

06.4-3 ELECTRON MOMENTUM DISTRIBUTION IN AMORPHOUS AND CRYSTALLINE TiCu AND TiCuH_x VIA γ -RAY COMPTON SCATTERING.* BY G. Bambakidis, Physics Department, Wright State University, Dayton, Ohio U.S.A., and I. Theodoridou and N. G. Alexandropoulos, Physics Department, University of Ioannina, Ioannina, Greece.

The one-dimensional electron momentum distribution for amorphous and crystalline samples of TiCu and TiCuH_x was deduced from the Compton line profile $J(q)$. The profile was obtained using a Compton spectrometer and a 500 mCi ²⁴¹Am annular source, following the same procedure utilized previously in a study of the NbH_{1.2} system (Theodoridou and Alexandropoulos, Zeit. Phys. B, to be published). The experimental results are compared to the momentum distribution obtained from a cluster calculation of the electronic structure of TiCu and TiCuH_x, based on the Johnson-Slater X α -scattered wave method.

The TiCu-H system has been better characterized than most crystalline/amorphous hydrides, which together with the availability of appropriate samples make this system an attractive one for isotropic Compton scattering studies.

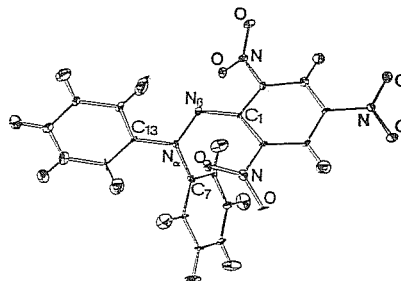
*partially supported by a NATO Research Collaboration Grant.

06.4-4 ON THE STRUCTURAL FACTORS OF BRAGG REFLECTIONS IN DIAMOND AND SILICON CALCULATED BY THE METHOD OF BONDING FUNCTIONS. By N.V. Shokhirev, Inst. of Chem. Kinetics, Sib. Branch of the Academy of Sciences, 630090 Novosibirsk and Yu.A. Rosenberg, L.I. Kleshchinsky, L.G. Andrievskaya, Inst. of Transp. Engineers, 664074 Irkutsk, USSR.

The wave function for the ground state of crystals with a diamond structure consists of bonding functions and atomic orbitals of the core, the overlap of the inner orbitals of a given atom and the valence orbitals of neighbours is neglected. These wave functions are used to calculate X-ray structural factors. The calculations take into account the overlap density of neighbouring $(2N+1)^2-1$ diatomic cells. The overlap integral matrix is inverted by the three-dimensional Fourier transformation. The calculations are carried out for $N=2$; a further increase in N does practically not affect the data obtained. The calculated results demonstrate a weak dependence of the ratio between S- and P-orbit populations upon the hybridization degree. The calculated structural factors of the Bragg reflections differ from those in experiment by no more than 1% in silicon and by 3% in diamond. The structure factors of the forbidden 222 reflection are systematically twice as low as those in experiment which results from the quality of the atomic orbitals employed (B. Roos, P. Seigbahn, Theor. Chim. Acta 17, 209, 1970) and from the neglect of anti-bonding orbits at deriving the wave function.

06.4-5 DETERMINATION BY POLARIZED NEUTRON DIFFRACTION OF THE SPIN DENSITY DISTRIBUTION IN A NON-CENTROSYMMETRICAL CRYSTAL OF DPPH: C₆H₆. By J.-X. Boucherle, B. Gillon, J. Maruani and J. Schweizer, CMOA du CNRS, DRF/DN du CENG and ILL, BP 156X, 38042 Grenoble Cedex, France.

The spin density distribution of the stable free radical diphenylpicrylhydrazyl has been studied in the crystalline form DPPH: C₆H₆ (Acta Cryst., to be published) at low temperature, with the magnetic moments oriented by an external field. It has been represented by a multipolar expansion on the different atoms, the coefficients of which have been determined by comparison with the flipping ratios measured by polarized neutron diffraction (Boucherle, Gillon and Schweizer, Proc. Int. Symp. Neut. Scat., Amer. Inst. Phys. (1982), 333). The spin density distribution thus obtained confirms and specifies the results from magnetic resonance, particularly the wide delocalization of the unpaired electron, including π - π and π - σ spin polarization effects, and the theoretical models used to relate hyperfine couplings to spin populations and conformational angles (Mol. Phys., to be published).



The structure of DPPH in DPPH:C₆H₆

06.5-1 THE EFFECT OF ANHARMONIC MOTIONS ON ATOMIC POSITIONS, BOND LENGTHS AND DEFORMATION DENSITIES. By C. Scheringer, Institut für Mineralogie der Universität Marburg, D 3550 Marburg, Federal Republic of Germany.

The positions of the atoms, i.e. the positions of the origins of the probability density functions (pdf's), depend on the definition of the pdf and the temperature factor which is actually used in the refinement. If there are no first order terms in the reciprocal lattice vector h , the mean positions (means of the pdf) are determined. If there are first order terms in h , other positions are defined. It is shown how the mean positions can be calculated from the temperature factors. When the temperature factor is formulated in the isolated - atom - potential approach, the maximum of the pdf is determined in the refinement. For temperature factors which contain the bond-length correction of molecular librations, correspondingly altered positions are determined.

Defining the temperature factor so that the mean positions are obtained, is advantageous in several respects. No first order terms of h need be considered in programming. The harmonic temperature factor is a simple Gaussian function. Anharmonic expansions need not be corrected for terms which are merely due to the choice of the origin of the pdf other than its mean.

In least-squares refinements, with the same set of data, harmonic and anharmonic temperature factors usually do not give the same estimates of the mean positions and, hence, not the same estimates of the bond lengths. The problem of parameter bias that arises here, is analyzed. It