EXPERIMENTAL DETERMINATION OF $\Delta f''$ FOR INDIUM BY X-RAY DIFFRACTION

R.Saravanan and S.K.Mohanlal,
School of Physics,Madurai Kamaraj University,Madurai-625021.

X-ray anomalous scattering is well known and considered as an important crystallographic technique with several applications.For its valid application, precise values of real and imaginary anomalous dispersion correction terms are needed. Although various methods of theoretical calculations are available in literature it will be appropriate that more experimental determination of such terms are useful for comparison.

In the present experimental work accurate measurements of X-ray intensities of Bijvoet pair reflections were carried out using an extended face of InP single crystal.The choice is made because of the simplicity of the non-centrosymmetric (ZnS type) struture and availability of pure flat plate crystal for such studies. The experimental data for CuK_α radiation were collected following the method of Barnea /1/ who discussed specific advantages of using flat plate crystals instead of spherical samples employing a home-built manual x-ray diffractometer. As shown in table, the close agreement of the measured Bijvoet ratio with the calculated values indicates the accuracy of the present measurements and justifies the determination of $\Delta f''$ values for the heavier atom In. The appreciable intensities for the even type Bijvoet reflections, which are forbidden in principle, show the effect of anharmonicity and bonding features in InP. Following the theory and application of Engel and Sturm /2/ the present experimental data were processed to yield the imaginary anomalous dispersion correction term $\Delta f''(In) = 5.03 \pm 0.3$ which compares very closely with the theoretically obtained value /3/ $\Delta f''(In) = 5.045$ for CuK_α radiation.

hkl	Bijvoet ratio			
	Measured	Calculated	Calculated*	X
111	0.069	0.085	0.120	0.58
311	0.089	0.093	0.138	0.64
331	0.125	0.112	0.161	0.78
511	0.128	0.123	0.180	0.71
531	0.149	0.135	0.197	0.76
533	0.159	0.144	0.210	0.76
222	0.007	0.000	0.000	-
422	0.011	0.000	0.000	-
200	0.015	0.000	0.000	-
400	0.013	0.000	0.000	-
600	0.018	0.000	0.000	-

*Without dispersion correction for light atom.

References:

/1/ Z. Barnea- in "Anomalous Scattering " Ed. by S.Ramaseshan and S.A.Abrahams, I.U.Cr, Munksgaard, Copenhagen, p.289(1975).
/2/ D.W.Engel and M.Sturm,ibid p.93 (1975).
/3/ International Tables for X-ray crystallography. I.U.Cr,Vol.IV The Kynoch press, Birmingham, p.949(1974).