

inhibitors with the main protease of the SARS coronavirus; and the progesterone receptor complex.

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Experimental and Theoretical Charge Densities in two polymorphic systems. Anna A. Hoser^a, Łukasz Dobrzycki^a, Matthias J. Guttman^b, Krzysztof Woźniak^a.
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Polymorphism is a very important phenomenon in crystallography, especially in designing new materials, and in pharmacy. In this study, we would like to verify if experimental or theoretical charge density studies may be helpful in analysis of small differences between polymorphs. For two different polymorphic forms of the hydrated and protonated N,N,N,N-tetra-(dimethylamino)naphthalene chloride, DMANH⁺x2Cl⁻xH₂O₂⁺ (triclinic P-1, and monoclinic P2₁/n) [1], and two different polymorphs of benzidine dihydrochloride (triclinic P-1, and orthorhombic Pbcn) [2] both experimental electron density distributions from the high resolution X-ray diffraction measurements and from theoretical calculations had been obtained and then analyzed. The differences between the charge density distributions in both polymorphs of both systems are surprisingly small. They are observed mainly as differing shape of the interaction paths between hydrogen atoms and the chloride anions. These deviations are generated by small differences in intermolecular interactions resulting from slightly different symmetry of the both systems.

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X-ray charge density analysis of vanadium diboride: A comparison of experiment and theory. Bürgehan Terlan, Horst Borrmann, Alexey Baranov, Carina Börrnert, Frank R. Wagner, Yuri Grin. *Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany.*

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The nature of the chemical bonding in intermetallic compounds is one of the open questions in inorganic chemistry. Experimental investigations of the electron density derived from diffraction data are very rare for intermetallic compounds. One of the main reasons is that the suitability of such compounds for charge density analysis is estimated to be relatively low as compared to organic compounds. The

electron density of VB₂ was reconstructed from room temperature high resolution single-crystal x-ray diffraction data using the multipole model by Hansen and Coppens [1]. The topological aspects of the electron density were analysed on base of the multipole parameters using Bader's Quantum Theory, *Atoms in Molecules* [2]. Comparison of the electron density both from experiment and theory reveals that topological features agree very well even at a quantitative level. The same number and type of critical points (CPs) are obtained, but only minor quantitative differences in the Laplacian of the electron density are observed. Successful reconstruction of the electron density from diffraction data for VB₂ provides new information for the understanding of chemical bonding in this compound.

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