06.7-6 ELECTROSTATIC PROPERTIES FROM ACCURATE X-RAY DIFFRACTION DATA. By K. Echchoura, Fachrichtung Kristallographie, Universität des Saarlandes, D-6600 Saarbrücken, Federal Republic of Germany.

Since X-ray structure factors are the Fourier components of the (charged) electron density in the unit cell, they can be used, at least in principle, to evaluate electrostatic quantities like inner and outer nuclear potential and field strength, and also to derive electrostatic part of molecular interaction energies. The results are limited by both the accuracy and the resolution of the X-ray experiment and it is best to restrict oneself to quantities which depend mainly on low-order reflections.

Outer moments may be obtained by either Fourier methods (Coppens & Hansen, I. r. J. Chem. (1977) 16, 163) or by least-squares fits ranging from simple L-shell refinement (Stewart, J. Chem. Phys. (1970) 52, 205) to the more involved multipole models (Stewart, Acts Cryst. (1976) A32, 565; Hirshfeld, Isr. J. Chem. (1977) 16, 226). Following Buckingham (Quart. Rev. (1959) 13, 183), these may then serve to expand the electric potential as a series of multipole moments. These possibilities can also be obtained by Fourier summation with modified coefficients F/πS, downgrading the effect of high-order data. The electrostatic potential may be interpreted as interaction energy of the (thermally smeared) electron density in the unit cell, they can be used, at least in principle, to evaluate electrostatic quantities like inner and outer nuclear potential and field strength, and also to derive electrostatic part of molecular interaction energies. The results are limited by both the accuracy and the resolution of the X-ray experiment and it is best to restrict oneself to quantities which depend mainly on low-order reflections.

This approach has been successfully used to study the influence of the short H-bridge (0...0 = 2.43 Å) in 1-hydroxypropyridinium trichloracetate on the electron density of bond systems, and to derive heights of barriers to internal rotation from multipole-multipole interactions in accord with experimental values.

06.7-7 CLUSTER CALCULATION OF ELECTRONIC STRUCTURE AND HYPERFINE INTERACTIONS FOR GARNETS. By S. Nagel and S.-S. Hafner, Institute of Mineralogy, University of Marburg, Lahnberge, 3550 Marburg, Germany (F.R.G.).

Because of their large spread in chemical composition, crystal structures of the garnet type Ca₃Al₂Si₃O₁₂ are excellent examples to test models of chemical bonding at atomic sites. We have applied the multiple scattering Xₚ method for studying the relationship between chemical bonding and nuclear hyperfine coupling measured with resonance techniques. Precise NMR data of 27Al, 69,71Ga, and Mössbauer data of 57Fe are well known for a large number of garnets. Calculations have been performed for Ï₆ and Ï₄ clusters with geometries as found in the garnets. c = Al, d = Ga and c = Fe, Ï₆. For stabilization we used the respective crystal potentials obtained for a point charge lattice. The second derivatives of the potential (Vₓₓ) at the a and Ï₆ positions were calculated from the cluster wavefunctions including those for the core electrons. Important contributions from ions not included in the cluster were obtained via lattice sums using the lowest multipole moments obtained for the cluster ions. Vₓₓ was found to be negative for both a and Ï₆ ions except for Ï₆ in Ca₃Al₂Si₃O₁₂. For 27Al and 67,71Ga the sign of the quadrupole coupling constant has not been determined experimentally. Our results are, however, consistent with the signs found from Mössbauer meas-

06.7-8 FORMAL ATOMIC CHARGES IN CUBIC BORON-NITRIDE BN. By A. Kirfel, B. Josten and G. Will, Mineralogisches Institut der Universität Bonn, Lehrstuhl für Mineralogie und Kristallographie, Poppelsdorfer Schloß, D-5300 Bonn, FRG.

Accurate measurements of X-ray structure amplitudes (up to s = 1.38 Å⁻¹) and ensuing structure refinements have been used to calculate structure factors for spherical charge integrations around the atomic sites (Sasaki et al., Acta Cryst. (1980) A36, 904). Charge values Z(R) were corrected for Fourier series termination effects and investigated in terms of radial charge distributions dZ/dR and their derivatives d²Z/dR² indicating effective atomic radii of 0.83 Å for N, and consequently 0.73 Å for B. The corresponding electron counts yield 5.99 el (N) and 3.04 el (B). Thus, the spheres describing 34.1 % of the unit cell volume contain 75.25 % of the electrons in the unit cell. Distributing the remaining more delocalized electrons equally on B and N renders a significant charge transfer T = 0.47 el from B to N emphasizing the ionic contribution to the B-N bond. Results are compared to corresponding calcula-

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