P14.07.13

Charge density of Ni(MePh₂)₂(C₆F₅)₂ (1) and the energy density in the Ni-C bond

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(1) was synthesised as a model compound for conducting metal-organic oligomers and polymers, and a charge density study was conducted in order to gain insight into the sigma carbon-nickel bond, which is often formally represented as $Ni^{2+}-C^-$. The results presented here, in combination with theoretically obtained values, demonstrate that the character of the Ni-C bond is far from ionic, and various parameters are presented that provide a much more nuanced image of this type of carbon-metal sigma bonding. Charges are calculated and compared with literature values, indicating that the nickel atom in this kind of compound is the most electron-rich nickel atoms known. The energy density is evaluated as a criterion for bond characterisation in this complex.

Keywords: charge density studies, metal organic compound, nickel compounds

P14.07.14

Experimental and theoretical charge density study of a compound containing linear tri-selenium bond

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The compound, 3,4-trimethylene-6a-selenasenophthene, is a planar molecule with two fused heterocyclic five-membered rings and a linear Se-Se-Se part. The electron density distribution is aimed at the understanding of the aromatic properties of the two five-membered rings and the rather unusual bond characters of Se-Se-Se bond. The electron density distribution will be derived both from accurate diffraction data experimentally and from the molecular orbital calculations theoretically. The experimental data were measured at 100K twice: one with wavelength of 0.5Å on a synchrotron source (SPring8 BL12B2); the other with Mo Kα on a in house CCD diffractometer. The deep violet rod crystal is rather small in two dimensions $\sim 30\mu$, it crystallized in orthorhombic space group *Pna*2₁ with unit cell dimension 11.2388(2), 16.4710(3) and 4.8867(1) Å. Two Se-Se bonds are 2.5486(5) and 2.5617(5)Å respectively. Detail comparison between two sets of data will be presented. Bond characterization will be given in terms of deformation density and the topological analysis. The corresponding theoretically calculated density is also going to be displayed. The topological properties associated with the chemical bond will be listed in comparison with the experimentally derived ones.

Keywords: charge density, selenium-selenium bond, synchrotron diffraction

P14.07.15

Population of atomic orbitals in silicide vanadium

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Based on a precision experiment carried out at room temperature (MoK-alpha, full sphere to sin teta/lambda 1.3) difference maps of electron density distribution in V3Si are draw. The achieved accuracy allows to calculate charge distribution numerical characteristics. A refining commonly used the overdetermined least-squares method can lead to rather deep but only local minimum values unless a multi-step selection and accounting of a large number of factors are made. This local minimum [s a results of corrections which may affect in different ways on the quality of a structural model. Therefore, the importance of our procedure is consecutive refinement of the structural model (to a level of R-values of around 1 per cent), initially without using a multipole model. This means that the introduction of several additional multipole parameters at the earlier achieved accuracy levels can lead to false R-factors reduction simply by increasing the number refined parameters. The required level has been achieved due to choosing a better strategy and by optimizing tactics of carrying out the experiment, data processing, and refinement of structural parameters especially. The calculation of atomic orbitals population made based on the experimental data and compared with theoretical calculation of the "first principles" done by B. Matheis (after expansion of his calculated electronic distribution in the same basis of atomic orbitals). The shown results speak of a good quality of the experiment and processing of the received data, as well as about the correct choice of a model made by B.Matheis. It should be noted that the results of other semi-phenomenological calculations show a significant difference in value as well, and sometimes in the transferred charge sign.

Keywords: higher accuracy, charge density distribution, atomic orbitals population

P14.07.16

Structural phase transitions in Rb₂Mn₂(SO₄)₃: A charge density study

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The langbeinite family of sulfates with the general formula $A_2B_2(SO_4)_3$ with A = Li^+, Na^+, K^+, Rb^+, Cs^+, $(NH_4)^+$ and B = Mg^{+2}, Mn^{+2}, Ni^{+2}, Ca^{+2} represents a class of ferroelastic and ferroelectric materials (1). X-ray diffraction studies have shown that crystals of these materials have a cubic structure with space group $P2_13$ at room temperature with a lattice parameter of nearly 10 Å and four formula units per unit cell. Theoretical calculations by Dvorak (2) suggest that these crystals can transform to low temperature phases with several possible space groups $P2_1$, $R3$, $P1$ and $P2_12_12_1$.So far in the literature there have been two different sequences of phase transition identified (3), one with cubic to orthorhombic distortion and the other with cubic - monoclinic - triclinic - orthorhombic distortion. Very high quality crystals of Rb₂Mn₂(SO₄)₃ were grown from slow evaporation of equimolar aqueous solution of the respective salts [Rb₂SO₄:2MnSO₄].The charge density data sets for this material