06.3-05   ELECTRONIC CHARGE AND MOMENTUM DENSITY DISTRIBUTIONS IN IONIC CRYSTALS: Li_3N and $Mg(OH)_2$

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Using these examples we wish to show how the understanding of the bonding mechanism in solids is widened by combining results from X-ray diffraction and Compton scattering experiments.

Schulz and Schwarz (Acta Cryst.(1978)A34,999) measured X-ray structure factors for Li_3N, and concluded from their analysis of the data that the crystal could be considered purely ionic. We have measured 6 Compton profiles along directions perpendicular to the hexagonal symmetry axis. The Fourier transform of the Compton profiles will be compared with the 1-electron wave function autocorrelation function calculated from two different models: 1. An LCAO calculation (O. Aikala, Turku University) which takes the ionic model as a starting point and then corrects for overlap of the atomic orbitals.
2. A self-consistent pseudopotential calculation (G. Kerker, MPI, Stuttgart, to be published). We confirm the ionic picture for Li_3N in which the N^{3-} ion is cosiderably distorted due to overlap with neighbouring ions.

We have measured Compton profiles perpendicular and parallel to the O-H bond in $Mg(OH)_2$. Our data agree well with the results of an extensive study on LiOH by Heuser and Weyrich (TH, Darmstadt). The anisotropy of the Fourier transform of the profiles for the two compounds are very similar around $1\overset{\circ}{A}$ (distances corresponding to the bond length in the OH^- ion). We therefore compare the measurements with theoretical calculations on the isolated ion (Cade, J.Chem. Phys.(1967)47,2390). We will furthermore compare the 1-electron density derived from this wave function with the results of an analysis of X-ray diffraction data on LiOH (Mair, Acta Cryst.(1978)A34,542).

06.4-01   DEFORMATIONS OF IONS IN IONIC CRYSTALS (NaF, KCl): A VARIETY OF THEORETICAL ESTIMATES, G. Bübel, P. Cortona and F.G. Fumi, Istituto di Scienze Fisiche, Università di Genova and GNSM-CNR, Unità di Genova (Italy).

Various approaches of rather different sophistication have been used to investigate the effect of the crystal field on the free-ion wave functions in NaF and KCl, and the ensuing effects on the structure factors of the lower order 'difference' (and 'sum') reflections, which have recently been measured with great accuracy by R. Colella of Purdue University (see Abstract by Yoder & Colella). The approaches include: a simple 'scaling' of the Clementi-Roetti Hartree-Fock wave functions (E.Clementi & C.Roetti, Atomic Data and Nuclear Data Tables 14, 177 (1974)), the representation of the Madelung field acting on a central ion by the charged Watson sphere (R.E.Watson, Phys. Rev. 111, 1108 (1958)), using both Hartree-Fock (E.Paschalis & A. Weiss, Theor. Chim. Acta 13, 381 (1969)), and Dirac-Kohn-Sham wave functions for the central ion, the use of Kunz's 'localized orbitals' wave functions for Na^+ and F^- in NaF (D.R.Jennison & B.Kunz, Phys. Rev. B13, 5597 (1976)); and finally the use of the crystal wave functions given by the density-functional method (P.Hohenberg & W.Kohn, Phys. Rev. 136, B864 (1964); W.Kohn & L.J.Sham, Phys. Rev. 140, A1133 (1965)). The comparison of the computed and measured structure factors will be discussed in detail. A comparison will also be made with previous calculations using different approaches.

06.4-02   ELECTRON DENSITY IN SODIUM FLUORIDE. By D. Yoder and R. Colella, Physics Department, Purdue University, W. Lafayette, IN 47907.

Several structure factors with $\sin\theta/\lambda$ ranging between 0.22 and 1.08 have been measured with high accuracy on an absolute basis in extinction-free conditions using a thin NaF crystal slab (t_0=0.325 mm) and short wavelength radiation. A gamma ray diffractometer (λ=0.12Å) available at the Research Reactor of the University of Missouri has been used for this experiment. It is found that even the strongest reflection, the (200), is extinction-free. The experimental values of the (hkl) experimental intensities are compared with two sets of values calculated using different Hartreee-Fock wavefunctions for free Na^+ and F^- ions (Cromer and Waber, Acta Cryst. (1965) 18, 104; Cromer and Mann, Acta Cryst. (1968) A24, 321). The observed intensities are generally greater than the calculated values, indicating that the wavefunctions in the crystal are, on average, compressed by the Madelung potential. Surprisingly, it is found that a better description for the crystal electron density is obtained when the relativistic Dirac-Slater wavefunctions are used instead of those obtained by the Hartree-Fock method. The effect of the Slater's approximation for the exchange correction is to contract the wavefunctions, thereby improving the agreement with experiment. The (111) reflection is 11% more intense than the calculated value, indicating that the ionic exchange between Na^+ and F^- is less than one electron.