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Of particular interest is the relationship between chemical bonding and property for polymer materials since the number of X-ray charge density study was very few due to the difficulty of crystallinity control of single crystal sample. Thus, the charge density study of polymer material is a challenging task. In order to reveal the bonding nature, MEM (Maximum Entropy Method) charge density study of the polyoxymethylene (POM, -$[CH_2O]_n$-) were carried out by synchrotron radiation (SR) X-ray diffraction experiment using the best quality single crystal at SPring-8 BL02B1.
The data with high counting statistics were measured at 123 K by the combination of high brilliance SR and the large cylindrical Imaging Plate (IP) camera. From the fiber pattern of POM recorded on IP, the integrated intensities of each Bragg reflections were obtained and corrected to the observed structure factors. The obtained X-ray pattern represented a typical feature of uniaxially-oriented POM structure on the basis of helical chain molecule.
The preliminary structure analysis was done by SHLEX-97 software with the 9/5 helical chain structure model reported by Hengstenberg *et al.* in 1927[1]. However, the analysis presented an inconclusive answer even for the fundamental structure and the *R*-factor was 17.1%. This result coincides with the existence of the none-indexed X-ray spots of the present pattern. The possibility of another structure model such as the 29/16 helical chain model by Tashiro *et al*. [2] should be also examined.
The MEM ought to allow visualizing charge density, which is consistent with the observed data. In fact, the MEM charge density based on the 9/5 helical chain model revealed the charge densities based on the mixture of several helical period structures. Even though the examination of bonding nature is still in progress, the existence of disordered and/or random feature of helical POM is uncovered in the charge density level for the first time.

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Keywords: polymers, maximum-entropy method, charge density studies

FA4-MS37-P08

Electron charge density and topological analysis of coumarin dye.

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The electron-density distribution of coumarin-102, a laser dye has been investigated from high-resolution X-ray diffraction data collected at 100K, and from data based on theoretically calculated structure factors (VASP)[1], using the Hansen & Coppens[2] multipolar atom model. Topological properties of the refined charge density have been determined using the Bader[3] "atoms in molecules" theory. Analysis of deformation electron density peak heights and topological features indicate that the chromen-2-one ring system has a delocalized π electron cloud in resonance with the N amino atom. The molecular electrostatic potential and dipolar moment were estimated from both theoretical and experimental multipolar models, and reveal an asymmetric character of the charge distribution along the molecule. This polarization effect is due to a substantial charge delocalization within the molecule. Moreover, C—H…O contacts are observed in the crystal packing, and are confirmed as true hydrogen bonds by the presence of (3,-1) critical points along H…O paths.

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Keywords: electron-density distribution, high-resolution X-ray diffraction, topological properties of charge

FA4-MS37-P09

ELECTRON CHARGE DENSITY DISTRIBUTION IN AN ORGANIC COMPOUND : THE 4,4 DIMETHYL CYANO BIPHENYL (DMACB).

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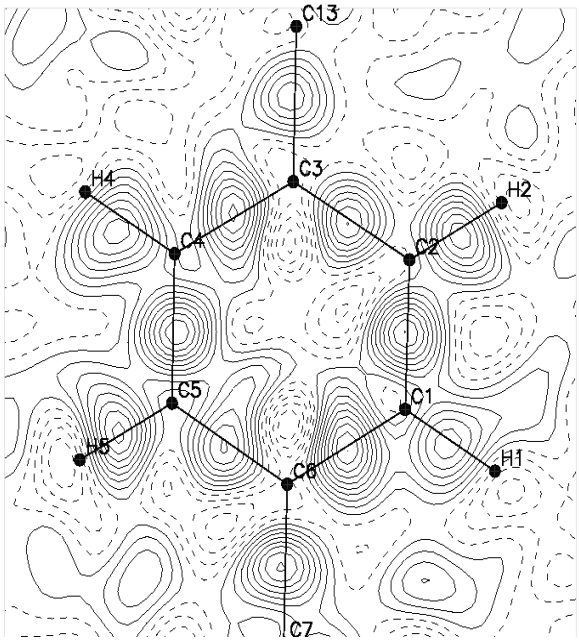
At room temperature, the 4,4 dimethylamino-cyanobiphenyl (DMACB) appears in two polymorphic structures: orthorhombic and monoclinic forms. In the present work, we shall focus on the monoclinic form of this compound which has a centrosymmetric structure with the space group Cc. The molecular dipole moment has been estimated experimentally [1].
High resolution single crystal diffraction experiment was performed at low temperature with MoKα radiation. The crystal structure was refined using the multipolar model of Hansen and Coppens (1978) [2]. The molecular electron charge density distribution is described accurately. The study reveals the nature of inter-molecular interactions including charge transfer. The results could be analyzed in more detail, if they were complemented by a quantum chemistry calculation. The electronic structure of this molecule has been investigated theoretically by the Semi-empirical and Ab initio calculations. The agreement between the experimental and theoretical results such as: atomic net charge, molecular dipole moment, electrostatic potential and electron density was satisfactory. All these results will be presented in the meeting. The figure below gives the charge density distribution in the phenyl plane.



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Keywords: charge density, XD Software

FA4-MS37-P10

The electron density of isoindole derivatives from synchrotron diffraction data. Lilianna Chęcińska[a], Magdalena Małecka[a] Agnieszka Rybarczyk-Pirek[a], Carsten Paulmann[b,c], Simon Grabowsky[d], Peter Luger[d]
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The isoindolin-1-ones are the important structural units found in natural products, biologically active substances and synthetic intermediates [1], [2]. Here, the electron density of two isoindole derivatives is considered: 3-hydroxy-2-phenyl-2,3-dihydro-isoindol-1-one (I) and 5-hydroxy-6-phenyl-5,6-dihydro-pyrrolo[3,4-*b*]pyridin-7-one (II).
The high-resolution synchrotron-diffraction data sets were collected at beamline F1 at Hasylab/DESY (Hamburg, Germany). The *XDS* [3] was used for an integration of frames and data reduction. Initial spherical refinements were performed with *SHELXL97* [4] providing starting values for subsequent aspherical-atom least-squares refinements with *XDLSM* of *XD2006* program package [5].
Two analyzed molecular structures of I/II consist of isoindol-1-one/aza-isoindol-1-one moiety substituted by phenyl and hydroxyl groups at position *2* and *3*, respectively. The geometry of the investigated molecules is similar but not identical, but their arrangement in the crystal structures is different.
In I, the molecules are linked by intermolecular hydrogen bond O-H···O (½-x,½+y,z) forming an infinite chain along [010] direction. In the aza-isoindole derivative (II) additional nitrogen atom is an accepting centre of hydrogen bonding, instead of oxygen atom, and O-H···N (x,½-y,½+z) is observed. This interaction generates an infinite chain along [001] direction.
The qualitative and quantitative analysis of the electron density distribution within isoindole moieties and hydrogen bonding areas will be presented in the poster.

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Acknowledgements: The research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013) under grant agreement No 226716.
The authors thank Professor Andrzej Jóźwiak, University of Łódź, Poland, for supplying substances to research.

Keywords: structure and charge-density analysis, synchrotron X-ray diffraction, isoindole derivatives

FA4-MS37-P11

Mismatched interactions in bis(phenolato) metal complexes Thomas S. Dols[a,b], Thomas P. Spaniol[a], Jun Okuda[a], Christian W. Lehmann[b], [a] *Institut für anorganische Chemie, RWTH Aachen University, Germany,* [b] *MPI für Kohlenforschung, Mülheim, Germany*
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Three-dimensional crystal structures have become an indispensible tool in modern catalyst research. To improve the product properties, the structural changes of homogeneous catalysts and their precatalysts are correlated with their impact on polymerization. We are investigating transition metal complexes with bridged bisphenolato ligands that are used in olefin-polymerization. The molecular structure of the ligand has a strong influence on the stereochemistry of the resulting polymer[1,2]. For this reason, the bis(phenolate) ligands have been tuned by different substituents on the aromatic rings as well as by modifying the bridging unit. S atoms as part of the bridge can improve the catalytic activity, obviously as a result of hemilabile interactions between the soft donor S atom and the hard metal center [3].
In several S-C-C-S-bridged bis(phenolato)titanium complexes, the M···S interactions lead to a stereorigid O,S,S,O-tetradentate coordination in solution [4]. Such a system has made it possible to polymerize styrene in homogeneous phase to give isotactic polystyrene for the first time [1]. The results prove the high conformational stability of the metal complexes under the conditions of polymerization.
The focus of our investigations is on metal complexes where, according to the HSAB principle, the hard metal centers are interacting with the sulfur atom of the bisphenolato ligand. It