radiation, a judgment can be made as to the structure of the band edges in a doped semiconductor material, this structure determining most of the optical and electrophysical properties of semiconductors [5]; also, the wavelength of the maximum in the recombination radiation can be evaluated.

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LITERATURE CITED


DISTRIBUTION OF INTENSITY IN ABSORPTION AND FLUORESCENCE SPECTRA
OF 1,2-DI-8-NAPHTHYLETHYLENE IN NAPHTHALENE CRYSTAL AT 4.2°K

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It has been shown in a number of studies that the distribution of intensity in progressive, fully symmetric vibrations in the absorption and fluorescence spectra of complex molecules is determined by both the Franck-Condon (FC) and Herzberg-Teller (HT) mechanisms of electronic-vibrational interaction [1, 2]. Qualitatively, the effect of joint influence of the FC and HT interactions is manifested in a departure from mirror-image correspondence of the absorption and fluorescence spectra. The parameters of the FC and HT interactions have been determined on the basis of fluorescence and excitation spectra [3], or on the sole basis of fluorescence spectra [4]. In determining the parameters of FC and HT interactions, it is of interest to perform a joint analysis of the adsorption and fluorescence spectra of an impurity introduced into a crystal lattice.

With the aim of determining the parameters of FC and HT interactions, we investigated the absorption and fluorescence spectra of 1,2-di-β-naphthylethylene (DBNE) in a crystal of naphthalene at 4.2°K.

The DBNE molecule consists of two naphthyl radicals connected by an ethylene group. The first electronic transition in the molecule is allowed, ϵ ∝ 10^6 [5].

Single crystals of naphthalene doped with DBNE were grown by the Bridgman method in glass ampuls. The absorption and fluorescence spectra at 4.2°K were photographed with a DKSSh-120 lamp in a DFS-13 spectrograph. The fluorescence spectra of the impurity were excited through the matrix (λ = 313 nm). The concentration of impurity in the specimen was determined from the absorption spectrum of a toluene solution at room temperature. The line intensities were averaged for several spectra and were recalculated to account for the spectral sensitivity of the film and the frequency factor. The error in determining the relative line intensities was approximately 10%.

The DBNE impurity is readily soluble in the naphthalene crystal; the naphthyl radicals replace naphthalene molecules in adjacent planes ab; the ethylene group is located between...
the layers along the c-axis. The impurity molecule in effect "cross-links" the ab planes of the naphthalene crystal [6].

The distribution of intensity in the absorption and fluorescence spectra of DBNE was investigated on specimens with a concentration of 2.2 \times 10^{-6} \text{ mole/mole}, for which the fluorescence spectra are not distorted by reabsorption. A detailed vibronic analysis of the electronic vibrational absorption and fluorescence spectra of DBNE in the naphthalene crystal at 4.2^\circ\text{K} was performed in [7]. An investigation of the polarization of radiation of the naphthalene crystal doped with DBNE showed that the radiation consists of polarized and depolarized components. After segregation of the polarized component, a determination was made of the angles between the radiating dipole and the crystal axes of the naphthalene. The angle with the a axis is 49\degree, coinciding within the limits of error with the angle determined from the absorption spectrum. An analysis of the vibrational structure of the polarized absorption and fluorescence spectra showed that vibrations that are not fully symmetric do not take part in forming the spectra.

In Fig. 1 we show the normalized absorption and fluorescence spectra of DBNE in the naphthalene crystal, corrected for spectral sensitivity. It can be seen that in the absorption and fluorescence spectra of the DBNE, formed by fully symmetric vibrations, a disruption of mirror symmetry is observed in the distribution of intensity; this may be related to a manifestation of HT interaction.

The general formula for calculating the integral intensity of a vibronic band with an arbitrary dependence of the electron matrix element on the coordinates of the nucleus has the form [1]

$$I^g(\omega) = I_0 \left\{ \delta(\omega - \epsilon) + \sum \left( \frac{\alpha_\kappa}{2} \pm a_\kappa \right)^2 \delta(\omega - \epsilon \mp v_\kappa) + \right.$$ 

$$+ \frac{1}{2l} \sum \left( \alpha_{\kappa 1} \frac{a_{\kappa 2}}{2} \pm a_{\kappa 1} \alpha_{\kappa 2} \right) \left( \alpha_{\kappa 1} \pm \alpha_{\kappa 2} \right) \delta(\omega - \epsilon \mp v_{\kappa 1} \mp v_{\kappa 2}) + \ldots \right\} , \quad g = 0, e,$$

where the upper sign is for absorption spectra (g = e) and the lower sign is for fluorescence spectra (g = o); \kappa = (c, s); \alpha and s are the respective indices of not fully symmetric and fully symmetric vibrations; \alpha_{\kappa 1}/2 is the FC parameter of displacement of the equilibrium position of the normal coordinate; \alpha_{\kappa} is the parameter of HT interaction.

When we account for the joint influence of FC and HT interactions on the fully symmetric vibrations, the observed spectra can be described by a theoretical model in which

$$\frac{\alpha_c}{2} \neq 0 \quad \frac{\alpha_s}{2} \neq 0$$

Correspondingly, we have used the following formulas to work up the absorption and fluorescence spectra of the DBNE: