# APPENDIX - I

## A CALCULATION OF QUADRUPOLE MOMENT AND QUADRUPOLE COUPLING CONSTANTS OF $^3D_2$, $^3D_1$ AND $^1D_2$ LEVELS OF $^{105}Pd$

Nuclear quadrupole resonance (NQR) spectra result from transitions between energy levels that arise from the interaction of electric field gradients produced by the surrounding electrons with the electric quadrupole moment of the nucleus. Nuclear quadrupole coupling constants (B) and quadrupole moments (Q) provide very valuable information about the atoms. The values of quadrupole coupling constants of $^{105}Pd$ atom for its $^3D_3$ and $^3D_2$ levels have been determined experimentally by channappa and Pendlebury (1965) through atomic beam resonance studies. However, quadrupole moment of $^{105}Pd$ and B values for $^3D_1$ and $^1D_2$ levels of $^{105}Pd$ atom are not available in the literature. These values have been calculated using the experimentally determined value of B pertaining to the $^3D_3$ level.

The energy levels $^3D_3$, $^3D_2$, $^3D_1$ and $^1D_2$ of $^{105}Pd$ atom arising from the configuration $4d^9\ 5S$ are shown in figure 1. The quadrupole coupling constant B is defined by the equation

$$Q = B \frac{h}{e^2 q_J} \qquad \ldots (1)$$

where Q is the nuclear quadrupole moment and $q_j$ is the electric field gradient. In the present case (sd), which is a two electron problem of the configuration s l, the field gradient is due to a single d electron only because the charge distribution of the electron is spherically symmetric. The field gradient $q_j$ is directly related to $\langle 1/r^3 \rangle$ where r is the distance of the d electron from the centre of the nucleus. The relation between the two quantities $g_1$ and $\langle 1/r^3 \rangle$ (Lucken, 1969) is given by

$$q_j = \sum_{nlm} A^2_{nlm} \left[ \frac{3m^2 - l(l+1)}{l(2l+3)} \right] \frac{2l}{2l+3} \left\langle \frac{1}{r^3} \right\rangle_{nlm} R \quad \cdots (2)$$

The field gradients arising from the configuration s.l are particularly easy to deal with since there is only one orbital giving rise to the field gradient. This configuration, in the limit of Russel-Saunders coupling, gives four terms $^3L_{l+1}$, $^3L_l$, $^3L_{l-1}$ and $^1L_l$. Spin-Orbit coupling only mixes states having the same value of l, hence the field gradients in the terms $^3L_{l+1}$ and $^3L_{l-1}$ are independent of the coupling. Substitution of the well-known Clebsch-Gordan coefficients in equation (2) yield,

$$q_{j=l+1} = \frac{-2l}{2l+3} \left\langle \frac{1}{r^3} \right\rangle R \quad \cdots (3)$$

$$q_{j=l-1} = \frac{-2(l-1)}{l(2l-1)} \frac{(l+1)(2l-3)}{(2l+1)} \left\langle \frac{1}{r^3} \right\rangle R \quad \cdots (4)$$

The field gradient for the $^3L_1$ term for intermediate coupling is given by

$$q_{j=l} = \left[ C_1^2 \frac{(2l-1)(l+2)(2l)}{(l+1)(2l+1)(2l+3)} R' + C_2^2 \frac{2(l-1)}{(2l+1)} \cdot R'' - \frac{12 C_1 C_2}{(2l+1)} \frac{\sqrt{l(l+1)}}{(2l+3)} S_r \right] K \quad \ldots (5)$$

where R, R', R" and Sr are relativity corrections and $C_1$, $C_2$, $\theta_0$ and $\theta$ are given by

$$C_1 = \sin(\theta_0 - \theta), \quad C_2 = \cos(\theta_0 - \theta),$$

$$\theta_0 = \tan^{-1}\sqrt{l(l+1)}, \quad \sin^2\theta = \frac{\Delta}{D} \quad \ldots (6)$$

D is the separation between the levels $^3L_1$ and $^1L_1$ and $\Delta$ is the deviation of the term $^3L_1$ from the position it would have had in the case of pure Russel-Saunders coupling.

EVALUATION OF QUADRUPOLE MOMENT

We have (Kopferman, 1958),

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{\Delta T}{R \alpha^2 Z_i a_0^3 \, H_r(l, Z_i)\,(l + 1/2)} \quad \ldots (7)$$

where $\Delta T$ is the separation between the levels $^3D_3$ and $^3D_1$ and is equal to 3529.81 $cm^{-1}$ (figure 1), R, the Rydberg constant, $\alpha$, the fine structure constant, $Z_i$, the effective atomic number, Hr, the relativistic correction factor, and $a_0$ is the Bohr radius.

On substitution of the value of $\Delta$ T and the values of R, $\alpha$, $Z_i$ and Hr from the tables listed by Kopfermann (1958), the equation (6) reduces to

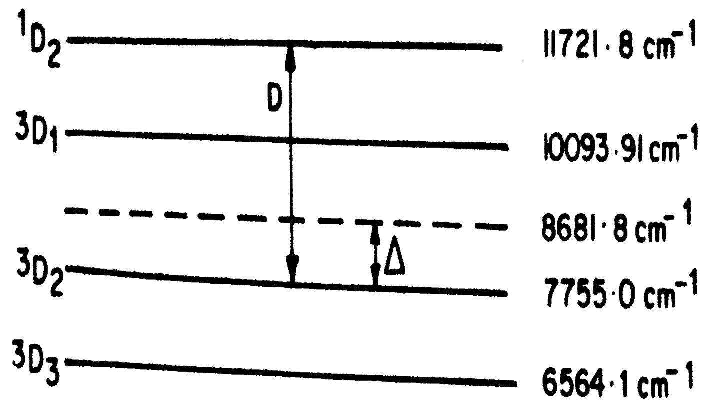


Fig. 1. Diagrammatic energy levels of $^{105}Pd$ atom

$$\langle \frac{1}{r^3} \rangle = 6.850\ a_0^{-3} \qquad \ldots (8)$$

Combining equations (1), (3) and (7) and using the value of B for $^3D_3$ level as 652.9 MHz, given by Channappa and Pendlebury (1965), we get the nuclear quadrupole moment of $^{105}Pd$ atom as $0.6923 \times 10^{-24}$ cm$^2$.

Using the above procedure one can estimate the value of Q in the case of atoms having 4d configuration. (Single 1 electron).

EVALUATION OF COUPLING CONSTANTS:

Quadrupole interaction constants for various levels are given by (Lurio et al., 1962),

$$B\ (^3L_{l+1}) = b_{l+1/2} \qquad \ldots (9)$$

$$B\ (^3L_{l-1}) = \frac{(2l-3)(2l+2)}{2l(2l-1)}\ b_{l-1/2} \qquad \ldots (10)$$

$$B\ (^3L_l) = \frac{(2l-1)(2l+4)}{(2l+1)(2l+2)}\ c_1^2\ b_{l+1/2} + c_2^2\ b_{l-1/2} - \frac{12 c_1 c_2 S_r}{2l\ (2l+1)} \left(2l/2l+2\right)^{1/2} b_{l+1/2} \qquad \ldots (11)$$

$$B(^1L_l) = \frac{(2l-1)\ (2l+4)}{(2l+1)\ (2l+2)}\ c_1'^2\ b_{l+1/2} + c_2'^2\ b_{l-1/2} - \frac{12 c_1' c_2' S_r}{2l\ (2l+1)} \left(2l/2l+2\right)^{1/2} b_{l+1/2} \qquad \ldots (12)$$

where $C_1'$ and $C_2'$ are correction factors similar to $C_1$ and $C_2$ ($C_1' = C_2$, $C_2' = -C_1$), Sr is another correction factor and b's are the single electron quadrupole elements given by the equation

$$b_j = \frac{2j-1}{2j+2}\ \frac{e^2Q}{h} \langle \frac{1}{r^3} \rangle R_j \qquad \ldots (13)$$

$R_J$ is a relativistic correction factor.

The various quantities required to calculate the B values for the different levels (through equations 9 to 12) are found and are given below.

$D = 3966.8\ cm^{-1}$; $\Delta = 926.8\ cm^{-1}$ (from Fig. 1).

Using equations (6) the constants C's are estimated as

| | | | |
|---|---|---|---|
| $C_1$ | = 0.1763 | $C_1'$ | = 0.9847 |
| $C_2$ | = 0.9847 | $C_2'$ | = -0.1763 |

Sr = 1.0213, from Kopfermann's (1958) table.

RESULTS AND DISCUSSION:

Using the calculated values of $Q$, $\langle 1/r^3 \rangle$ and other parameters, the values of quadrupole coupling constants for the different levels are calculated and found to be

$B\,(^3D_2)$ = 402.56 MHz,
$B\,(^3D_1)$ = 228.40 MHz, and
$B\,(^1D_2)$ = 577.27 MHz.

The calculated value of B for the $^3D_2$ level agrees very well with the experimental value of 398.19 MHz reported by Channappa and Pendlebury (1965). No comparison could be made of the values calculated for the other two levels as no experimentally determined or calculated values for these levels appear to be available at present.

## REFERENCES


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