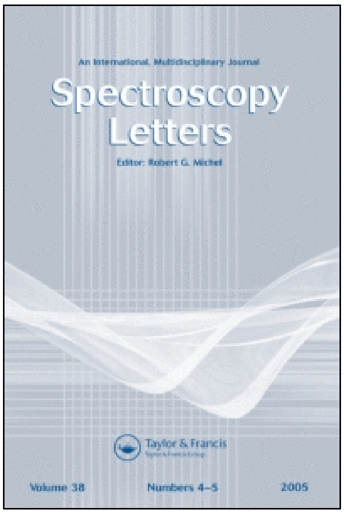

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CALCULATION OF ABSORPTION INTENSITIES OF Cr^{3+} ION PAIR LINES IN RUBY

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 Cr^{3+} 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 Cr^{3+} 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]

$$H_{ef}({}^4A_2{}^2E) = K_1 + K_{2\mu} X^{(E)}_{\mu}(2) + [J_1 + J_{2\mu} X^{(E)}_{\mu}(2)] (Q_1^{(1)} Q_2^{(1)}) + \lambda X^{(A_2)}_{(2)} Q_0^{(1)}(2) + \sqrt{\frac{2}{3}} D Q_0^{(1)}(1) + \sqrt{\frac{2}{3}} J_{z2} [Q_1^{(1)} Q_2^{(1)}]^2_0 + A [Q_1^{(1)} Q_2^{(1)}]^1_0 \qquad (1)$$

The parameters of EH (1) were varied to obtain the best agreement with experimentaly found scheme of levels [2] . The eigenfunctions of EH (1) $|{}^4A_2{}^2E,K,\bar{S},|M_{\bar{S}}|>$ (where K=±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

$$W=\sum_{\alpha,\nu,q} E_\alpha\left[\gamma^{\alpha}_{\nu q}\, X^{(E)}_{\nu}(2)\, Q^{(1)}_{q}(2)+\mathcal{T}^{\alpha}_{\nu}\, X^{(E)}_{\nu}(2)\left(Q^{(1)}_{1}Q^{(1)}_{2}\right)\right] \qquad (2)$$

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 $\Delta\bar{S}=0,\pm1;\ \Delta\mu=\pm1$ where $\Delta\mu$ is the change of the quasi-momentum projection[3] and those due to the second term in(2) are $\Delta\bar{S}=0;\ \Delta\mu=\pm1$

The intensity of the electro-dipole transition between the multiplets $({}^4A_2{}^4A_2SM_S)$of the ground pair states and the excited levels $({}^4A_2{}^2E,K,\bar{S},|M_{\bar{S}}|)$has been calculated by the formula

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

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. π-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

Table I. Absorption intensities at 77°K (4th nn.).
The experimental data are borrowed from Kisliuk et. al. [4]

	π		σ	
	Exp.	Theor.	Exp.	Theor.
4A2	0	0.1	1d	0.6
4B2	0	0.2	1d	0.6
4A1	5	3.6	4	2.5
4B1				
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. σ-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 Cr^{3+} ions in ruby. The auther 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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