

$$D = \frac{4\lambda^2(\Delta_0 - \Delta_1)}{\Delta_0 \Delta_1} \quad (3)$$

is valid for the zero-field splitting parameter D in the second order of perturbation theory. The notation is the same as in equation (2).

If both Δ_0 and Δ_1 do not essentially change then the change of D must be the result of a change in the difference, $\Delta_0 - \Delta_1$, which is equal to the splitting of the Γ_5 triplet by the trigonal distortion. This assumption and the experimental results permit to evaluate the change of g -tensor components described by equation (2).

Increasing the pressure from 0 to 12 kbar leads to a change of D by $180 \times 10^{-4} \text{ cm}^{-1}$ with $\lambda \approx 45 \text{ cm}^{-1}$ (for a crystal) and $\Delta_0 \approx \Delta_1 \approx 12000 \text{ cm}^{-1}$, then the g -tensor components should change by 0.0005, that is within the experimental error.

The change of hyperfine interaction can be evaluated by means of the change of D in the framework of the model used. The hyperfine field H^{hf} , acting on a nucleus is estimated by the numerical expression (4) (in G)

$$H^{\text{hf}} = 1.25 \times 10^5 \left\langle \frac{1}{r^3} \right\rangle \Delta g_L. \quad (4)$$

The value $\left\langle \frac{1}{r^3} \right\rangle$ is expressed in atomic units. The shift $\Delta g = -8\lambda/\Delta_0$ is written as Δg_L to outline that the shift of the g -factor has orbital nature and is not connected with the admixture of other spin substates to the ground state. This condition is fulfilled in the case of V^{2+} in octahedral surroundings, as the ground state of the ion is a singlet one.

From equation (4) using formulas (2) and (3) one can evaluate the change of the orbital hyperfine field (in G):

$$\delta H^{\text{hf}} = 1.25 \times 10^5 \frac{4}{3\lambda} \delta D \left\langle \frac{1}{r^3} \right\rangle. \quad (5)$$

For the V^{2+} ion $\left\langle \frac{1}{r^3} \right\rangle = 2.75$ at. units. Using the experimentally obtained change of D one finds $|\delta H^{\text{hf}}| \approx 190 \text{ G}$. At $p = 0$ $\Delta g_L = -0.02$ and $H^{\text{hf}} = -6.88 \text{ kG}$. With increasing pressure $|\Delta g_L|$ decreases and consequently $|H^{\text{hf}}|$ decreases, too,

which results in a decrease of the hyperfine structure constant.

References

- (1) E.S. ITSKEVICH, Prib. i Tekh. Eksper. 4, 148 (1963).
- (2) B. BLEANEY and R.S. RUBINS, Proc. Phys. Soc. 77, 103 (1961).
- (3) A. ABRAGAM and B. BLEANEY, Electron Paramagnetic Resonance of Transition Ions, Clarendon Press, Oxford 1970 (p. 431).
- (4) Hyperfine Interactions, Ed. A.J. FREEMAN and R.B. FRANKEL, Academic Press, New York/London 1967 (p. 118).

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