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8,10,12-tetrafluoro-o-carboline) and metallocarboranes (CpFe(dicarb) and CpCo(dicarb) (Cp=C5H5, dicarb=dicarbollide) proving the absence of electron density accumulation inside the carbaborane cage and multicenter bonding at the triangular faces of the isoceles-triangular. Among the organometallic compounds the metalocene derivatives Cp2V, Cp2FeCp* (Cp*=C5Me5) and CpTi(η4-C8H8) were studied. On the contrary to the disordered ferrocene, the structure of Cp2V and Cp2FeCp* are ordered at low temperature and the asymmetry of the 3d-electron distribution around metal atoms and the nature of metal-ligand bond were analyzed. The observed EDDs in the molecules studied are essential for analysis of chemical bond features.


Using high-resolution (sin θ/λ ≤ 1.0 Å⁻¹) low temperature (120-140 K) X-ray diffraction data electron density distribution analysis in the new nitrogen-containing heterocycles (1-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 nearby the mid-points of the chemical bonds except for the exocyclic 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 tetrazacetopentalene (II) and tetrazine derivative (III) the strong π-component on the C-C, C-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 showed to determine the contribution of the different resonance forms in the electronic structure. In the tetrizene derivative (III) high maxima on the DED maps corresponding to 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 SnO2. By V.S. Urusov*, O.V. Fakubovich and N.N. Eremin, Moscow State University, Russia.

The precise X-ray investigation, including 6p maps calculation was carried out to study peculiarities of chemical bonds in crystals of cassiterite SnO2 grown by oxidation of metallic tin (Sn=a, 4.739(1), c=3.1877(9) A, sp. gr. P4/nnm, Z=2, ρc=6.99 g/cm³, µ=0.9, λ=0.6608 Å, 2θ=26.8°). Scanning, sin θ/λ=0.08 Å⁻¹, 141 independent reflections. Parameters of the high-angle (sin θ/λ=0.6 Å⁻¹, 104 θ=71°) refinement are: R=0.0062, wR=0.0072, S=1.1777. The deformation electron density (6p) maps for characteristic sections show main features common with 6p maps of isostructural rutile TiO2 (R.Restorff, D.Schwarzenbach and J.R.Schneidner, Acta Cryst. (1987), B43, 251-257) and stilbovin SnO2 (M.A. Stackman, R.J. Hill and C.V. Gibbs, Phys. Chem. Miner. (1987), 14, 139-150). However, there are some peculiarities due to a more polarizable electron shell of Sn²⁺ compared to Ti⁴⁺ or Si⁴⁺ ions.


Y2BaCuO5 has a tightly packed structure with all cations and the O3 anion co-planar in a mirror plane with y=0.25. There are O1 and O2 atom pairs above and below that plane. Analysis of synchrotron data for a small Y2BaCuO5 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 map in the y=0.25 plane displayed in the Figure shows that electron density is strongly depleted along the shorter links in that grid.