

The present result is closer to that of Kipic, *et al.*, which in turn means that the present value indicates a different penetration parameter. Using the present experimental value for the L-shell conversion coefficient and the theoretical 'no penetration' values, the penetration parameter is estimated to be $\lambda = 11 \pm 3$. The value is not inconsistent with the systematics of Subba Rao⁹, who fitted the penetration parameters in an empirical relation with $M 1$ retardation factors.

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ON THE CONVERSION OF THE 192 keV TRANSITION IN ^{114}In

THE 192 KeV transition in the decay of the isomeric state ^{114m}In , is extensively used as a standard gamma ray for energy and efficiency calibration of NaI(Tl) and Ge(Li) detectors. The most widely referred to conversion work on this transition is that of Hoffmann¹ who employed an anthrasene split crystal and obtained using peak-to-beta counting method $\alpha_{\gamma} = 4.3 \pm 0.4$ and $\alpha_{\beta} = 2.8 \pm 0.5$. The latter value was extracted using the K/L value of 2.0 ± 0.6 . The values of K/L and K/L + M obtained by other authors² were at variance with the value obtained by Hoffmann, values of 1.12 to 2.0 being

reported. A careful measurement of the K-conversion coefficient is therefore carried out in the present study. In view of the simple decay scheme associated with this isotope, K X-ray-to-gamma ray method is applicable in this case. However, a Ge(Li) spectrometer system is employed to separate out the interfering events from the genuine ones.

It is well established² that ^{114m}In decays by the isomeric transition in 96.6% of the cases and by electron capture to levels in ^{114}Cd in the remaining 3.4% of the cases. The ground state decay of the ^{114}In is mostly associated with the negatron decay to ^{114}Cd . The nature of the 192 keV isomeric transition is established to be E4, the connecting state characteristics being well established to be 5 and 1+. The internal conversion of the 192 keV transition in ^{114}In gives rise to In K X-rays while the electron capture decay contributes to the X-rays of Cd. However, since the energy difference of these X-rays is small, they are counted together. The total contribution of the X-rays through the electron capture is estimated employing the percentage branches, the K-capture probability P_K , the internal conversion associated with the gamma rays associated with Cd and the fluorescent yield of Cd. The K-capture probability is estimated using the relations furnished by Martin *et al.*³. The K-conversion coefficients are obtained from literature⁴ and the fluorescent yields are obtained from the data of Bambynek *et al.*⁵. The total contribution to the X-ray peak thus estimated is found to be 6%, the remaining 94% being due to the conversion of the 192 keV transition. Since the contribution is small, the error associated with the contribution could be neglected. Thus, after correcting for the small other contributions, the K X-ray intensity could be used together with the gamma ray intensity to evaluate the K-conversion coefficient using the relation

$$\alpha_K (192 \text{ keV}) = \frac{N_x}{N_\gamma} \cdot \frac{\epsilon_\gamma}{\epsilon_x} \cdot \frac{1}{\omega_K} \quad (1)$$

where N's are the intensities, ϵ 's are the relative photopeak efficiencies and ω_K is the K-shell fluorescent yield in In.

The radioactive source ^{114m}In is obtained from the Isotope Division, BARC as InCl_3 in HCl solution and a few drops of the source liquid dried over a mylar foil over a perspex frame are employed for the determination of the conversion coefficient. The source is directly mounted on the cryostat arm of the 35 cc coaxial Ge(Li) detector and the spectrum is recorded on a ND 512 channel analyzer. The relative efficiency calibration is carried out using auxiliary sources ^{152}Eu , ^{133}Ba , ^{75}Se and ^{57}Co . Using the intensities N_x and N_γ under the X-ray

and gamma lines together with the relative efficiencies and $\omega_k = 0.850 \pm 0.029$ taken from the data of Bambynek *et al.*,⁵ the final value of α_k is obtained as

$$\alpha_k (192 \text{ keV}) = 2.00 \pm 0.09$$

The error is mostly contributed by that in the fluorescent yield, the error in the statistics of counting being only of the order of 1%. The present value is more accurate than the value reported in the Nuclear Data Sheets. The theoretical value obtained from the computer interpolation programme of Hager and Seltzer⁶ for a 191.6 keV transition of E4 type is 2.48. The present value of the experimental conversion coefficient is smaller than the theoretical value by $(19 \pm 4)\%$. It may be recorded that Raman *et al.*⁷ concluded in their survey that the conversion coefficients of high multipole transitions (E3, M4) to show discrepancies between theory and experiment. The present transition which is an E4 follows the same trend, but it is of interest to note that deviation is much larger. The gamma ray transition probability is found to show a hindrance of about 30 over the single particle estimate (Moszkowski), in correlation with the present anomalous conversion coefficient. This is indicative of the differences in the structure of the connecting states.

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THE CRYSTAL STRUCTURE OF TRIGLYCINE CALCIUM BROMIDE

THE crystal structure of diglycine calcium chloride tetrahydrate was already reported¹ and the structure determination of the addition compound of glycine with calcium iodide is under progress. This is a preliminary note reporting the atomic coordinates

in the crystal structure of triglycine calcium bromide.

The single crystals of triglycine calcium bromide $[(\text{NH}_2\text{CH}_2\text{COOH})_3\text{CaBr}_2]$ were grown from a saturated aqueous solution containing glycine and calcium bromide. The crystal data are as follows: $a = 8.97$, $b = 14.74$, $c = 20.30$ Å, $V = 2681.5$ Å³, $F. W = 425.1$ gm., $D_{\text{meas}} = 2.06$ gm. cm⁻³, $D_{\text{cal}} = 2.10$ gm. cm⁻³, $Z = 8$, $\mu (\text{CuK}\alpha) = 114.7$ cm⁻¹ and the space group is $\text{Pbc}2_1$ which is confirmed by structure analysis. The density was measured by flotation, in a mixture of bromoform and carbon tetrachloride.

The three-dimensional intensity data (Hkl , $\text{H} = 0$ to 8, $\mu r \approx 1.02$; hKl , $\text{K} = 0$ and 1, $\mu r = 1.21$) were collected using $\text{CuK}\alpha$ radiation by the multiple-film equi-inclination Weissenberg technique. The spot-shape, absorption, Lorentz and polarisation corrections were applied in the usual way. Peaks with coordinates $(0, 0, w)$ were absent in the Patterson synthesis indicating that the space group is non-centric. From sharpened and unsharpened three-dimensional Patterson syntheses, as well as from a three-dimensional minimum function, the positions of the four bromine atoms and the two calcium atoms in the asymmetric part were determined.

Thereafter, successive Fourier and difference Fourier syntheses revealed the rest of the structure. With isotropic thermal parameters for all the atoms, least-squares refinement was carried out using the LALS program (originally written by Gantzel, Sparks and Trueblood and modified later by Liminga of Uppsala and also in the University of Madras) on the IBM 370/155 computer, at the Indian Institute of Technology, Madras. For 1576 observed reflections, the residual index at present is 0.13. Further refinement is under progress. The present fractional atomic coordinates are recorded in Table I.

Each of the calcium atoms is coordinated to five oxygen atoms of the carboxyl groups and a bromine atom. The Ca-O distances range from 2.01 to 2.72 Å, and the Ca-Br distances are 2.93 Å and 3.02 Å. The glycine molecules have the normal bond distances and bond angles as found in other similar structures². The hydrogen bonds are between the nitrogen, oxygen and bromine atoms.

This compound was earlier assigned the chemical formula $(\text{NH}_2\text{CH}_2\text{COOH})_3\text{CaBr}_2 \cdot 4\text{H}_2\text{O}$, similar to that of the diglycine calcium chloride tetrahydrate¹. But, the present structure analysis undoubtedly confirms the chemical formula $(\text{NH}_2\text{CH}_2\text{COOH})_3\text{CaBr}_2$, the molecular weight of which is more or less the same as that of diglycine calcium bromide tetrahydrate,