Modification of The Atomic Scattering Factor in Electric Field

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Quantum mechanical calculations of a modification of the X-ray scattering form factor of an atom/ion in an electric field using a three parameter wave function have been performed. These calculations are compared with the previous two parameter wave function calculations. The X-ray atomic scattering factor for an unperturbed atom with N electron is given by:

$$f_0 = \sum_{j=1}^{N} \psi_0^* \exp(i\chi S \cdot r_j)\psi_0 d\tau = \sum_{j=1}^{N} \psi_0^* \exp(iKr_j \cos\theta_j)\psi_0 d\tau$$

In the presence of an electric field F, the wave function is perturbed,

$$f = f_0 + if_1F + O(F^2) \text{ where } if_0F = 2F \sum_{j=1}^{N} \int \psi_0^* \exp(iKS \cdot r_j)\psi_1 d\tau$$

We use the Kirkwood - Pople-Schofield approach for the wave function

$$\psi = \psi_0 \left[1 + \sum_j u(r_j)\right] \text{ where } u(r) = F(\mu r + \nu r^2 + \eta r^3) \text{ and the } f_1 \text{ is given by}$$

$$if_1F = 2F \sum_i \sum_j \psi_0^* \exp(iKS \cdot r_j)(\mu r_i + \nu r_i^2 + \eta r_i^3) \cos\theta_i \psi_0 d\tau$$

The optimal values of μ, ν and η are determined variationally and calculated from various moments of the unperturbed charge distribution using a single Slater determinant.

	Ne		Na^+		Fe^-	
K	(a)	(b)	(a)	(b)	(a)	(b)
0.2	0.522	0.524	0.206	0.207	2.19	2.21
0.6	1.330	1.314	0.563	0.542	4.520	4.450
1.0	1.620	1.581	0.775	0.743	3.932	3.661
1.4	1.450	1.391	0.821	0.806	2.378	2.239
1.8	1.043	1.004	0.731	0.716	0.991	0.930
2.2	0.604	0.583	0.566	0.560	0.012	0.006
2.6	0.206	0.201	0.383	0.371		
3.0	0.023	0.020	0.211	0.200		

(a) Two parameter wave function
(b) Three parameter wave function

Table 1: *The magnitude of the modified X-ray scattering factor per unit applied field with scattering vector K in inverse atomic units.*

References

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