s2.m2.p1 **Development of Vacuum Camera Imaging Plate method (VCIP) for the measurements of Electron density distribution in metal complexes.** [A]K.Tanaka, [A]S. Takagi,[B]Y.Takenaka & [C]V.V.Zhurov, [A]*Dept. of Mat. Sci. and Eng., Nagoya Inst.Tech., Japan,* [B]*Hokkaido Univ. Edu. at Hakodate and* [C]*Karpov Res. Inst. Phy. Chem., Russia.* Keywords: VCIP, electron density, metal complexes.

Vacuum camera (VC) is an evacuated cylinder with an Imaging plate (IP) attached on the inside wall. It enables to measure X-ray intensities under vacuum. A He-cryostat can be installed in it. The aim of the research is to develop VCIP as one of the devices for super accurate structure factor measurement with 0.5% accuracy in a near future.

The measurement by VCIP at Spring-8 with 50keV SR revealed almost zero background at high angles. The measurements by VCIP and a four-circle diffractometer of the electron density of $KNiF_3$ gave almost the same electron densities. However the R-factors were 0.8% and 0.4% for VCIP and four-circle measurements, in spite of the advantage of low background in VCIP. In the four circle measurement multiple diffraction (MD) was avoided utilizing accurate orientation matrix of the crystal.

Since VC is an off-line IP device, orientation matrix necessary for MD avoidance should be determined with the camera parameters for each measurement. A least-squares program was developed to refine these parameters. Slant incidence of diffracted X-rays on the IP is another problem. The absorption of the emitted light from Bragg peaks by the phosphor layer of the IP itself has been taken into account.

The VCIP method was successfully applied to $KNiF_3$ and LaB_6 measured at laboratory and Spring-8. Peak positions were fitted within one pixel and the lattice parameters conform to the cubic system within the error.

VCIP is still in progress. The absorption correction and the evaluation of MD for non-spherical crystals are being developed. VCIP will be a tool more accurate than the four-circle diffractometer because of its low background.

s2.m2.p2 **Atomic properties from experimental electron densities: Program Newprop-int.** M. Souhassou *LCM3B, BP 239,54506 Vandoeuvre les Nancy France.* Keywords*:* topology, electron density, critical points.

The theory of atoms in molecules is a powerful tool to investigate molecular and atomic interactions in term of the topological properties at the critical points of the total electron density. The gradient path trajectories around a nucleus define atomic basins, over which the integration of the electron density allow to derive atomic properties, such as net atomic charges and dipole and higher moments that can be used calculate electrostatic properties such as electrostatic potential.

From an electron density distribution obtained either in analytical form or on a three dimensions grid, topological properties are derived for different compounds and analyzed in terms of critical points and their classification and the integration over the atomic basins.

This method was used to investigate: charge transfer in TTF-BQ molecular conductors (Theoretical 3D grid density), in molecular magnetic materials for which the charge transfer is responsible for magnetic coupling; and in zeolites to derive net atomic charges, that can be used for modeling the electrostatic properties to calculate sorption energies.

The presentation will summarize topological properties and discuss the outcome of these results.