

at 200K (Cubic, $P2_13$) and at 100K (Orthorhombic, $P2_12_12_1$) respectively were collected and analyzed by using XD2006 package (4). The topological analysis and calculation of relevant properties bring out the salient features which allow for a clear distinction in bond paths, Laplacian maps and electrostatic potential isosurfaces in both metal coordination and sulfate tetrahedra across the phase transition.

References:

- (1) Zemann, A. and Zemann, J.; 1957, *Acta Cryst.* **10**, 409.
- (2) Dvorak, V.; 1972, *Phys Status Solidi* **B52**, 93.
- (3) Yamada, N.; *et al.* 1981 *J. Phys. Soc. Jpn.* **50**, 907.
- (4) XD2006 - A computer program for multipole refinement, topological analysis of charge densities and evaluation of intermolecular interaction energies from experimental or theoretical structure factors. Volkov, A. *et al.* 2006.

Keywords: charge density, mineral structures, sulfates

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Tartaric acid gyration tensor components from charge density distribution

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L-tartaric, (+)-(2R,3R)-2,3-dihydroxybutanedioic, acid crystallizes in non-centrosymmetric space group $P2_1$. Experimentally determined principal components of the gyration tensor [1] and the optical rotation calculated from the structural data using Pauling's atom volume polarizabilities [2] differed significantly. Since the contribution of the molecule itself to optical activity of the crystal was estimated as relatively small, the predominating intermolecular effects were expected to be responsible for the high gyration tensor components. To get necessary information, charge density analysis was performed [3] using the program package XD [4] and low-temperature (80 K) X-ray diffraction data. The results of the topological analysis of $\rho(r)$ at the bond critical points gave a quantitative description of the hydrogen bonds whereas the properties of charge density distribution enabled the derivation of atom volume polarizabilities [5,6] which in turn were utilized for the determination of gyration tensor components. This work is partially supported by the Polish Ministry of Education and Science (grant No. N204 124 32/3169).

[1] Mucha D., Stadnicka K., Kaminsky W., Glazer A.M., *J. Phys.: Condens. Matter*, 1997, 9, 10829.

[2] Mucha D., Stadnicka K., Glazer A.M., Devarajan V., 1996 *J. Appl. Crystallogr.*, 29 304.

[3] Pitak M., PhD Thesis, 2006, Jagiellonian University.

[4] Koritsanszky T., Howard S.T., Macchi P., Gatti C., Farrugia L.J., Mallinson P.R., Volkov A., Su Z., Richter T., Hansen N.K., *XD - A Computer Program Package for Multipole Refinement and Topological Analysis of Charge Densities from Diffraction Data*, 2003.

[5] Coppens P. *X-ray Charge Densities and Chemical Bonding* 1997, IUCr Oxford University Press,

[6] Matsuzawa N., Dixon D.A., *J. Phys. Chem.*, 1994, 98, 2545.

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Chemical bonding in energetic RDX: An experimental and theoretical study

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Accurate X-ray diffraction data at 20K and 120K were obtained for the alpha-form of the 1,3,5-trinitrohexahydro-1,3,5-triazine (RDX) crystal using a Rigaku R-Axis Rapid high-power rotating anode diffractometer with a curved image plate detector. Data were integrated with the program VIIPP [1] using the predicted reflection positions from the program HKL2000 [2], scaled and averaged with SORTAV [3], and the multipole refinements performed with the XD program package [4]. The experimental electron density (ED) obtained at two temperatures has been analyzed in terms of the Quantum Theory of Atoms in Molecules, and compared with the ED calculated theoretically. Features of the intra- and inter-molecular bond critical points and the oxygen atom lone-pair locations are discussed. Hydrogen bonding, O · · · O, O · · · N and N · · · N intermolecular interactions are reported. Atomic charges, features of the electrostatic potential and the molecular dipole moment are discussed.

1. Zhurov, V. V. *et al.* (2005) *J. Appl. Cryst.*, 38, 827; Zhurova, E.A. *et al.* (1999) *Acta Cryst.* B55, 917.

2. Otwinowski, Z.; Minor, W. (1997) *Methods Enzymol.*, 276A, 307.

3. Blessing, R. H. (1987) *Cryst. Rev.*, 1, 3.

4. Koritsanszky, T. *et al.* (2003) *XD - A Computer Program Package for Multipole Refinement and Analysis of Electron Densities from Diffraction Data*; Tech. Rep.; Freie Universität Berlin: Berlin, Germany.

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Application of the aspherical scattering formalism on the refinement of macromolecules

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The conventional modelling of an X-ray diffraction experiment makes use of the "Independent Atom Model (IAM)", which ignores a priori electron density asphericities caused by the interaction of atoms. The Hansen&Coppens multipole model allows for a non-spherical atomic description but may require more than 40 parameters per atom and therefore needs high resolution diffraction data ($d < 0.5 \text{ \AA}$), which is mostly far beyond the scattering power of macromolecules. The recently introduced invariom model overcomes this limitation by assignment of individual aspherical scattering factors (multipoles) to each chemically unique atom in a structure. This permits to refine only atomic positional and vibrational parameters and thus to use data sets of medium resolution ($d < 0.9 \text{ \AA}$). The invariom library covers all bonding situations in polypeptides. Numerous tests on small molecules showed that this approach improves the accuracy of the molecular geometry, yields a better description of the displacement parameters and more accurate Flack parameters even in the case of limited resolution. But so far