

in which

$$A = \sum_{MK} f_K(\epsilon) \int |D_{MK}|^2 d\Omega = \frac{16\pi^2}{5} (f_{\uparrow\uparrow} + f_{\perp}), \quad (8)$$

$$B_m = 8\pi^2 \sum_{MK} (-1)^{M-K} f_K(\epsilon) \begin{pmatrix} 2 & 1 & 1 \\ -m-M & M & \end{pmatrix} \begin{pmatrix} 2 & 1 & 1 \\ 0 & -K & K \end{pmatrix} \delta_{m_0} = \\ = 16\pi^2 (0, 1825)^2 (-2f_{\uparrow\uparrow} + f_{\perp}). \quad (9)$$

Here  $f_{\uparrow\uparrow}$  corresponds to oscillation along the axis of symmetry,  $f_{\perp}$  to oscillation perpendicular to that axis, and  $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$  are (3 - j) symbols [2].

We have  $\beta \approx 0.15$  for heavy strongly deformed nuclei; (7) gives the greatest anisotropy for isolated peaks at about 5%.

We can find  $f_K$  as a function of  $\epsilon$  from experiment (no satisfactory theoretical relation is available). All of the above formulas correspond to a single  $\gamma$ -ray energy, but the  $\gamma$ -ray source may be a betatron, in which case the angular distribution is governed by the maximum energy  $E_{\gamma m}$ :

$$w(\epsilon_m, \delta) = C' \{ J_{\uparrow\uparrow} (1 - 0,33 \beta Y_{20}) + J_{\perp} (1 + 0,17 \beta Y_{20}) \},$$

in which

$$J_{\uparrow\uparrow} = \int_{E_t}^{E_{\gamma m}} \frac{f_{\uparrow\uparrow}(\epsilon) d\epsilon}{\epsilon}, \quad J_{\perp} = \int_{E_t}^{E_{\gamma m}} \frac{f_{\perp}(\epsilon) d\epsilon}{\epsilon}.$$

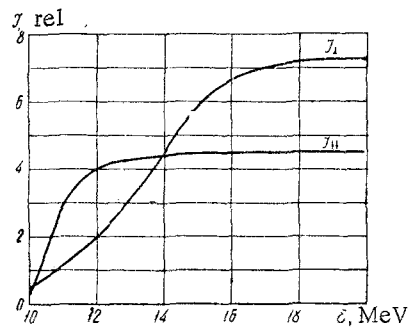


Fig. 1

Figure 1 shows  $J_{\uparrow\uparrow}$  and  $J_{\perp}$  as functions of  $E_{\gamma m}$  for typical values of the position and width of the giant resonance in strongly deformed nuclei. Here the anisotropy is about 3% in the most favorable cases.

Nuclei near  $A = 25$  have marked deformation, the most deformed being Mg-24 (ratio of semiaxes 1.8 : 1) [3], with  $\beta = 0.67$ . The anisotropy is about 27% for a line spectrum and 7% for a betatron spectrum ( $E_{\gamma m}$  at the maximum of the giant resonance). The smallness of the effect for heavy nuclei (about 3%) makes it difficult to observe, whereas for  $A \approx 25$  the effect is large enough (about 7%) to be observable.

#### REFERENCES

1. J. Levinger, Nuclear Photo-Disintegration [Russian translation], IL, 1962.
2. A. Edmonds, collection: Deformation of Atomic Nuclei [Russian translation], IL, 1958.
3. E. V. Inopin and B. I. Tishchenko, ZhETF, 37, 1308, 1959.

19 February 1964

Kirov Polytechnical Institute,  
Tomsk

#### SELECTION OF AN ABSOLUTE INTENSITY SCALE FOR RAMAN LINES

N. K. Sidorov and L. S. Stal'makhova

Izvestiya VUZ. Fizika, No. 3, pp. 162-163, 1965

Bernstein and Allen's formula [1]  $S = \frac{(5b'^2 + 7g'^2)_{\Delta\nu}}{(5b'^2 + 7g'^2)_{459}}$  for the standard intensity is used for determining absolute Raman intensities;  $b'$  is the trace of tensor  $\alpha'$  for the derivative of the polarizability with respect to the normal coordinate,  $g'$  being the anisotropy of that tensor. The unit of intensity on this scale is the quantity  $(5b'^2 + 7g'^2)_{459}$  found for the  $459 \text{ cm}^{-1}$  line, whose absolute value is  $34 \times 10^{-8} \text{ cm}^4/\text{g}$  [2]. If we use as standard the  $802 \text{ cm}^{-1}$  line of  $\text{C}_6\text{H}_{12}$ , the measure of the absolute intensity in the scale  $S = \frac{(5b'^2 + 7g'^2)_{\Delta\nu}}{(5b'^2 + 7g'^2)_{802}}$  is  $(5b'^2 + 7g'^2)_{802} = 24 \cdot 10^{-8} \text{ cm}^4/\text{g}$  [3].

But uniform illumination of the vessel in a plane perpendicular to the axis (as in the standard elliptical illuminator) makes it preferable to use the scale  $R = \frac{(5b'^2 + 13g'^2)_{\Delta\nu}}{(5b'^2 + 13g'^2)_{802}}$ , because this ratio can be evaluated by experiment with-

out measuring the degree of depolarization  $\rho$ , which has to be measured in order to obtain S [1].

Naberukhin [4] (see also [5]) has shown that  $f(\rho)$ , the relation of the measured integral intensity to  $\rho$  and to the geometry of the illumination in an elliptical system, varies by not more than 4% for  $\rho$  from 0 to 6/7.

Placzek's theorem gives [1, 3] that

$$R = \frac{(5b'^2 + 13g'^2)_{\Delta\nu}}{(5b'^2 + 13g'^2)_{802}} = \frac{Q}{Q_{802}} \frac{n^2}{n_{C_6H_{12}}^2} \frac{\sigma}{\sigma_{802}} \frac{M}{d} \left( \frac{d}{M} \right)_{C_6H_{12}} \frac{\Delta\nu}{802} \left( \frac{\nu - 802}{\nu - \Delta\nu} \right)^4 \frac{f(\rho)}{f(\rho_{802})}. \quad (1)$$

Here Q is the area under the line, n is the refractive index of the liquid,  $\sigma$  is the spectral sensitivity of the photomultiplier, M is molecular weight, d is density, and  $\Delta\nu$  is line frequency. It is simple to show that  $f(\rho)/f(\rho_{802})$  and  $f(\rho)/f(\rho_{459})$  may vary from 1 to 1.03 for the elliptical system for  $\rho$  between 0 and 6/7, so we may put  $f(\rho)/f(\rho_{802}) = 1$ , and R is virtually independent of  $\rho$ . This produces an error less than that from substituting in  $f(\rho)/f(\rho_{802})$  for the measured  $\rho$ , because the latter have 5-10% error. All the other quantities on the right in (1) can be found by experiment.

To find S requires measurement of  $\rho$ , whereas to find R does not, so  $(5b'^2 + 13g'^2)_{\Delta\nu}$  can be found without direct measurement of  $\rho$  (which is a difficult task). Also, the  $(5b'^2 + 7g'^2)_{\Delta\nu}$  arising in the determination of S differs from  $(5b'^2 + 13g'^2)_{\Delta\nu}$  in that the latter directly characterizes the absolute intensity, because Placzek's theory gives  $I_{\Delta\nu}$  as proportional to  $(5b'^2 + 13g'^2)_{\Delta\nu}$ , not to  $(5b'^2 + 7g'^2)_{\Delta\nu}$ . Then  $(5b'^2 + 13g'^2)_{802} = (5b'^2 + 7g'^2)_{802}(1 + \rho_{802}) = 26 \cdot 10^{-8} \text{ cm}^4/\text{g}$ , because  $\rho_{802} = 0.07$ . Measurement of R gives us the absolute line intensities as

$$(5b'^2 + 13g'^2)_{\Delta\nu} = R \cdot 26 \cdot 10^{-8} \text{ cm}^4/\text{g}.$$

#### REFERENCES

1. A. J. Bernstein and G. Allen, J. Opt. Soc. Amer., 45, 237, 1955.
2. J. Brandmüller and H. Schrötter, Zs. Phys., 149, 131, 1957; H. W. Schrötter, Zs. Electrochem., 64, 853, 1960.
3. N. K. Sidorov, L. S. Stal'makhova, and L. I. Bratanova, Optika i spektroskopiya, 13, 783, 1962.
4. Yu. I. Naberukhin, Optika i spektroskopiya, 13, 498, 1962.
5. P. A. Bazhulin and M. M. Sushchinskii, UFN, 68, 135, 1959.

15 April 1964

Chernyshevskii University,  
Saratov

#### BASIS FOR NEGLECTING OVERLAP INTEGRALS IN CALCULATIONS ON MOLECULAR SYSTEMS

V. G. Plotnikov

Izvestiya VUZ. Fizika, No. 3, pp. 163-164, 1965

The most usual method in calculations on molecules, MO-LCAO, employs parameters calculated by Mulliken's method [1], which has the disadvantage of neglecting overlap integrals without giving a convincing reason for this. The basic equation in MO-LCAO may be put as

$$Fc_{j\kappa} = \varepsilon_j Sc_{j\kappa}, \quad (1)$$

in which F is the matrix for the Fok hamiltonian, S is the matrix for the overlap integrals, the  $c_{j\kappa}$  are the coefficients in the expansion for the molecular orbital, and the  $\varepsilon_j$  are the energy levels.

The nondiagonal elements of (1) take the following form in the semi-empirical MO-LCAO method:

$$\beta_{i\kappa} - S_{i\kappa}\varepsilon_j, \quad (2)$$

in which

$$\beta_{i\kappa} = \frac{1}{2} S_{i\kappa}(\alpha_{ii} + \alpha_{\kappa\kappa}), \quad (3)$$

the  $\alpha$  being the diagonal elements.

We see from (2) and (3) that both terms in (2) are of the same order in S, so it would seem impossible to neglect