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

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_o and Δ_1 do not essentially change then the change of D must be the result of a change in the difference, $\Delta_o - \Delta_1$, 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 180x $\times 10^{-4}$ cm^{-1} with $\lambda \approx 45$ cm^{-1} (for a crystal) and $\Delta_o \approx \Delta_1 \approx 12000$ 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)

$$H^{hf} = 1.25\times10^5 \left\langle \frac{1}{r^3} \right\rangle \Delta g_L . \qquad (4)$$

The value $\left\langle \frac{1}{r^3} \right\rangle$ is expressed in atomic units. The shift $\Delta g = -8\lambda/\Delta_o$ 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):

$$\delta H^{hf} = 1.25\times10^5 \, \frac{4}{3\lambda} \, \delta D \left\langle \frac{1}{r^3} \right\rangle . \qquad (5)$$

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 $|\delta H^{hf}| \approx 190$ G. At $p = 0$ $\Delta g_L = -0.02$ and $H^{hf} = -6.88$ kG. With increasing pressure $|\Delta g_L|$ decreases and consequently $|H^{hf}|$ 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).

(Received August 1, 1975)