij}| = \begin{vmatrix} k^2 - \bar{k}_0^2 & K^2 C \chi_{-g} \\ K^2 C \chi_g & k^2 - \bar{k}_g^2 \end{vmatrix} \\ = k^4 - (\bar{k}_0^2 - \bar{k}_g^2) k^2 + \bar{k}_0^2 \cdot \bar{k}_g^2 - K^4 C^2 \chi_g^2 = 0, \quad (1)$$

where $|\chi_{-g}| = |\chi_g|$, $\bar{k}_g = \bar{k}_0 + \vec{g}$ (\vec{g} is the reciprocal lattice vector) and others are in general usage. The diagonal terms of S_{11} and S_{22} in eq. (1) represent the same two circles intersected at two points and the dispersion relations from eq. (1) near Brillouin zone boundary should be carefully examined. The roots of k^2 in eq. (1) could be given by

$$k^2 = \frac{1}{2} \left\{ (\bar{k}_0^2 + \bar{k}_g^2) \pm \sqrt{(\bar{k}_0^2 - \bar{k}_g^2)^2 + 4 |K^4 C^2 \chi_g^2|} \right\}. \quad (2)$$

In case of $|\bar{k}_0^2| \cong |\bar{k}_g^2|$, eq. (2) could be expanded as

$$= \frac{1}{2} (\bar{k}_0^2 + \bar{k}_g^2) \pm |K^2 C \chi_g| \pm \frac{1}{8 |K^2 C \chi_g|} (\bar{k}_0^2 - \bar{k}_g^2)^2 \pm \dots \quad (3)$$

After mild calculation, the 2nd and 3rd terms in eq. (3) show hyperbola and ellipse in form like

$$y^2 = b^2 \pm (bx/a)^2 \quad (4)$$

as dispersion curves and the parameter $2b$ in eq. (4) is simultaneously not only the transverse axis of hyperbola but also the diameter of ellipse. Therefore, the Bragg gap could not exist. By roughly approximating S_{11} and S_{22} at $k^2 - \bar{k}_0^2 \cong 2\bar{k}_0 \cdot \Delta k \cong 2K \cdot \xi_0$ and $k^2 - \bar{k}_g^2 \cong 2\bar{k}_g \cdot \Delta k \cong 2K \cdot \xi_g$, since eq. (1) could be shared half and half by the central surfaces of the second order in eq. (4) and one half of a pair, i. e., ellipse has been eliminated by rough approximation, consequently another half of hyperbola of the popular dispersion curve could be given by

$$|S_{ij}| = \begin{vmatrix} 2\xi_0 & KC\chi_{-g} \\ KC\chi_g & 2\xi_g \end{vmatrix} = 4\xi_0\xi_g - K^2 C^2 \chi_g^2 = 0, \quad (5)$$

which could be defined by that products of the perpendiculars from an arbitrary point on hyperbola to its two asymptotes is a constant. The rough approximation that makes biquadratic eq. (1) a quadratic eq. (5) could not be accepted with no proofs and remarks. Further, all of drawings in eq. (5) in almost all

references have been shown by a simple coordinate mix-up. It is something very strange from mindlessness.

Keywords: dynamical theory of X-ray diffraction, Laue method, dispersion.

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Experimental charge density studies, electrostatic and topological analysis of 1-(2'-Aminophenyl)-2-methyl-4-nitro-1H-imidazole crystals. Agneszka Paul^{a,b}, Maciej Kubicki^a, Claude Lecomte^b, Christian Jelsch^b. ^aAdam Mickiewicz University in Poznań, Poland. ^bNancy University, CNRS, France.

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High resolution diffraction data of crystals of small organic molecules, such as 4-nitro-1H-imidazole derivatives, are achievable within a period of days, thanks to the development of the measurement devices.

Processing these data in the standard manner to solve and refine the structures and to obtain the information about the geometry and interactions is usually performed applying the Independent Atom Model (IAM). Within this approximation all atoms are treated as 'spherical balls' with the electron density concentrated around the nuclei. However, this assumption neglects transfer of the charge density into the bonding regions – especially for the covalent bonds – and the transfer associated with the intermolecular interactions.

To improve the electron density distribution model and to allow for the detailed analysis of the intra- and interactions in the molecules and in the supramolecular assemblies, such as the 1-(2'-Aminophenyl)-2-methyl-4-nitro-1H-imidazole, the Hansen-Coppens formalism [1] and Atoms-in-Molecule approach [2] for topological analysis are used. The multipole model has been implemented in the MoPro program suite [3] and allows electrostatic and topological calculations for both small molecules and biological macromolecules at subatomic resolution.

Within this poster the experimental charge density distribution of the title compound will be presented. The crystal structure of this 4-nitroimidazole derivative was published recently, using standard resolution data [4], however no detailed analysis of the influence of the substituents on the electron distribution was performed. The main observed interactions are the strong and weak hydrogen bonds (N-H...N, N-H...O and C-H...O, C-H...Cg (centroid of the aromatic ring), respectively). These regions, with a special attention paid to the nitro group (as hydrogen bond acceptor), will be analysed. This is a part of our project to investigate the weak interactions in the series of 4-nitro-1H-imidazole derivatives, to examine the influence of the different substituent groups on the charge density distribution within the aromatic ring.

[1] Coppens P., Koritsanszky T.S., Chem. Rev. (2001). 101, 1583-1627. [2] Bader R.F.W. (1990). Atoms in Molecules: A Quantum Theory. Oxford University Press. [3] Jelsch, C., Guillot B., Lagoutte, A. & Lecomte C.J. Applied Crystallography (2005). 38. 38-54. Advances in protein and small-molecules charge-density refinement methods using MoPro. [4] Kubicki M., Wagner P., Acta Cryst. (2007). C63, o454-o457.

Keywords: 4-nitro-1H-imidazole derivatives, multipole refinement, high resolution diffraction