DREAM (Blessing, 1986) and the recently developed multipole refinement and analyses package XD (Koritzantszky et al., 1994, we will present charge density analyses results on Creatine Monohydrate using both the Seed-Skewness method and the elliptical peak-mask method.

An interactive version of this abstract can be obtain from the URL: http://www.cf.ac.uk/uwcc/chemy/bracke/iucr/iucr96.html

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PS09.01.09 ANHARMONICITY IN MnF_2 AT LOW TEMPERATURE: BEYOND THE FROZEN-CORE APPROXIMATION.

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Antiferromagnetic order in MnF_2 induces a dipolar distortion of the fluorine inner electron shell. The core-deformation generates a substantial electric field at the nucleus, which is not compensated by peripheral lattice contributions, thus giving rise to an apparent Coulomb force on the nucleus. The force exerted on any nucleus should vanish in the stable equilibrium configuration. A local source of an opposing electric field could consist in a small skewness of the fluorine nuclear vibrational distribution which should persist even in the limit of zero temperature. This model rests upon the assumption that the electron deformation does not rigidly follow the nuclear motion.

Pulsed single-crystal neutron diffraction (T = 15 K) at the spallation source IPNS has been used to test this hypothesis. Data have been collected up to very high diffraction vectors, $(\sin\theta/\lambda)_{max} = 2.75$ Å^{-1}. The harmonic mean-square displacement parameters are in excellent agreement with previous results from both gamma-ray and neutron diffraction. Statistically significant third-order coefficients of a Gram-Charlier expansion could be extracted from the experiment. The shape of the antisymmetric part of the nuclear distribution function substantiates a subtle balance between the mean thermal electric fields due to the electronic and the nuclear charge density distribution. The sense of the skewness around the equilibrium position is opposite to the one found previously for the paramagnetic state. It is to be noted that data from nuclear scattering alone can provide valuable indications concerning a local redistribution of electron density.

Experiment thus confirms the conclusion that the core polarization in antiferromagnetic MnF_2 is dynamically stabilized. A theoretical description of the detailed physical mechanism is lacking at present.

PS09.01.10 ELECTRON DENSITY AND PROPERTIES OF ROCK-SALT TYPE CRYSTALS

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The X-ray diffraction studies of the electron density (ED) of the crystals with rock-salt structure, traditional test crystals in solid state computational methods, should provide the basis for direct comparison of the theoretical and experimental data. However-

er, the severe extinction and sometimes ignoring TDS distort the diffraction intensities and the problem of description of highly ionic electronic states exists in theoretical calculations for these crystals. Therefore the reliable estimation of real today's level of both experimental and theoretical results concerned with electronic properties of these crystals is needed.

We have performed the accurate X-ray diffraction experiments and theoretical calculations by non-empirical Hartree-Fock method for LiF, NaF, NaCl and MgO crystals. In addition, the electron diffraction measurement of electrostatic potential in MgO was done. The quasi-static structure amplitudes reconstructed from the X-ray experiments were compared with theoretical ones calculated with different basis sets at experimental geometry. It was found that the extended optimised basis sets result to close agreement with experimental data, including low-angle "extinctional" reflections. The analysis of the ED (both experimental and theoretical) in terms of deformation density maps and Bader's quantum-topological theory was done. The electrostatic potential was calculated and compared with electron-diffraction data.

PS09.01.11 CHARGE DENSITY STUDIES OF TRANSITION METAL SULFIDES.

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The electron density distributions of transition metal sulfides MS_2 (pyrite structure) for M = Mn, Fe, Co, and Ni have been analyzed by multipole refinement and topological analysis using the XD program package (1), with data reported previously (2). The metal d-orbital populations and deformation density maps confirm that the transition metal in MnS_2 is in a high spin state, while low spin states occur in the other solids. The electron density at the M-S bond critical points decreases as the bond length increases, indicating decreasing bond strength. The Laplacians at the S-S and M-S bond critical points are all positive. Their values do not correlate well with the bond lengths or densities. The structure factors from a theoretical DFT calculation on FeS_2 (3), have been analyzed with the multipole formalism. Experimental and theoretical multipole parameters and density maps will be compared.

The effect of the use of selection of different form factors (non-relativistic, relativistic and modified relativistic) will be discussed.

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