

the insensitivity of $R_w(F^2)$ to the polarizing functions is evidently attributable primarily to their strong correlations with the atomic coordinates rather than to their inaccessibility with the present X-ray data. These correlations are a consequence of an overall similarity between the scattering factors φ'_0 and the derivatives of the structure factors (of the static density) with respect to the corresponding atomic coordinates. They are therefore unlikely to be substantially reduced even at much lower temperatures and with much higher resolution. A more promising strategy might be the collection of extremely precise neutron data sufficient to establish the nuclear positions to within about 0.0001 Å. If the core polarization is indeed of the form given by the functions ρ'_0 defined above, an uncertainty Δr in atomic position corresponds to an approximate uncertainty in electric field, due to the correlation between them, of

$$\Delta E \sim 2Z^3 \Delta r / 3a_0^3.$$

This assumes an error in the coefficient of ρ'_0 sufficient

to displace the centroid of the two-electron core by $\sim \Delta r$. For the atoms C, N, and F, an error in position of 0.0001 Å as derived by neutron diffraction would lead to an error of about 0.10, 0.15, and 0.33 eÅ⁻², respectively, in the field at the nucleus from this source alone if the coefficients c'_0 were refined without constraint.

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