approach. This simulated energy surface is thus only dependent on the charge density. Preliminary calculations seem quite encouraging. This may be of interest for Molecular Dynamics, since such methods rely totally on the assumed energy surface. The method we propose is also quite adapted for critically reducing the number of leading conformational parameters in complex molecules.

We also considered polarisation effects in fragments. For exemple, for simple molecules, we study the evolution of fragments when changing interatomic distances. Simple and general trends appear, that can be empirically modelled and related to polarisabilities or vibrational parameters.

The method can be used either with theoretical or experimental densities.

PS.09.02.07 PROPERTIES OF THE PROMOLECULE. B. Etschmann, E. N. Maslen. Crystallography Centre, The University of Western Australia, Nedlands, 6907, Australia

The power of the promolecule model, which consists of a (Hartree) product of the free atom wave functions, can be partly attributed to the number of chemical and physical properties that are unique functionals of the one-electron density[1].

Evaluating atomic charges on overlapping neutral atoms in a promolecule may appear anomalous, but the close relationship between bonding and potential energies makes it physically reasonable to subdivide electron density in proportion to each atom's contribution to the electrostatic potential.

Atomic radii are determined in two stages. An invariant component of the radius associated with the atomic cores is first equated to the value at which the integral of the density equals the number of core electrons. The second most significant contribution is from the valence electrons, which must be treated as penetrable. The main requirement when evaluating atomic radii from atomic electron densities is to evaluate the penetrability of the valence subshells.

The promolecule also gives a good first order prediction of bonding energies for atoms extending across the whole periodic table[2]. Energies predicted for diatomic molecules containing a monovalent anion an cation at the equilibrium spacing approximate bonding energies more accurately than integral point charges at those locations.

Values for these properties predicted by the promolecule model will be compared with experimentally measured equivalents for the garnet $Yb_3Al_5O_{12}$.

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PS09.02.08 QUANTUM CHEMICAL AND EXPERIMENTAL STUDY OF UREA. Dirk Feil and Roelof de Vries, Chem. Phys. Lab, University of Twente P.B 217, 7500 AE Enschede, Netherlands; Vladimir Tsirelson, D. Mendeleev University of Chemical Technology, Moscow, Russia

Introduction

In urea crystals one finds a considerable interaction density due to the network of strong hydrogen bonds distorting the molecular electron density distribution. The infinite size of the network requires, strictly speaking, band structure calculations to determine this effect.

Crystal Hartree-Fock-calculations (HF) have been carried out by Dovesi et al while DFT-calculations on clusters and on the crystal were carried out with ADF and the Amsterdam BAND program, respectively, as part of the present study. The outcome of the calculations are compared with the experimental results of Swaminathan et al and of Zavodnik et al.

Results

- The difference between the HF and the DFT exceeds experimental uncertainty.
- The description of the atoms is an important part of the discrepancy between HF and experiment.
- The interaction densities, resulting from HF and DFT calculations, do not differ significantly.
- Band structure calculations are not essential for the determination of the interaction density; with well-chosen parts of many-molecule clusters one can construct molecules that hardly differ from molecules in the crystal. Cluster calculations allow the use of larger basis sets.

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PS09.02.09 THE CHARGE DENSITY OF DL-ASPARTIC ACID. R. Flaig, T. Koritsánszky, P. Luger, D. Zobel, Institute for Crystallography, Freie Universität Berlin, Germany

A full topological analysis [1] of the electron density of DL-aspartic acid extracted from low temperature (20 K) X-ray data collected with solid state detector and AgKα radiation has been completed and the results compared with those obtained from Hartree-Fock wavefunctions.

The multipole refinement of the diffraction data was performed with the XD program package [2]. The static electron density, its Laplacian and various one-electron properties were derived. All critical points of the electron density and the Laplacian were located to characterize the covalent bonds and intermolecular interactions.

Experimental topological parameters for C-O bonds were found to be sensitive to the refinement model applied in the multipole treatment of the X-ray data. The ab initio calculations [3] at the Hartee-Fock level show considerable basis set dependence of the bond topological parameters. To mimic the intermolecular forces in the crystal calculations on molecular clusters were also carried out. The effect of the inclusion of the neighbouring molecules on the topology of the charge density especially in the C-O bond has been analyzed.

A comparative study based on diffraction data collected with solid state detector and MoKα radiation is in progress.

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PS09.02.10 ASPHERICITY SHIFTS FROM AB-INITIO DENSITIES COMPARED WITH EXPERIMENTAL RESULTS. S. Harkema, B.J.M. Fransen, J.A. Romein and D. Feil, Chemical Physics Laboratory, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

It is well known that positional and thermal parameters derived from X-ray and neutron diffracton experiments differ. These differences are caused by deviations from local spherical symmetry in the electronic charge density due to chemical bond formation. These asphericity shifts are most pronounced for H-atoms, but have also been detected for other atoms (F.H. Allen, *Acta Cryst.* (1986), B42, 515). In order to study these effects in a quantitative way structure factors were calculated from ab-initio electron densities for urea-phosphoric acid, for which compound a very extensive X-ray data set is available. The calculated structure factors were used as input for a spherical atomic refinement and theoretical asphericity shifts were determined. The shifts observed are a function of S.