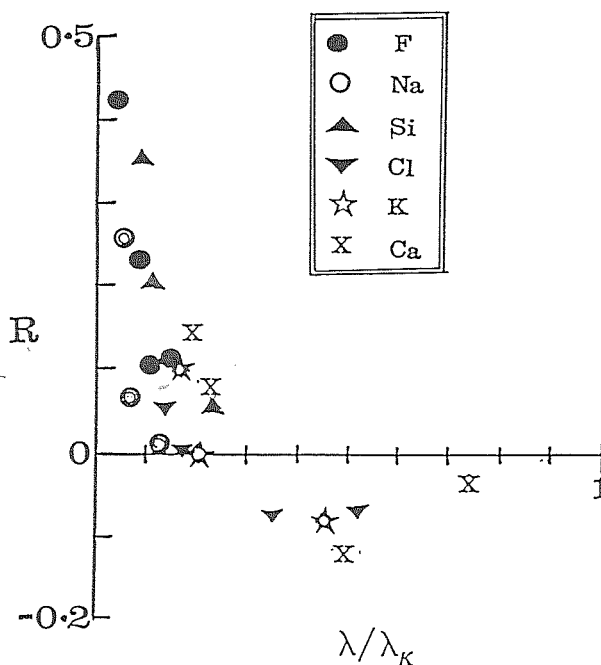


06.7-3 PSEUDOATOM SEPARATION METHOD AND CHARGE MOMENTS CALCULATIONS FROM ELECTRON DENSITY DISTRIBUTION. By G.A. Ivanov-Smolenskij, V.G. Tsirel'son, R.P. Ozerov, Mendeleev Institute of Chemical Technology, Moscow, USSR.

The results of pseudoatomic fragments (pseudoatoms) charge moment calculations according to formula $\langle A \rangle_i = \int_V g(\vec{r}) \hat{A}(\vec{r}) w_i(\vec{r}) dv$ are presented. Here $\langle A(\vec{r}) \rangle$ is the average value of operator $A(\vec{r})$ with pseudoatom in the crystal, $g(\vec{r})$ - X-ray electron density function, $w_i(\vec{r})$ - separation function responsible for the volume of i th pseudoatom. Charge Q , mean distance of electrons from nucleus $\langle r \rangle$ and diamagnetic susceptibility of pseudoatom χ have been determined. The separation functions suggested by Coppens (FC) (Adv. Quant. Chem. (1977) 10, 1) and Hirschfeld (FH) (Theor. Chim. Acta (1977) 44, 129) were used for calculations. Modification of FC in which atom radii were substituted by $\langle r \rangle / Q$ is suggested. Self-consistent results can be obtained with this modification. Application to χ determinations has shown that the experimental magnetic measurement values agree well with the results of calculations. Using FH there produced χ values unreasonably higher than the measured ones. This reflects the fact that FH describe the inner electrons better than the outer ones. Modification of FH in which free atom density function g , replaced by g^N is proposed. The calculated values of Q , $\langle r \rangle$ and χ converge to constants at $N > 6$. The methods were tested on some alkali halides.



06.7-4 EVIDENCE OF A SYSTEMATIC ERROR IN THE TABULATED VALUES OF $f'(\omega, 0)$. D.C. Creagh, Physics Department, Royal Military College, Duntroon, A.C.T. 2600, AUSTRALIA.

Both conventional LLL and Ångström ruler interferometers have been used to measure the x-ray refractive index and hence $f'(\omega, 0)$ for six low atomic number elements at the characteristic $K\alpha_1$ wavelengths of Ag, Mo, Cu, Fe and Cr. The results presented pertain to F, Na, Si, Cl, K and Ca. Significant differences from the theoretical calculations are apparent for the short wavelength measurements whereas the difference is small at longer wavelengths.

Most argument between those interested in the theory of x-ray scattering has centred on the type of analysis considered to be appropriate: whether one should use non-relativistic second order perturbation theory, or whether one should use relativistic quantum mechanics. The tabulation in International Tables IV is derived using relativistic Dirac-Hartree-Fock-Slater techniques. These results differ from those derived by using the Kramers-Kronig transform of the atomic photo-electric scattering cross-sections by the addition of a constant term related to the total self consistent field energy of the electrons. The application of relativistic methods of analysis causes a SHIFT IN POSITION of the $f'(\omega, 0)$ curve but no change in shape.

That the results of the interferometer experiments show that a CHANGE IN SHAPE occurs is demonstrated in the figure where the relative error $R = (f'_{\text{exp}} - f'_{\text{theor}}) / |f'_{\text{theor}}|$ is plotted in terms of the dimensionless parameter (λ / λ_K) for all six elements. λ_K is the wavelength of the K-shell absorption edge.

If the theoretical and experimental values of $f'(\omega, 0)$ differ only by a constant a hyperbolic curve would be expected for each atom. The more complicated dependence of R with (λ / λ_K) indicates that a wavelength dependent correction term is required in the relativistic theory.

06.7-5 ELECTROSTATIC PROPERTIES OF PHOSPHORYLETHANOLAMINE AT 123 K FROM CRYSTAL DIFFRACTION. By B. M. Craven and S. Swaminathan, Department of Crystallography, Univ. of Pittsburgh, Pittsburgh, PA 15260 USA, H.-P. Weber, Max-Planck-Inst. f. Festkörperforschung, Heisenbergstr. 1, D-7000 Stuttgart 80, FRG, and R. K. McMullan, Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973 USA.

The charge density and electrostatic potential have been calculated for the PEA zwitterion at 123 K from neutron (2527 reflections, $\sin\theta/\lambda \leq 0.79 \text{ \AA}^{-1}$) and X-ray diffraction data (4150 reflections, $\sin\theta/\lambda < 1.3 \text{ \AA}^{-1}$) using Stewart's rigid pseudoatom model. Net charges are $-0.64(11)e$ for the PO_4 -group and $+0.49(5)e$ for the NH_3 -group, with molecular dipole moment $13(2) \text{ D}$. A layer of zwitterions from the PEA crystal structure is used as a model for the outer surface of a phospholipid bilayer. The electrostatic potential in sections parallel to this layer shows a checkerboard pattern of positive and negative regions.

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