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CALCULATION OF ABSORPTION INTENSITIES OF Cr³⁺ ION PAIR
LINES IN RUBY

KEY WORDS: exchange-coupled pair, optical absorption intensities

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The calculation of relative intensities of the optical absorption lines of the fourth order pair of Cr³⁺ ions in ruby has been performed assuming the electro-dipole character of the transitions.

In paper [1] the semiempirical method of the effective Hamiltonian (EH) has been applied to interpret the energy spectrum of the lowest excited states of 4th order pair of Cr³⁺ ions in ruby. The purpose of the present article is to calculate the absorption intensities of zero-phonon pair lines using the results of [1].

EH constructed of spin $Q^{(k)}$ and orbital $X^{(r)}$ irreducible tensorial operators has the following form [1]

$$H_{\text{eff}}(A_2 E) = K_1 + K_{2M} X_M^{(E)}(2) + [J_1 + J_{2M} X_M^{(E)}(2)] (Q_1^{(4)} Q_2^{(4)}) + \\ + \lambda X_{(2)}^{(A_2)} Q_0^{(4)}(2) + \sqrt{\frac{2}{3}} D Q_0^{(4)}(1) + \sqrt{\frac{2}{3}} J_{22} \left[Q_1^{(4)} Q_2^{(4)} \right]_0^2 + A \left[Q_1^{(4)} Q_2^{(4)} \right]_0^4 \quad (1)$$

The parameters of EH (1) were varied to obtain the best agreement with experimentaly found scheme of levels [2].

The eigenfunctions of EH (1) $|{}^4A_2^2 E, K, \bar{S}, |M_{\bar{S}}\rangle >$ (where $K=\pm 1$ is an orbital index, \bar{S} is the total spin of the pair)may be used for calculation of the optical absorption intensities. The operator of the electro-dipole transition may be written in the framework of EH sceme as

$$W = \sum_{\alpha, \nu, q} E_{\alpha} \left[\gamma_{\nu q}^{\alpha} X_{\nu}^{(\epsilon)}(2) Q_q^{(1)}(2) + \tilde{\gamma}_{\nu}^{\alpha} X_{\nu}^{(\epsilon)}(2) (Q_1^{(1)} Q_2^{(1)}) \right] \quad (2)$$

where the first term in brackets describes the electric dipole perturbed by both the odd parity field and the spin-orbit interaction, the second term denotes the exchange induced electric dipole. The selection rules for the transition due to the first operator in(2) are $\Delta \bar{S}=0, \pm 1; \Delta M=\pm 1$ where ΔM is the change of the quasi-momentum projection [3] and those due to the second term in(2) are $\Delta \bar{S}=0; \Delta M=\pm 1$

The intensity of the electro-dipole transition between the multiplets $({}^4A_2, {}^4A_2 S M_{\bar{S}})$ of the ground pair states and the excited levels $({}^4A_2^2 E, K, \bar{S}, |M_{\bar{S}}\rangle)$ has been calculated by the formula

$$I(S \rightarrow \bar{S}, |M_{\bar{S}}\rangle, K) \sim e^{-E_S/kT} \sum_{M_S, M_{\bar{S}}} K S M_S |W| \bar{S}, |M_{\bar{S}}\rangle, K \rangle^2 \quad (3)$$

The parameters in (2) were varied to obtain the best agreement with the experiment [4]. The comparison with the experiment has been done in two cases (Table 1).

1. $\tilde{\gamma}_{\nu}$ -polarised transitions. At this polarization the single ion mechanism of transition is non effective what is confirmed by the polarizational dependence of R-lines of dilute ruby and also by the weakness of the pair lines

ABSORPTION INTENSITIES OF Cr³⁺ IONS

Table I. Absorption intensities at 77°K (4th nn.).

The experimental data are borrowed from Kisliuk et. al. [4]

| | $\bar{\pi}$ | | $\bar{\sigma}$ | |
|-----|-------------|--------|----------------|--------|
| | Exp. | Theor. | Exp. | Theor. |
| 4A2 | 0 | 0.1 | 1d | 0.6 |
| 4B2 | 0 | 0.2 | 1d | 0.6 |
| 4A1 | | | | |
| 4B1 | 5 | 3.6 | 4 | 2.5 |
| 4A0 | 0 | 0 | 0 | 0 |
| 4B0 | 0 | 0 | 0 | 0 |
| 4C3 | 0 | 0 | 2d | 2.2 |
| 4D3 | 0 | 0 | 2d | 2.0 |
| 4E3 | 0 | 0 | 2d | 1.1 |
| 4C2 | 4 | 4 | 2 | 2.5 |
| 4D2 | 3 | 3 | 2 | 2.1 |
| 4E2 | 3 | 1 | 2 | 0.8 |
| 4C1 | 0 | 0 | 0 | 0.5 |
| 4D1 | 0d | 0 | 1d | 0.5 |
| 4E1 | 0 | 0 | 0 | 0.2 |
| 4F2 | 2d | 2 | 4 | 3.5 |
| 4F1 | 2 | 1.5 | 4d | 2.4 |
| 4F0 | 0 | 0 | 0 | 0 |
| 4G3 | 1d | 0 | 2 | 2.2 |
| 4H3 | 0 | 0 | 0 | 2.0 |
| 4I3 | 0 | 0 | 0 | 1.1 |
| 4G2 | 4 | 4 | 3 | 3.5 |
| 4H2 | 4 | 4 | 2 | 2.1 |
| 4I2 | 2 | 2 | 2 | 0.8 |
| 4G1 | 0 | 0 | 0 | 0.5 |
| 4H1 | 0 | 0 | 0 | 0.5 |
| 4I1 | 0 | 0 | obs. | 0.2 |

which are exclusively depended on this mechanism [4].

2. $\bar{\sigma}$ -polarized transitions. In this case the both mechanisms of transition are effective. Obtained relations for the

parameters explain well enough the relative intensities of R-lines in dilute ruby. A good agreement of experimental and theoretical values of the absorption intensities confirms the correctness of interpretation of the energy level scheme in papers [1,2].

Naito [5] proposed a new interpretation of the energy level scheme of 4th order pair of Cr³⁺ ions in ruby. The author used groundless assumption about invariability of one electron exchange parameters γ_{ij} in the ground and excited states of the pair and completely ignored the charge-dipole interaction in the excited state of the pair. In our opinion these two assumptions make Naito's interpretation rather questionable.

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