

PS02.09.15 PROBABILITY DISTRIBUTION OF STRUCTURE FACTORS AND THE ROLE OF ATOMIC HETEROGENEITY. Anuradha Mukhopadhyay*, G. B. Mitra† and G. Mostafa†, *Department of Physics, Jadavpur University, Calcutta-700032, †Indian Association for the Cultivation of Science, Calcutta-700032, India

The effect of atomic heterogeneity on the exact probability distribution of structure factors has been studied by regulating two factors $p=N_H/N_L$ and $g=f_H/f_L$ (N_H, N_L : number of heavy and light atoms in the asymmetric unit; f_H, f_L : atomic scattering factors for heavy and light atoms respectively). A number of real examples of various p and g values indicating different degrees of heterogeneity have been studied. We have defined a modified structure factor E' in cases of atomic heterogeneity and shown that E' is Gauss distributed irrespective of whether E is Gauss distributed or not. In general the curves of $P(E)$ vs E show humps, oscillatory in nature, the oscillations being about the Gaussian fall of $P(E')$ vs E' curve. Depending on the values of p and g the agreement between the two distributions vary from being poor to excellent. In cases where the agreement is excellent it should be possible in principle, to obtain the heavy atom position. Though it seems apparent that heterogeneity should increase with the increase of the number of heavy atoms present, it is a noteworthy observation that this is true upto a certain value of p following which any increase in p decreases the heterogeneity. An explanation for this observation has been attempted.

The correspondence for the above distribution with the truncated Cauchy distribution has been compared for different degrees of heterogeneity.