06.2—11 ELECTRONIC CHARGE DISTRIBUTION IN VO_2. By E. Nowack and W. Gonschorek, Institut für Kristallographie der RWTH, 5100 Aachen, Fed. Rep. of Germany.

The electronic charge distribution in monoclinic VO_2, slightly distorted rutile structure, has been determined from integrated X-ray intensities by refinement of multipoles 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) 4, 1200): on vanadium the observed multipolar charge distribution corresponds to a (x^2-y^2) orbital with maximum densities of .7 and .02 $e\text{Å}^{-3}$ towards the near and farther vanadium neighbours along tetragonal c and of .4 and .2 $e\text{Å}^{-3}$ 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 $e\text{Å}^{-3}$ 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 $e\text{Å}^{-3}$ are not involved in bonding. The O-O bonds lead to chains of octahedra along tetragonal b but not a. 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 MOLE= CULES BY THE LOCAL HYBRID ORBITAL APPROACH. By Z.B.Maksić[a] ,Lj.Vučković[b] and Lj.Vujisić[b], [a]The "Rudjer Bošković" Institute and The Fa= culty of Natural Sciences and Mathematics, The University of Zagreb, Zagreb Yugoslavia and [b]The "Boris Kidrič" Institute, Vinča, Beograd, Yugoslavia

The electron density contours in strained hydrocarbons involving three-and four-membe= red rings were studied by the local hybrid or= bital approach based on the idea of deformed atoms in molecules. Both total and deformati= on 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 ma= xima of the density in the strained bonds are placed off the straight lines connecting the chemically bonded nuclei. The need for a dis= tinction between the interatomic distances and bond lengths is stressed. The latter is defined in terms of the electron density.

06.2—13 ON THE STRUCTURAL FACTOR VALUE OF THE FORBIDDEN 222 REFLECTION IN DIAMOND. By Yu.A.Rosenberg,A.I.Kolosovsky,L.I.Kleshchinsky,I.L.Feldman,V.M.Kiselev,Inst.of Transp. Engineers,664074 Irkutsk and N.V.Shokhirev, Inst.of Chem.Kinetics,Sib.Branch of Academy of Sciences,630090 Novosibirsk,USSR.

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_{α} and CuK_{α}, that of 333 for MoK_{α} radiation. In the $CuK_{\alpha 1}$ radiation the value of 222 integrated reflecting power is in the interval $14-24 \cdot 10^{-7}$ and evaluating the structure factor makes from 0.95 (kinematically approximated) to 2.00 (after dynamical theory). The X-ray topography produces a striking difference between the most perfect to the least perfect crystals, demonstrating the validity of the kinematical calculation on bad crystals against the dynamical one on good ones. This is also confirmed by measurements of the integrated reflecting powers of other cases where the dislocation density in the crystals is from $5 \cdot 10^5 cm^{-2} - 8 \cdot 10^7 cm^{-2}$. It should be noted that in most perfect crystals in the case of Cu and Mo radiations extinction corrections for 222 are necessary. The obtained 222 structure factor value 0.95 ± 0.05 is in good agreement with the results of M.Renninger (Z.Krist. 97, 107, 1937) and R.J.Weiss and R.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, W.H., Acta. Cryst. 7, 305, 1954) has been re-examined to investigate the electron distribution in the bonds, lone pairs and hydrogen bonds.
X-ray diffraction data (ca. 15000 reflections) was collected at 105K, maximum $\sin \theta/\lambda=1.16 \text{ Å}^{-1}$. Using these data deformation density maps have been calculated $\Delta\rho=\rho(obs)-\rho(cal)$. The calculated density was obtained using parameters from high order data, $\sin \theta/\lambda \geq 0.80 \text{ Å}^{-1}$. 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 B-O bond regions the densities seem to be of equal 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 presented.
X-ray diffraction data of borax ($Na_2B_4O_5(OH)_4 \cdot 8H_2O$) has been recollected (Morimoto, N., 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.