and so on. For example, in the case of polyoxymethylene, synchrotron X-ray diffraction gave us the observed reflections more than 700, from which the details of the chain conformation and chain packing mode were derived accurately. The 2-dimensional neutron diffraction data collected for both of H- and D-polyoxymethylene samples allowed us to extract the H and D atomic positions exactly as shown in Figure. The similar results were obtained also for the other polymers listed above.

(a) POM-h$_2$ (b) POM-d$_2$
Fo(+)   Fo(-)   Fo(+)
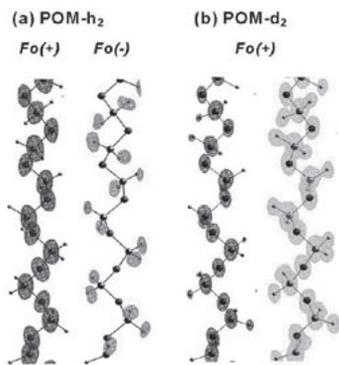
Keywords: deuterated polymers, neutron diffraction data, hydrogen atoms

P14.02.01

Invarioms for the DNA

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The application of the invariom database [1] of pseudoatom scattering factors that are transferable from one molecule to another (invarioms) in the refinement of single crystal X-ray diffraction data has so far been limited to amino acids / oligopeptide molecules and to a number of organic compounds. Nucleotide bases and the macromolecules they are part of form another class of compounds that are ideally suited for a database approach. An advantage of a scattering-factor database built by purely theoretical methodology is that the database can be extended to any chemical environment with ease. However, scattering-factor (invariom) assignment based on experimentally determined geometries is sometimes not unambiguous. This problem does occur more often for nucleotide bases, where the distinction of bond orders from the bond distance is more difficult. We present a new algorithm that circumvents these difficulties and have extended the invariom database also to nucleotide bases. Charge-density quality single-crystal X-ray diffraction data on thymidine [2], adenosine and the watson-crick base pair 1-methyl-adenine-1-methyl-thymine provide real-life examples to validate these database entries. To highlight their applicability to larger systems, initial refinement results of X-ray data of a DNA-porphyrin complex [3] are also presented. Diffraction data to 0.86 Å resolution were retrieved from the Protein Data Bank (1EM0).

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P14.01.02

Charge density and X-ray absorption studies on heterobimetallic phosphido-bridged Mo and W complexes

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The heterobimetallic phosphido-bridged complexes, $CpW(CO)_2(\mu$-$PPh_2)Mo(CO)_5$ (1) with W-Mo distance 3.1723(4)Å and $CpW(CO)_3(\mu$-$PPh_2)Mo(CO)_5$ (2) with W-Mo distance 4.510(4)Å have been reported with special chemical reaction properties because of the interaction between W and Mo: complex 2 can be converted into 1 after irradiation with UV or heating at reflux temperature. In order to correlate how the chemical bond of Mo-W affect the chemical reaction in complex 1 and 2, the accurate single crystal diffraction data of both complexes at 100 K are collected and the experimental electron density in terms of multipole model are derived to investigate the electron density distribution and chemical bonds. All chemical bonds will be characterized based on atoms in molecule theory, and classified by the location of the bond critical point (BCP) and its associated topological properties. The bonding characters will be complemented with x-ray absorption spectroscopy of Mo K-edge. All experimental observations will be compared with the density functional theory calculation. A reasonable explanation will be given in relation with the different chemical reaction properties between 1 and 2.

Keywords: charge denstiy, X-ray absorption spectroscopy, density functional theory

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Generalized library of experimental multipolar atoms

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A library of average multipole populations describing the electron density of common chemical groups is being built. The library values are obtained from several small peptide or organic compound crystal structures refined against available ultra-high-resolution X-ray diffraction data [1]. The atom types are defined on the basis of their chemical environment and local symmetry. New local coordinate axes systems have been defined in special cases. The introduction of optimal constrains and restrains allows for reduction of the number of multipolar parameters. As a consequence more meaningful results and stable refinements are gained. We will present the latest advancements of the crystallographic software MoPro suite [2] for the estimation of protein-ligand electrostatic interaction energy. Aldose reductase (hAR) is an enzyme involved in diabetes complications and the inhibition of the protein is a therapeutic way to treat them. The electrostatics interactions of the Fidarestat inhibitor with the enzyme active site have been characterized using the library electron density modelling. This information is useful to understand the affinity and specificity of Fidarestat with hAR compared to other