In NSNO, diagonal-stripe charge ordering is observed at x = 1/3 [1] in contrast to LSCO with vertical-stripe charge ordering at x = 1/2 [2]. NSNO also shows checkerboard (CB) charge ordering at x = 1/2 [3]. This system undergoes an insulator-metal transition with melting of its charge ordered state but shows no superconductivity up to x = 1.6 [4]. Hitherto there has been no study of the electronic structure in the insulator-metal critical region. The comparison between these layered nickelate and cuprate Mott transition systems will be of benefit for understanding the uniqueness of high-Tc cuprates.

We have investigated the resonant x-ray diffraction (RXD) at Ni K-edge (~8.3 keV) photon energy to clarify the electronic structure in CB-type charge order phase in Nd$_2$Sr$_2$NiO$_6$ (x=0.5). In the present case, we consider a dipole transition between Ni 1s and 4p. The 4p-level are influenced by their interaction with the e$_g$ electrons. In CB-type order phase, we have succeeded in observing the non-zero RXD signal at (100) for an incident x-ray polarization E||a, whereas there is no RXD signal for E||c. The polarization dependence of (100) diffraction suggests that the (x$^2$-y$^2$)-type hole orbital order of e$_g$-state is realized in x=0.5. The charge disproportionation is estimated less than 0.2, thus the CB-type modulation of electronic structure should be originated from the orbital order rather than the charge order.

As decreasing temperature, the material undergoes a tetragonal-orthorhombic structural transition at around 250 K. Upon the transition the polarization dependence of the RXD signal changes, that is, the (x$^2$-y$^2$)-type hole orbital order transmutes into the (3z$^2$-r$^2$)-type order in accordance with the orthorhombic transition. The tilting of NiO$_6$-cage should affect the e$_g$ orbital state. We consider that the (3z$^2$-r$^2$)-type orbital order plays an important role in the insulator-metal transition.

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**Keywords:** resonant diffraction, orbital order, charge order

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**Preliminary deformation density studies of Z-DNA hexamer duplex d(CGCGCG),**

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Crystals of the left-handed Z-DNA duplex have the potential to diffract X-rays to the highest resolution. Recently, using synchrotron radiation, we have measured X-ray diffraction data extending to 0.55Å resolution for a single crystal of d(CGCGCG), crystal, and described its high-quality structural model obtained through conventional least-squares refinement (R=7.77% [1]). At the very high resolution of the diffraction data, not only are the positions of the hydrogen atoms clearly revealed, but there are also indications of electron density related to bonding electrons visible well above the map noise level. The high ratio of observations to individual atom parameters makes it possible to carry out a deformation density study of this DNA model.

We have used the program MOPRO [2] for the high-order refinement and consequently for the transfer of the ELMAM library [3] data to build a starting model for a multipolar refinement. The results show the importance of deformation effects, visible both in successful convergence of the refinement (for instance, systematic decrease of residual densities) and in the drop of the R-factor. The transferred and refined multipolar parameters will allow us to analyse electron-density-derived properties of the DNA molecule, including topological analysis, base pairing, hydrogen bonding, etc. The Figure shows the static deformation density for one of the cytosine fragments at the current stage of MOPRO refinement (contours at 0.0x e.Å$^2$ interval, dashed for negative values).

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**Keywords:** polarized neutron diffraction, spin density, magnetic field density,
Charge density studies on N-n-butyltetrachlorophthalimide
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The charge density distribution in N-n-butyltetrachloro-phthalimide has been determined by means of high-resolution X-ray diffraction at 100K. The supramolecular structure of the title compound is stabilized by intermolecular halogen bonds C-Cl-O and intermolecular Cl-Cl interactions [1]. In the current presentation the deformation density distribution of electron density and topological analysis of electron density clearly indicates a significantly anisotropic distribution of density for the title compound crystal are shown. The deformation density distribution after crystal structure refinement with Invarions. The comparison of molecular electrostatic potentials has important implications on their function as anti-infective agents. Molecular electrostatic potentials for the same protonation states show a striking degree of similarity for the whole class of compounds. The relevance of this similarity for rational drug design and optimization of lead structures is discussed. The rapid calculation of electrostatic potentials directly from the invarion database makes the procedure suitable for high-throughput screening.

Deposited, newly determined and re-measured single-crystal diffraction data of varying quality were evaluated in this manner. The structure of lomefloxacin hydrochloride tetrahydrate is reported for the first time and the structural model of enoxacin methanol solvate as reported by Yoon et al. [2] needed revision: it turns out to be a water solvate. An in silico validation procedure for invarion database entries [3] is presented.

Keywords: Z-DNA, sub-atomic resolution, deformation density


Dipole moment determination in push-pull chromophores from charge density data
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Push-pull chromophores find use in organic optical materials and for many applications their ground state dipole moment and polarizability are important properties. [1] In the condensed phase intermolecular interactions influence these properties and may lead to an enhancement of the dipole moment. The crystalline state provides a rigid surrounding for the intermolecular interactions, thus maximizing the effects. Experimental charge density studies facilitate the determination of molecular “in-crystal” dipole moments. However, the dipole moment values determined in this way have to be examined critically and are prone to systematic errors. [2] In this study dipole moments obtained from multipole refinements of structure factor amplitudes determined experimentally by diffraction and theoretically by ab-initio calculations are compared. The applicability of the invarion model [3]