06. CHARGE, SPIN AND MOMENTUM DENSITIES

06.X-5 From Spin Densities to the Ground State of Unpaired Electron Systems

P. Becker
Institut Laue-Langevin, 156X, 38042 Grenoble Cedex

It is first shown that the parameters which govern charge and spin densities are essentially of same origin and relations among them are specified. However, there are subtleties apparent in the spin density \( \rho_s - \rho_p \) which are hardly seen.

After a review of the theoretical aspects and of the possible modelisation of polarised neutron data, a few examples will be discussed, including organic radicals and more common transition metal compounds. The examples will be discussed, including organic radicals and more common transition metal compounds. The emphasis will be put on the comparison between charge deformation or valence density and unpaired electron density. The case of non pure spin case (occurrence of unpaired electrons) will be discussed. The comparison with magnetic resonance data will be commented on specific examples.

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06.X-6 THEORETICAL AND EXPERIMENTAL STUDIES OF MOMENTUM DENSITIES IN METALS, SEMICONDUCTORS AND INSULATORS.* By Vedene H. Smith, Jr., Department of Chemistry, Queen's University at Kingston, Kingston, Ontario, K7L 3N6, Canada.

From Compton scattering of X-rays or \( \gamma \)-rays and from the angular correlation of \( 2\gamma \)-annihilation in positron experiments, one may obtain information about the momentum density, \( \rho (\mathbf{p}) \). Since \( \rho (\mathbf{p}) \) is defined from the square of the electron wavefunction in momentum space whereas \( \rho (\mathbf{r}) \) is defined from the square of the electron wavefunction in position space, complementary and independent information on that provided by X-ray and \( \gamma \)-ray diffraction experiments is available. The relationship among these various electron distributions and their transforms (\( \rho (\mathbf{p}) \) and \( \rho (\mathbf{r}) \)) will be discussed. Emphasis will be placed on examples drawn from recent experiments and calculations for metals, semiconductors and insulators.

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