# LETTERS TO THE EDITOR

## E 2 CONVERSION COEFFICIENTS

IN general the theoretical internal conversion coefficients are supposed to be accurate. But recently Raman et al.[1] showed that E3 and M4 theoretical values are over-estimations by a few per cent. Hence in the present investigations a comparison of the accurate experimental results and theoretical E2 K-conversion coefficients $(a_k)$ of Hager and Seltzer[2] is attempted to search for the possible discrepancies.

The method of Internal External Conversion (IEC) Technique for the measurement of internal conversion coefficients is standardised by Hultberg et al.[3] and many measurements are reported. However, the theoretical photoelectric cross sections used, are in general those of Grodstein[4] (accuracy ~5 to 15%) and Nagel et al.[5] (accuracy ~2%) which are not very accurate. In recent years, Scofield[6] reported very accurate theoretical photoelectric cross sections (accuracy ~0·1%). The validity of these values is established[7] Hence, most of the available E2 experimental internal conversion coefficients measured by the IEC technique[8-21] are corrected using the recent values of Scofield[6], thus improving the accuracy. To study the discrepancies between the theory and experiment, plots of [(Theory—Expt.)/Theory]% with proton number neutron number and transition energy are shown in Fig 1. In Fig. 1 the latest square fitted lines are also shown to study the variation of the discrepancy

From a study of Fig. 1. the following conclusions can be drawn: (1) The theoretical E2 conversion coefficients are over-estimations by a few per cent and
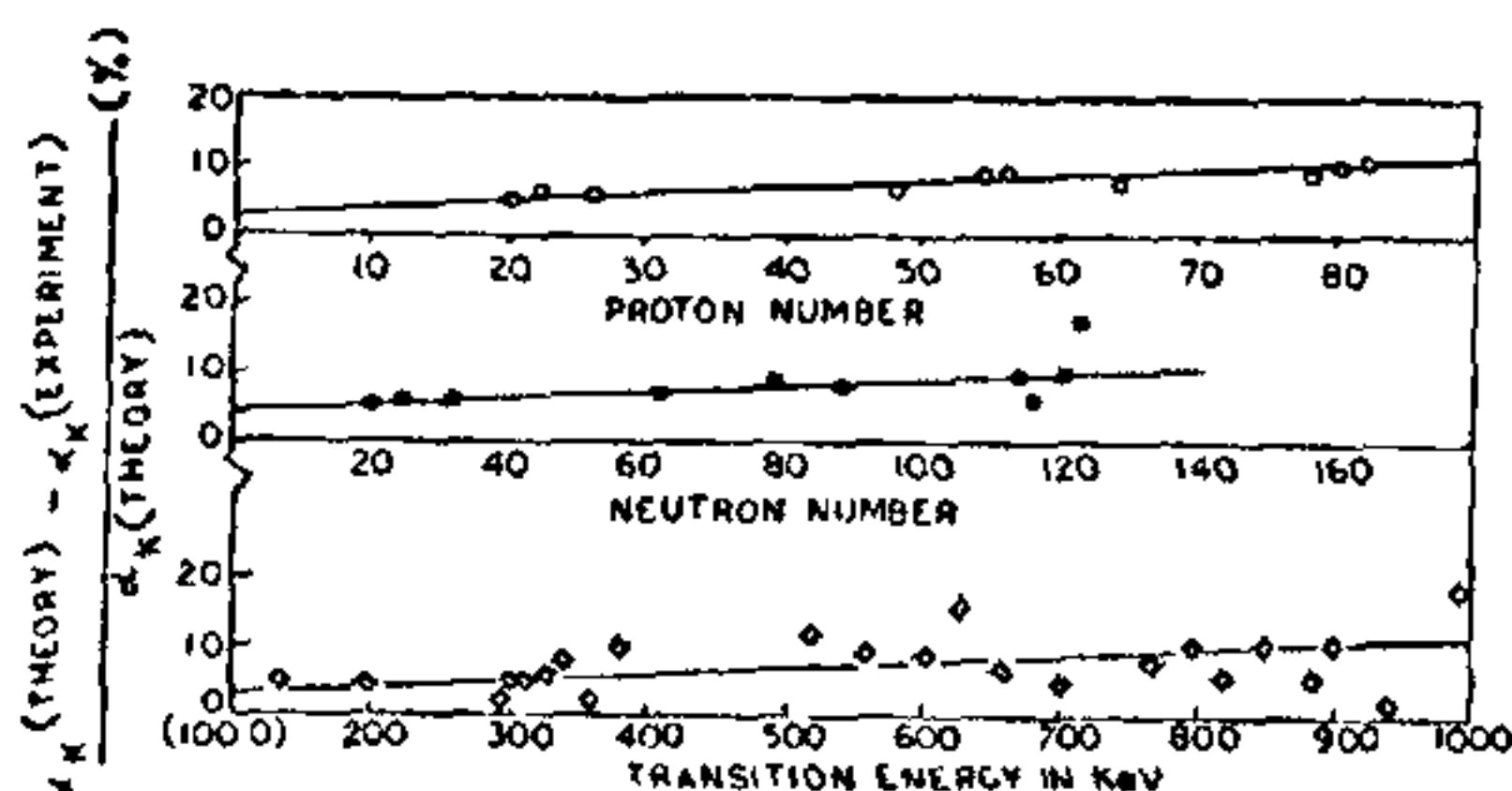


[ FIG. 1. Comparison between theoretical and experimental E2 conversion coefficients.

(2) the deviation between theory and experiment seems to increase with proton number, neutron number and the transition energy. These deviations may be due to the theoretical insufficiencies in the theoretical data of Hager and Seltzer[2].

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## STRUCTURAL STUDY OF ZnNbCuO₄

DURING the course of a of detailed study on ternary (XYZO₄ spinels) oxides[1], we could find that hardly any work is carried out on niobium-spinels, except Zn₂.₈₃ Nb₀.₀₇O₄[2] and ZnLiNbO₄[3]. Romeijn[4] has studied the spinel structure from geometrical considerations which lead to a condition for formation of oxidic spinel, i.e., the cationic radii should lie between 0·45 Å to 0·96 Å. The ionic radius[5] of Nb⁴⁺ and Nb⁵⁺ is 0·74 Å and 0·70 Å respectively,

As the ionic radius of niobium lies well within the spinel formation region, we thought it interesting to study $ZnNbCuO_4$. The compound has been prepared for the first time by intimately mixing together the reacting oxides of A.R. grade in proper molar ratio, under acetone. The mixture was heated in a platinum boat in air in an electric furnace at 900° C for about 70 hours. The sample was cooled in the furnace. The formation of the compound was checked by X-ray diffraction patterns taken on Debye-Scherrer camera of 114·6 mm diameter, using filtered copper radiation. The pattern indicated a single phase and absence of ines due to the reacting oxides.

The crystallographic results are included in Table I. All the observed reflections are indexed for orthorhombic unit cell with dimensions $a = 9.006$ Å; $b = 8.619$ Å and $c = 9.253$ Å. It is evident from the observed reflections that the compound crystallises in a face-centered Bravais lattice.

TABLE I

*Crystallographic data of $ZnNbCuO_4$*

| $d$(observed) in Å | $d$(calculated) in Å | $h\ k\ l$ |
|---|---|---|
| 3·231 | 3·228 | 2 2 0 |
| 2·737 | 2·712 | 3 1 1 |
| 2·583 | 2·583 | 2 2 2 |
| 2·313 | 2·313 | 0 4 0 |
| 2·117 | 2·154 | 0 0 4 |
| 2·026 | 2·024 | 4 2 0 |
| 1·868 | 1·857 | 2 4 2 |
| 1·759 | 1·774 | 1 5 1 |
| 1·674 | 1·665 | 1 1 5 |
| 1·599 | 1·613 | 4 4 0 |
| 1·515 | 1·516 | 6 0 0 |
| 1·440 | 1·434 | 0 0 6 |
| 1·369 | 1·367 | 5 3 3 |

$a = 9.006$ Å;    $b = 8.619$ Å    $c = 9.253$ Å

It is clear from the observed orthorhombic symmetry and the existence of planes like (420), (600), etc., that the compound is not a spinel. Though the ioric radius of $Nb^{5+}$ is suitable for the formation of a spinel structure, large difference of ionic radii (0·70 ∼ 0 96 Å) and charges of $Nb^{5+}$ and $Cu^{1+}$ might have been probably responsible for the instability for spinel structure.

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## METHOD OF DETERMINING AN INDEX OF THE INFLUENCE OF VIBRATION-ROTATION INTERACTION ON FRANCK-CONDON FACTORS IN 2-ATOM MOLECULES

IN the study of intensities of electronic spectra of diatomic molecules, it is usual practice to ignore the effect of vibration-rotation interaction[1] in the calculation of Franck-Condon (FC) factors. Learner and Gaydon[2] were the first to show the error resulting from the neglect of centrifugal distortion of the potential curve in the case of OH. Since the relative intensity distribution in the diatomic molecular band system is understood in terms of FC factors, the dependence of these quantities on the rotational quantum number J has been studied by several investigators[2-10] and is shown to be significant for some molecular transitions. It is the purpose of this note to report a simple method for understanding the dependence of FC factors on J.

The effective potential for a vibrating rotator has a minimum given by

$$r_0 = r_e\,[1 + 4\,B_e^2\,J\,(J + 1)/\omega_e^2] \tag{1}$$

which is more nearly tde equilibrium internuclear distance for the rotating molecule on the basis of the Morse-Pekeris model[11] with slight modifications[7] where $r_e$, $B_e$ and $\omega_e$ are the usual spectroscopic constants. Thus a principal effect of vibration-rotation interaction[6] is the displacement of the radial co-ordinate of the minimum to larger $r_0$ values with increasing J. The FC factor depends on $\Delta r_e$ ($= r_e' \sim r_e''$), the separation between the minima of the potential energy curves[12-14] for the two participating electronic states. Similarly FC factor $(q_{v'J'}^{v''J''})$ depends on $\Delta r_0$ ($= r_0' \sim r_0''$) in the present case. The difference ($\Delta r_0 - \Delta r_e$) could serve as an index for the influence of vibration-rotation interaction on FC factors.

The values of $r_0$ for different J have been calculated using the expression (1) for the various electro-