

s2.m1.p17 **Determination of atomic domains and coordinations from a procrystal electron density calculation.** T. Balic-Zunic, *Geological Institute, University of Copenhagen, Denmark.*

Keywords: electron density.

Many important crystal chemical properties can satisfactorily be defined from the analysis of an approximate electron density calculated from the sum of theoretical electron densities for isolated atoms placed at atomic positions in a crystal structure (procrystal model).

The procrystal model is used to determine the shape and size of atomic structural domains which have polyhedral properties with faces representing bonding contacts between atoms. The approach enables determination of atomic coordinations for a great number of known crystal structures for which measured or calculated accurate electron densities have not yet been determined.

The polyhedra with faces defined by minimum surfaces in electron density represent natural atomic domains of atoms and give more reliable information about atomic coordinations than Voronoï/Dirichlet polyhedra in which the boundaries between the atoms are defined from purely geometrical rules.

While the local electron density properties at the bond critical points are rather sensitive to the applied model for calculation, the position of a minimum density surface is much less sensitive to the small deviations from the real density when applying the procrystal model. Therefore are the atomic coordinations determined from the shapes of atomic domains expected to be more reliable than those based on the search for bond critical points in a procrystal electron density map.

The approach will be illustrated by examples from several inorganic crystal structures with largely different characteristics. From light elements (Be) to the heavy ones (Sb) and chemical bond interactions ranging from closed shell to shared, the calculations gave satisfactory results. In some of them significantly different and more realistic coordinations have been determined than by other recently applied methods.

The concept of atoms as polyhedral moieties, with characteristic general volumes and shapes depending on the element type and valence state, could prove to be a much more valuable basis for theoretical modelling of crystal structures than a simple set of atomic radii. The present model gives a starting tool for a systematic collection of the characteristic parameters.

s2.m1.p18 **Topological Analysis of the Electron Density Distribution of Two Nickel Complex.** I-J. Hsu, C.-C. Wang, and Y. Wang. *Department of Chemistry, National Taiwan University, Taipei, Taiwan.*

Keywords: charge spin densities.

Electron density distribution of the compound, Ni(disn)(tfd) [disn = C₄N₄H₂, andiiminosuccinonitrilo; tfd = C₄S₂F₆, 1,2-trifluoromethylethene-1,2-dithiolate], is studied in terms of multipole model based on the X-ray diffraction data and of the molecular orbital calculation. The compound appears to have significantly different dipole moment when it is in ground state and when it is in excited state. This special physical property may be due to uneven ligand coordination, one (disn) and the other (tfd). The Ni metal ion of Ni(disn)(tfd) is bonded to two N-atoms and two S-atoms. In contrast to the complex Ni(disn)₂ where Ni is bonded to four N atoms. The comparison will be made in terms of the topological analysis of the electron density distribution between the Ni(disn)(tfd) and the Ni(disn)₂ compounds. All topological properties, including the bond critical points (BCP), Laplacian of the electron density, electron density at the BCP and Fermi-Hole function of these two compounds, will be presented both from X-ray diffraction experimentally and from molecular orbital calculation theoretically.

Special attention is made on the radial function of the multipole term in the multipole model, especially for the 3d-transition elements. The effect ζ value on the electron density at the vicinity of the metal ion will be discussed.