of the complexes has been investigated by theoretical calculations[2], but is still in controversy. Here we show the bonding nature of the 1-zirconacyclopent-3-yne complex by means of experimental charge density analysis.

Diffraction data were collected using synchrotron radiations at KEK PF-AR NW2 beam line by Rigaku Mercury CCD diffractometer up to $\sin\theta / \lambda = 1.0$ Å$^{-1}$. Multipole expansion method was applied for modeling of atoms. Final $R$ was 0.027 for reflections with $I > 1.5\sigma(I)$.

The 1-zirconacyclopent-3-yne moiety is planar. Valence shell charge concentrating region on each of the C atoms on the α positions extends toward the charge depressing regions on the Zr atom. Bond critical points and bond paths were found on the Zr-C(α) bonds. The bond paths curve inwardly near the C(α) atoms. These suggest that both of the $\eta^2$-σ, σ and $\eta^4$-π, π structures contribute to the bonding. No bond paths, in contrast, were found on the Zr-C(β) bonds. In conclusion, bonding of 1-zirconacyclopent-3-yne is in resonance between $\eta^2$-σ, σ and $\eta^4$-π, π structures.

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**Keywords: charge density, chemical bonding, zirconium compounds**

## P.14.07.9
**Different Approaches to Absorption Corrections for Charge Density Analyses**
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In order to increase the accuracy of high-angle diffraction data for multipole refinement with XD, crystals with diameters of up to 0.5 mm were measured. Bigger crystals give intensity data with higher signal-to-noise ratios, especially for high-angle reflections, but large crystals also make accurate absorption and extinction corrections a necessity, especially for crystals of *3d*-coordination compounds. Extinction corrections require values of TBAR, the absorption-weighted mean sum of incident and diffracted beam path lengths through the crystal, and anisotropic extinction corrections require also the direction cosines of the incident and diffracted beams [1].

Several absorption correction methods were compared based on crystallographic R-values, maximum and minimum values of residual densities, and the *d*-orbital populations from the experimental electron density studies of several *3d*-coordination compounds [2-3]. Valuable additional information was obtained from quantum chemical calculations and subsequent topological analysis of both experimental and theoretical electron densities [4].

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**Keywords: charge density, copper compounds, properties**

## P.14.07.10
**Chemical Bonding Based on Charge Density Calculations for Solids**
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We calculate the electronic structure of solids within density functional theory (DFT) and use the WIEN2k code [1] that is based on the full-potential augmented plane wave (APW) method. The key quantity is the electron density, which can be decomposed into contributions according to core and valence regions or even a small energy region (an energy sub band) that gives more insight into the chemical bonding than the total density. The partial densities of states (DOS) partitioned into atomic ℓ- and m-like contributions provide further details in chemical bonding.

Recently the experimental determination of the electronic charge density has been greatly improved, e.g. due to synchrotron radiation which allows to obtain structure factors with high accuracy [2]. Although the comparison between theory and experiment is made difficult by T=0 calculations vs. finite temperature experiments with absorption and extinction, fine details can be extracted that often agree well and lead to a better understanding of chemical bonding.

Such comparisons will be shown for a selected class of materials from oxides, $SiO_2$, silicates to highly correlated systems as the high-temperature superconductor $YBa_2Cu_3O_7$ [2] or the pyrochlore compound $Y_2Nb_2O_7$ [3]. A special feature appears in $BaCoO_3$ for which orbital is found to occur along the Co chains.

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**Keywords: DFT, charge density distribution, chemical bonding**

## P.14.07.11
**Electron-density Properties of the Functionally-substituted Hydropyrimidines**
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This work reports the results of the study of electron density and electronic energy density in the new functionally substituted hydropyrimidines. We performed the accurate X-ray diffraction measurements at 110 K and reconstructed the electron density and electronic energy density for three compounds of this series. *Ab initio* calculations were performed for different molecular conformations as well. In this work, we shall focus on the study of ethyl 4,6-dimethyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate. The topological analysis of the experimental and theoretical electron densities was fulfilled for all the conformations and the bonding network was quantitative described in terms of the electron density and energy density topological features. In addition, the analysis of critical points of molecular orbitals (i.e. HOMO, LUMO) has been performed. Similar considerations were done for the other functionally substituted hydropyrimidines. New electron-localization/delocalization indices like the exchange energy density and correlation energy density and its Laplacians are introduced. The electron-density-based similarity of the pharmacophoric parts of the conformers of the hydropyrimidines studied has been estimated using new original algorithm.
**Keywords: electron density, accurate measurements, ab initio calculations**

## P.14.07.12
**Electron Density Study of 2,5-Dimethyl-3,4-trimethylene-6a-thiathiophthene Using XRD, XAS and DFT Calculations**
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Thiathiophthene, a planar molecule with two fused heterocyclic five-membered rings and essentially a linear S-S-S bond, is a molecule of great interest due to the unusual bonding characters and the possible aromatic properties of the two five-memberd rings. In order to understand the remarkable bonding properties, the electron density distribution of one of the derivatives, i.e. 2,5-dimethyl-3,4-trimethylene-6a-thiathiophthene ($C_{10}H_{12}S_3$), was investigated both by