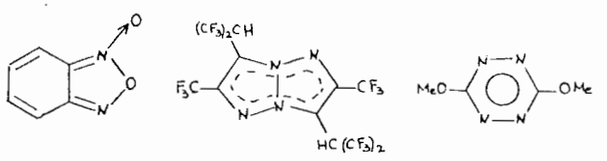
14-Diffraction Physics and Optics

8,9,10,12-tetrafluoro-*o*-carborane) and metallacarboranes CpFe(dicarb) and CpCo(dicarb) (Cp=C_5H_5, dicarb=dicarbollide) proving the absence of electron density accumulation inside the carborane cage and multicenter bonding at the triangular faces of the icosahedron. Among the organometallic compounds the metallocene derivatives Cp_2V, CpFeCp* (Cp*=C_5Me_5) and CpTi(η^8-C_8H_8) were studied. On the contrary to the disordered ferrocene, the structures of Cp_2V and CpFeCp* are ordered at low temperature and the asymmetry of the *3d*-electron distribution around metal atoms and the nature of metal-ligand bonds were analyzed. The observed EDD's in the molecules studied are essential for analysis of chemical bond features.

PS-14.02.11 ELECTRON DENSITY DISTRIBUTION IN THE NITROGEN-CONTAINING HETEROCYCLES. By *E.A.Kuz'mina, M.Yu.Antipin* and Yu.T.Struchkov.* A.N.Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russian Federation.

Using high-resolution (sin $\theta/\lambda \leq 1.0$ Å^{-1}) low temperature (120-140 K) X-ray diffraction data electron density distribution analysis in the new nitrogen-containing heterocycles (I-III) was performed in order to elucidate essential features of the chemical bonding.



A conventional high-angle (R=3.0-4.0%) and multipole refinement (MOLLY program) procedures were used for constructing the dynamic and static deformation electron density (DED) maps, calculation of atomic charges and multipole parameters (final R values after multipole refinement were in the range of 1.9-2.4%). For the benzofuroxane molecule (I) atomic charges were found to be small, positive DED peaks were localized nearly at the mid-points of the chemical bonds except for dative N→O bond,where the corresponding maximum was shifted to the O atom. An essential delocalization of the electron density in the π-region was found in this heterocycle. In the fluorinated tetraazapentalene (II) and tetrazine derivative (III) the strong π-component on the C-C, N-N and C-N bonds in the rings was established, testifying to the aromatic character of these heterocycles. Atomic charge distribution in (II) based on the multipole refinement data allowed to determine the contribution of the different resonance forms in the electronic structure. In the tetrazine derivative (III) high maxima on the DED maps corresponding to the lone pairs were found near N atoms in the molecular plane. The DED peaks on the C-N and N-N bonds were found to be shifted towards the centre of the heterocycle (bent bonds) probably due to the electrostatic repulsion between lone pairs and chemical bond electron density.

PS-14.02.12 ELECTRON DENSITY DISTRIBUTION IN CASSITERITE SnO_2. By V.S.Urusov*, O.V.Yakubovich and N.N.Eremin, Moscow State University, Russia.

The precise X-ray investigation, including δρ maps calculation was carried out to study peculiarities of chemical bonds in crystals of cassiterite SnO_2 grown by oxidation of metallic tin: a=4.739(1), c=3.1877(9) A, sp.gr. $P4_2/mnm$, Z=2, ρ_c=6.99 g/cm^3, μr=0.9, λ MoKα, 2θ-θ scanning, sin $\theta/\lambda \leq 1.08$ A^{-1}, 141 independent reflections. Parameters of the high-angle (sin $\theta/\lambda \geq 0.6$ A^{-1}, 104 refl.) refinement are: R=0.0062, wR=0.0072, s=1.1777.
The deformation electron density (δρ) maps for characteristic sections show main features common with δρ maps of isostructural rutile TiO_2 (R.Restory,D.Schwarzenbach and J.R.Schneider, Acta Cryst. (1987), B43, 251-257) and stishovite SiO_2 (M.A.Spackman, R.J.Hill and G.V.Gibbs, Phys.Chem.Min. (1987), 14,139-150). However, there are some peculiarities due to a more polarizable electron shell of Sn^{4+} compared to Ti^{4+} or Si^{4+} ions.

PS-14.02.13 SECOND-NEAREST-NEIGHBOUR INTERACTIONS AND THE ELECTRON DENSITY DISTRIBUTION IN Y_2BaCuO_5
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Y_2BaCuO_5 has a tightly packed structure with all cations and the O3 anion coplanar in a mirror plane with *y/b* = 0.25. There are O1 and O2 atom pairs above and below that plane. Analysis of synchrotron data for a small Y_2BaCuO_5 crystal shows that second nearest neighbour interactions dominate the redistribution of electron density. Within the mirror plane the cations are aligned in the sequence Ba—Y2—Cu—Y1—Ba over a total length of 13.10 Å. Atoms in those lines are cross-linked by zigzag connections along the *a* axis. The difference electron density Δρ in the *y/b* = 0.25 plane displayed in the Figure shows that electron density is strongly depleted along the shorter links in that grid.

