

Poster Sessions

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Polymorphism studied with invariom-derived cluster dipole moments

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Polymorphism, the phenomenon that a compound occurs in more than one form in the solid state, is commonplace, but not well understood. While the research area of crystal structure prediction is most successful in predicting polymorphism for relatively small and rigid structures at high computational cost [1], to date no simple way of predicting polymorphism exists. Energetic considerations of packing energies as for example those obtained from the PIXEL approach [2] share computational requirements to some degree.

Our approach towards attempting an understanding of polymorphism is to exploit the benefits of invariom refinement [3]. First of all accurate molecular structures as obtained after invariom refinement [4] make subsequent energetic considerations from experimental coordinates generally more reliable. Furthermore, going beyond molecular properties in the gas-phase is required for understanding solid-state phenomena. We therefore look at dipole moments and electrostatics of clusters of molecules of a number of polymorphic structures. Cluster sizes are chosen as to grant successful optimization of a central molecule within a two-layer ONIOM approach [5]. We assume that such clusters are a suitable model for a molecular packing environment. Quantum chemical results for such clusters are compared to results from a superposition of isolated molecules, where the invariom approach is used to generate the non-spherical density of the isolated molecule. We look at trends that emerge from this comparison.

Polymorphic molecules investigated include glycine, dihydro-carbamazepine, the new case of hydroxylysine hydrochloride, and a number of other published cases, where intensities for invariom refinement were available from the IUCr webpage.

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Charge density analysis of the [RhCp*(N-Me-L-Pro)Cl] rhodium complex

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Organometallic chiral-at-metal rhodium or iridium complexes are commonly used in homogeneous catalysis as they lower the energy barrier and improve the selectivity in cycloaddition reactions [1]. Due to the presence of a second or third-row transition metal (with a large number of core electrons) the overwhelming majority of their structural studies have been carried on "in a classical way", using the independent atom model (IAM). However, a more accurate description of the metal bonding, as well as the most common ligands, becomes necessary as it may help in the understanding of their catalytic activity.

Here we present the analysis of the charge density of the rhodium complex [RhCp*(N-Me-L-Pro)Cl] obtained from high-resolution X-ray diffraction. Special features of the multipolar model refinement, as the choice of the electronic configuration and the radial function of the metal; the anharmonic nuclear motion, and the anisotropic thermal refinement of hydrogen atoms will be discussed. The electronic bonding distribution in the proline ligand will be compared to those in other proline derivatives. The deformation density has been interpreted according to the Quantum Theory of Atoms in Molecules [2]. Topological analysis allows for a description of the nature of the bonding involving the metal atom, in terms of charge density, laplacian and energy density at bond critical points.

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A qualitative and quantitative analysis of dynamic charge densities

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The dynamic electron densities of the amino acids α -Glycine and D, L-serine have been determined to understand the nature of the chemical bonds. Multi-temperature data sets of serine have been used to analyze the effect of thermal vibrations on the charge density distribution. Diffraction data of α -Glycine have been kindly supplied by Destro et al [1] and of D L-Serine by Dittrich et al [2]. Multipole refinements have been performed for both compounds, employing the computer program XD [3]. The dynamic densities have been obtained by an inverse fast Fourier transform (FFT) of the structure factors calculated from these models, employing the computer program PRIOR. Absence of series termination effects has been established for grid sizes smaller than 0.05 Å. The resulting densities are free of spurious critical points, and they exhibit maxima and bond critical points (BCPs) at expected positions. Topological analyses of these dynamic charge densities have been carried out according to Bader's quantum theory of atoms in molecules (QTAIM) [4], using the computer program EDMA [5]. The density and Laplacian at the bond critical point are obtained. The effects of thermal vibrations are clearly visible, especially in the values of the Laplacian at BCPs.

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