ionic crystals, the cluster method meets serious problems: What is the potential? How to account for periodicity?

The present calculations were performed using Bloch functions to account for periodicity and a potential calculated with the Ewald method (program ADF-BAND (te Velde et al, 1990)). Dynamic structure factors were calculated and compared with multipole refined low-temperature data (van Beek et al, 1996). The difference amounted to R(F)=1.6%.

Realizing that multipole refinement not only reduces noise, but also introduces bias, the theoretical data were refined with the same POP-multipole program. This reduced the difference with experiment to R(F)=0.8%, the remainder for the greater part due to the NH_4 group (R(F)=1.1%) and to a lesser part to the fluorine. Electron density maps corresponding with the various differences will be shown.

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PS09.02.16 TOPOLOGICAL PROPERTIES OF ELECTRON DENSITY OF PENTAFLUOROSULFANYL DERIVATIVES. G. J. Perpetuo, T. Koritsanszky, D. Preugschat, D. Lentz and P. Luger, Institute for Crystallography and Institute for Inorganic Chemistry Free University of Berlin, Germany

Topological analyses of experimental and theoretical electron densities and Laplacian functions of the title compounds (SF_5X, X = NC, NCO and CN) are presented. The parameters of a static density model based on the multipole formalism /1,2/ has been extracted from high-resolution X-ray diffraction data collected at 120 K. Ab-initio calculations /3/ have also been performed at the Hartree-Fock and MP2 level of theory utilizing 6-311G+(3df) and 6-311G* basis sets, respectively. Geometry optimizations were also carried out. In the case of SF_5NCO the asymmetric unit consists of two conformers; the isocyanate being in eclipsed and straggered position with respect to the equatorial SF_4 moiety. Calculations at the MP2 level show the latter to correspond to a transitional state. The experimental bond-topological properties /4/ (the electron density and its Laplacian at the bond critical points) occur to be overestimated compared to those calculated from wavefunctions. The application of high basis sets including polarization and diffuse functions is proved to be important. The degree of the covalent character of the S-F bonds in the different molecules is compared.

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PS09.02.17 THEORETICAL AND EXPERIMENTAL ELECTRON DENSITY ANALYSES OF DIHYDROXY BENZOPHENONE. F. K. Ross, Z. Hu, and R. Glaser, Research Reactor Center and Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211, USA

Detailed electron density distributions for dihydroxybenzophenone (DHBP, $C_{13}H_{10}O$) have been obtained from X-ray+Neutron (X+N) diffraction analysis and by ab initio molecular orbital calculations(1) for a closely analogous structure. Various mechanisms for accounting for H atom bond polarization in the X+N model are tested and compared with results from theory. Anharmonic thermal motion appears to be a significant effect and must be adequately modeled before good agreement of the two methods is achieved. Comparisons of charge density distributions, orbital population parameters, potential maps and critical points will be discussed.

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PS09.02.18 THE CRYSTAL STRUCTURE OF PALLADIUM DIPHENYLGLYOXIME; AN ANALYSIS OF STRONG HYDROGEN BONDS IN PALLADIUM-DIGLYOXIME COMPOUNDS. Ronald F. See, Christopher Curtis and William M. Strub, Department of Chemistry, Saint Louis University, St. Louis, MO 63103, Joseph W. Ziller, Department of Chemistry, University of California at Irvine, Irvine CA 92717

When the 2+ ions of group 10 metals, such as palladium, react with bidentate glyoxime-type ligands, the result is a four-coordinate, square-planar compound where the glyoxime moieties are linked by intramolecular strong hydrogen bonds of the O··H··O type. The nature of these strong hydrogen bonds has long been of interest, in as much as they offer a serious challenge to theories of chemical bonding. Palladium(II)-diglyoxime complexes provide an excellent opportunity to compare strong hydrogen bonds, as changes in the hydrogen bonds can be measured against the electronic effects of the substituent groups on the glyoxime backbone. The structure of the title compound, $Pd(dpgH)_2$ (dpg = diphenylglyoxime), was refined to R = 4.46% for 4σ data and 7.90% for all data. The distance between the oxygen atoms involved in the intramolecular hydrogen bond is 2.550(10) Å. There is strong evidence that the hydrogen atom involved in this hydrogen bond is in a nearly-centered (though asymmetric) position. This structure can be compared with those previously reported structures of palladium-diglyoxime compounds, which have the substituents -H, $-NH_2$, $-CH_3$ and α-furyl. Use of the Hammett parameters allows one to quantify the electronic effects of the substituent groups, and thus to investigate the response of the intramolecular hydrogen bond to changing electronic environments. These results indicate that electron-withdrawing groups tend to strengthen the hydrogen bond; it may be possible to explain this observation with reference to bond valence theory.

PS09.02.19 CHARGE DENSITY DISTRIBUTION IN $AgGaS_2$. Roland Spengler, Andreas Bram, Hans Burzlaff, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Universität Erlangen-Nürnberg, Bismarckstraße 10, 91054 Erlangen, Germany, Volker Krämer, Kristallographisches Institut, Universität Freiburg, Hebelstr. 25, 79104 Freiburg/Br., Germany.

$AgGaS_2$ is one of the most interesting materials for applications as photovoltaic semiconductor in sandwich photo cells because of its large band gap. Jaffe & Zunger [1,2] explained the energy gap by a strong contribution from the d-orbitals of the Ag-atoms following their pseudo-potential calculations.

Experimental measurements at 293K, 105K and 25K on a self-constructed 4-circle diffractometer using HUBER mechanics, an APD-cryostate and self-developed interfaces and software [3] show an increasing order of the non-spheric charge density at Ag and Ga with decreasing temperature [4]. It was posible to obtain information about the occupancy of the d_{z^2}, $d_{x^2-y^2}$, d_{xy}, $d_{xz,yz}$-orbitals.

These observations are in agreement with charge density calculations made by A. Shaukat et.al. [5]. Quantitative parameterization of the occupancy of the d-orbitals and a comparison of theory and experiment shall be presented.

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