

SHORT COMMUNICATIONS

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A note on the values of the ratio of the imaginary to the real part of the atomic scattering factors for the X-ray Kα<sub>1</sub> and Kβ<sub>1</sub> radiations.\* By V. PARTHASARATHI and S. PARTHASARATHY, Centre of Advanced Study in Physics, University of Madras, Guindy Campus, Madras-600025, India

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The values of the ratio (k) of the imaginary to the total real part of the atomic scattering factor are obtained for atoms with Z=10 to 98 for the Kα<sub>1</sub> and Kβ<sub>1</sub> radiations of Cr, Fe, Cu, Mo and Ag. Numerical tables contain the value of k corresponding to the forward direction (denoted by k<sub>0</sub>) and the average values of k for the ranges θ=0 to 50° and θ=0 to 90° (denoted by k̄<sub>50°</sub> and k̄<sub>90°</sub> respectively).

The probability distributions of quantities such as the normalized Bijvoet differences x and Δ (Parthasarathy & Srinivasan, 1964), Bijvoet ratio δ (Parthasarathy, 1967; Parthasarathy & Parthasarathi, 1973), anomalous phase angle α<sub>A</sub> (Parthasarathy, Sabesan & Venkatesan, 1970), and the phase angle error θ (Parthasarathy, 1965) are found to depend on the parameter k [=Δf''/(f<sub>0</sub>+Δf'')]† which is the ratio of the imaginary to the total real part of the atomic scattering factor of the anomalously scattering atoms in the unit cell. Further it can be seen (see the above references) that the distributions of x, Δ, δ, α<sub>A</sub> and θ are more sensitive to variations in the value of k than in the other parameter (i.e. σ<sub>i</sub><sup>2</sup>) defining the relevant distributions. It is therefore useful for the purpose of ready reference, to tabulate the values of k for various atoms for different X-radiations.

Though the value of the imaginary part Δf'' (which owes its existence to the inner-most electrons) of an atom for a given wavelength could be taken to be practically constant for various values of the Bragg angle θ, the quantity k will be a monotonically increasing function of (sin θ)/λ (abbreviated as s), owing to the marked fall of the atomic scattering factor f<sub>0</sub> with increasing s. The average values of k over the various values of s for a few atoms for Cu Kα and Mo Kα radiations have been calculated by Parthasarathy (1967) and it can be seen that the average value k (denoted hereafter by k̄) of an atom for a given wavelength is significantly different from the value corresponding to the forward direction (denoted by k<sub>0</sub>). Since, for the application of the theoretical distributions of x, Δ, δ, α<sub>A</sub> and θ the value of k̄ is more important than that of k<sub>0</sub>, we shall evaluate k̄ for atoms with Z=10 to Z=98. In some actual crystals, because of thermal vibrations, the reflexions for which θ is large (say, θ>50°) may be too weak to be measured (see Hall & Maslen, 1965). It would therefore be useful to have the values of k̄ for the range θ=0 to 50° as well. Since the

Table 1. Values (%) of the ratio of the imaginary to the total real part of the atomic scattering factors for the Kα<sub>1</sub> radiations of Cr, Fe, Cu, Mo and Ag

Table with columns for ATOM, CrKα1, FeKα1, CuKα1, MoKα1, and AgKα1, and sub-columns for k0, k50, k90. Rows list elements from Be to Pb.

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† The atomic scattering factor of an anomalous scatterer is a complex quantity and is usually written as f=f<sub>0</sub>+Δf'+iΔf''.

k<sub>0</sub> is the value of Δf''/(f<sub>0</sub>+Δf') corresponding to the forward direction (θ=0); the quantities k̄<sub>50°</sub> and k̄<sub>90°</sub> are the average values of k corresponding to the ranges θ=0 to 50° and θ=0 to 90° respectively.

