
The electronic charge distribution in monoclinic V0₂, slightly distorted rutile structure, has been determined from integrated X-ray intensities by refinement of multipole superimposed on neutral atoms. The multipolar charge distribution is represented by a Fourier transform of structure factors calculated from the refined multipoles. The result agrees in part with the band model first proposed by Goodenough (Bul. Soc. Chim. France (1965) 1200): on vanadium the observed multipolar charge distribution corresponds to a \((x^2-y^2)\) orbital with maximum densities of .7 and .02 \(e\cdot\text{Å}^{-3}\) towards the near and farther vanadium neighbours along tetragonal \(c\) and of \(.4\) and \(.2\) \(e\cdot\text{Å}^{-3}\) perpendicular to \(c\) bisecting O-V-O angles.

The two (crystallographically independent) oxygens show deformation densities corresponding to \(p\) orbitals. One lobe of each orbital with maximum \(.6\) \(e\cdot\text{Å}^{-3}\) is rather extended and overlaps with a similar lobe on a neighbouring (independent) oxygen with the same \(z\) parameter. The other small lobes with \(.2\) \(e\cdot\text{Å}^{-3}\) are not involved in bonding. The O-O bonds lead to chains of octahedra along tetragonal \(b\) but not \(c\). In contrast to rutile no charge accumulations are found between oxygens of the same octahedron and between oxygen and vanadium.

06.2-12 ISOPYCNIC MAPS OF ELECTRON CHARGE DISTRIBUTIONS IN SOME STRAINED ORGANIC MOLECULES BY THE LOCAL HYBRID ORBITAL APPROACH. By J.B.Maksic, Lj. Vučkovic and Lj. Vujisic, "Rudjer Boskovic" Institute and The Faculty of Natural Sciences and Mathematics, The University of Zagreb, Zagreb Yugoslavia and The "Boris Kidrič" Institute, Vinča, Beograd, Yugoslavia.

The electron density contours in strained hydrocarbons involving three- and four-membered rings were studied by the local hybrid orbital approach based on the idea of deformed atoms in molecules. Both total and deformation isopycnic maps were considered. The main facets of the electron charge distributions are well reproduced. One observes a drift of charge density from atomic peripheries into the regions between the bonded atoms. The maxima of the density in the strained bonds are placed off the straight lines connecting the chemically bonded nuclei. The need for a distinction between the interatomic distances and bond lengths is stressed. The latter is defined in terms of the electron density.


The 222 integrated reflecting power in natural diamond crystals has been measured on a double-crystal spectrometer at FeK\(_\alpha 1\), CuK\(_\alpha 1\) and MoK\(_\alpha 1\) radiations. The measurements were carried out in a symmetric Bragg position in a parallel scheme, crystal-monochromator - Silicon, where the reflection 111 is for FeK\(_\alpha\) and CuK\(_\alpha\), that of 333 for MoK\(_\alpha\) radiation. In the CuK\(_\alpha\) radiation the value of 222 integrated reflecting power is in the interval 1a-2a-10\(^{-7}\), and evaluating the structure factor makes from 0.95 ± 0.05 is in good agreement with the results of M. Renninger (Z. Krist. 97, 107, 1937) and R.J. Weiss and H. Middleton (Private comm., 1964).

06.2-14 THE DEFORMATION ELECTRON DENSITY IN BORIC ACID, B(OH)\(_3\), STUDIED BY X-RAY DIFFRACTION AND SCF-CI CALCULATIONS. By Michael Gajhede, Sine Larsen and Sten Rettrup, Department of Physical Chemistry, University of Copenhagen, Denmark.

The crystal structure of boric acid (Zachariasen, I.J.H., Acta. Cryst. 7, 305, 1954) has been re-examined to investigate the electron charge distribution in the bonds, lone pairs and hydrogen bonds. X-ray diffraction data (ca. 15000 reflections) was collected at 105K, maximum sin \(\theta/\lambda\) = 1.1 \(\text{Å}^{-1}\). Using these data deformation density maps have been calculated employing parameters from high order data, sin \(\theta/\lambda\) = 0.8 \(\text{Å}^{-1}\). The hydrogen positions were derived using distances from the neutron study (Craven, B.M., & Sabine, T.M., Acta. Cryst. 20, 214 (1966)). The map of the molecular plane shows maximum deformation density in the oxygen lone pair region. In the O-H and O-B bond regions the densities are of the same magnitude. The two molecules in the asymmetric unit show identical features. Ab-initio calculations were performed at the SCF and SCF-CI level. The theoretical density map shows no significant differences from the experimental map. This indicates that the population analysis can be used in the investigation of transfer of charge from boron to oxygen. These results will be compared with other experimental results. X-ray diffraction data of boric acid (\(\text{B(OH)}_3\)) has been recollected (Morimoto, K., Mineral J. 2, 1-18 (1956)) and experimental, as well as theoretical, maps are being calculated. Since the anion contains both planar and tetrahedral boron, this compound is suited for comparisons.