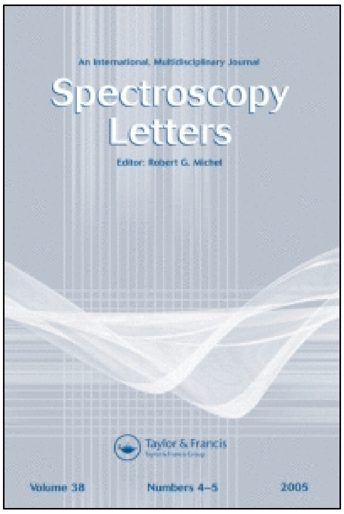

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POLARIZED LUMINESCENCE OF COMPLEX MOLECULES IN THE VAPOR PHASE

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ABSTRACT

For the lifetimes of luminescence essentially exceeding the mean period of free molecular rotation the manifestation of intramolecular orientation of absorption and emission transition dipole moments and of the principal inertia moments relation in the polarization of one- and two-photon excited luminescence and circularly polarized luminescence is analyzed. The degree of polarization of dinaphtho [2,1-b; 1',2'-d] furan, BPO, dibenz [def,mno] chrysene, triphendioxazine and perixanthenoxanthene diluted vapor fluorescence is measured and by comparison of experimental and calculated values the intramolecular orientation of fluorescent transition dipole moment is found.

INTRODUCTION

Convincing evidence of the existence of complex molecule polarized fluorescence in gas phase was obtained through theoretical and experimental studies

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of POPOP (1,4-bis[2-(5-phenyl-oxazolyl]-benzene) vapors [1,2]. Nano- and picosecond lasing with a degree of polarization up to 1.0 also pointed to the existence of optically induced anisotropy in POPOP vapors [1,3,4].

The large inertia moments and intensive intramolecular disturbances shade the rotational quantum effects and allow a classical approach to the description of reorientation dynamics of complex molecules. In the approach when the distribution density of the excited molecules $\rho(\Gamma,t)$ in the rotational phase space Γ of the excited state is much smaller than that of the ground state molecules $\rho_0(\Gamma)$ the master equation for $\rho(\Gamma)$ is

$$\frac{\partial\rho(\Gamma,t)}{\partial t} + i\hat{L}(\Gamma)\rho(\Gamma,t) = -\rho(\Gamma,t)/\tau + \rho_0(\Gamma)P_a(\Omega,t) \quad , \quad (1)$$

where τ is the excited state lifetime, $\hat{L}(\Gamma)$ is the Liouville operator of free rotation, $P_a(\Omega,t)$ is the rate of optical excitation, inducing anisotropy. The solution of eq. (1) for collisionless excited states is of the general form

$$\rho(\Gamma,t) = \rho_0(\Gamma)\int_0^\infty P_a(\Omega,t-t')\exp\{-(\tau^{-1}+ i\hat{L}(\Gamma))t'\}dt' . \quad (2)$$

The observed light intensity of given polarization is proportional to the differential cross-section of the emitting transition $\sigma(\Omega)$ averaged over the phase space density of excited molecules

$$W = \langle\sigma(\Omega)\rho(\Gamma,t)\rangle_\Gamma \quad . \qquad (3)$$

It is shown [1,2,5-6] that the orientational relaxation of anisotropic distribution of excited molecules in the solution of equation (1) is represented by the second-rank tensor correlation function calculated for the asymmetric-top molecules [7]. The analytical form of the solution [7] permits a detailed study of the properties of polarized luminescence and induced dichroism of molecular vapors, the time dynamics of optically induced anisotropy orientational relaxation as well as the character of subsequent stationary (residual) anisotropy observed in rarefied vapor fluorescence when the fluorescence lifetime τ exceeds the period ω_{rot}^{-1} of molecular rotation ($\tau >> \omega_{rot}^{-1}$) . The relaxing part of anisotropy carries a great deal of information. As yet no methods of subpicosecond resolution of anisotropy (polarization) measurements have been proposed, only polarized luminescence caused by the stationary part of induced anisotropy is discussed below.

One-Photon Excited Luminescence

The stationary part of the second-rank tensor correlation function allows a symmetric expression for the luminescence anisotropy [5] $r = (W_e^{\parallel} - W_e^{\perp})/(W_e^{\parallel} + 2W_e^{\perp})$:

$$\begin{aligned} 2r = {} & r_A((\alpha_1^2-\beta_1^2)(\alpha_2^2-\gamma_2^2) + (\alpha_2^2-\beta_2^2)(\alpha_1^2-\gamma_1^2)) + \\ & + r_B((\beta_1^2-\alpha_1^2)(\beta_2^2-\gamma_2^2) + (\beta_2^2-\alpha_2^2)(\beta_1^2-\gamma_1^2)) + \\ & + r_C((\gamma_1^2-\alpha_1^2)(\gamma_2^2-\beta_2^2) + (\gamma_2^2-\alpha_2^2)(\gamma_1^2-\beta_1^2)) \quad , \end{aligned} \qquad (4)$$

where the coefficients r_A, r_B, r_C are equal to luminescence anisotropies that could be observed for the coincident absorption $\vec{\mu}_a$ and emission $\vec{\mu}_e$ transition dipole moments oriented along the A, B, C principal inertia axes, respectively ($I_A > I_B > I_C$); α_1, β_1, γ_1 and α_2, β_2, γ_2 are the direction cosines of $\vec{\mu}_a$ and $\vec{\mu}_e$ in the principal inertia axes. The coefficients r_A, r_B, r_C are expressed by the stationary components G_A^2, G_B^2 and G_C^2 of the orientational second-rank correlation function $C_2(t)$ [5,7]:

$$r_{A,B,C} = 0{,}4\,G^2_{A,B,C} \;; \qquad (5)$$

$$G_A^2 = C_1' + C_3'' \,, \qquad G_B^2 = C_2' + C_2'' \,, \qquad G_C^2 = C_3' + C_1''$$

with

$$C_1' = \frac{1}{4}\int_{\varepsilon_0}^{1} f(F_1 - F_2)^2 d\varepsilon, \quad C_2' = \frac{1}{4}\int_{\varepsilon_0}^{1} f(F_1 + F_2)^2 d\varepsilon, \quad C_3' = \int_{\varepsilon_0}^{1} fF_2^2 d\varepsilon,$$

$$F_1 = 3\left[1 - \varepsilon^2 + \frac{\delta^2 + 2}{\delta^2}\,\varepsilon^2\left[\frac{E(\lambda)}{K(\lambda)} - 1\right]\right], \quad F_2 = 3\varepsilon^2\,\frac{E(\lambda)}{K(\lambda)} - 1,$$

$$f = \frac{K(\lambda)}{2\pi}\,\frac{I_A(1+\delta^2)^{1/2}}{(I_B I_C)^{1/2}}\left[1 + \frac{I_A - I_C}{I_C}\,\varepsilon^2\right]^{-3/2}, \quad \delta^2 = \frac{I_C(I_A - I_B)}{I_A(I_B - I_C)},$$

$$\lambda = (1-\varepsilon^2)^{1/2}/\varepsilon\cdot\delta \,, \qquad \varepsilon_0 = \delta/(1+\delta^2)^{1/2} \,,$$

$K(\lambda)$, $E(\lambda)$ are the complete elliptic integrals of the first- and second-kind, $C''_{1,2,3}$ are obtained from $C'_{1,2,3}$ by interchanging I_A and I_C.

Based on the polarization degree values P_A, P_B, P_C, which are tabulated in [5] and bearing in mind that $r = 2P/(3-P)$ it is possible to find the values r_A, r_B and r_C.

Thus, the intramolecular orientation of transition dipole moments and the ratios of principal inertia moments determine the luminescence anisotropy of complex molecule vapors when the excited state is collisionless. The luminescence is unpolarized when $\alpha_1^2 = \beta_1^2 = \gamma_1^2$ or $\alpha_2^2 = \beta_2^2 = \gamma_2^2$ or both.

Fig.1 illustrates the fluorescence anisotropy dependence calculated from (4) and (5) for planar molecules with the principal inertia moment ratio $I_A/I_B = 1.6$ (e.g. perixanthenoxanthene) on the intramolecular orientation of coincident transition dipole moments for $(\alpha_1 = \alpha_2, \beta_1 = \beta_2, \gamma_1 = \gamma_2)$ (Fig.1a) and with the fluorescent transition moment $\vec{\mu}_e$ fixed (Fig.1b). The isolines indicate the intramolecular directions of equal anisotropy. The radial coordinate R is the angle between the transition dipole moment $\vec{\mu}$ and the axis of the coordinate trihedron $(\alpha = \beta = \gamma)$; the azimuthal coordinate is the angle between the projections of $\vec{\mu}$ and the C-axis to the plane perpendicular to the axis $\alpha = \beta = \gamma$. It can be seen that the directions of equal anisotropy form irregular cones around the principal inertia axes.

Thus, the solution of the problem of finding an intramolecular orientation of the vibronic transition dipole moment using experimental polarization spectra of luminescence is as a rule many-valued. For a planar molecule, the moments of allowed transitions of π-electronic system are oriented in its plane and the space of the moments directions are shown in Fig.1 by the BC curve. In this case the solution is two- or four-valued. To reduce or resolve ambiguity additional information (molecular symmetry consideration, etc.) is needed.

It has been shown by this method that the fluorescent transition dipole moments of p-quaterphenyl, perylene and POPOP are oriented along the C-axes [8].

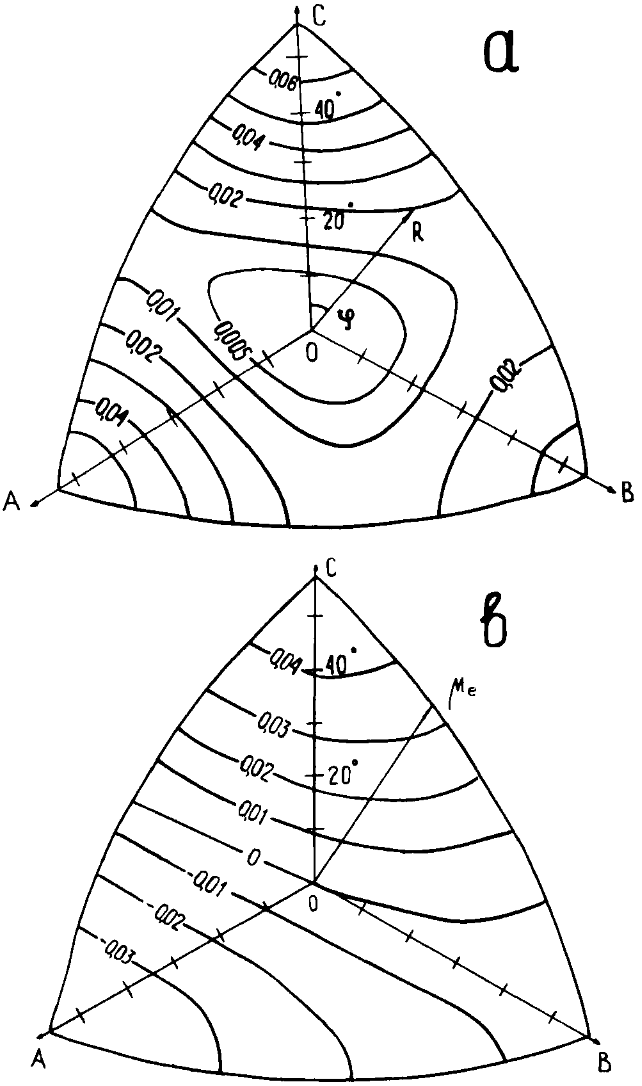
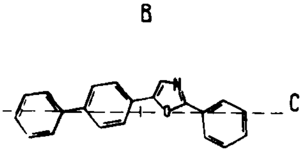


FIG. 1. Perixanthenoxanthene. Anisotropy of diluted vapor luminescence as a function of intramolecular transition moment orientation:
(a) absorbing and emitting oscillators coincide;
(b) luminescent oscillator is fixed in the molecular plane at 33.5° to the C-axis

We have studied the 2-(4-biphenylyl)-5-phenyloxazole (I), dinaphtho [2,1-b; 1,2-d] furan (II), triphendioxazine (III), dibenz [def, mno] chrysene (IV) and perixanthenoxanthene (V). The condensed polycyclic molecules II-V are planar. The torsional vibrations of BPO molecule cannot essentially change the intramolecular orientation of the C-axis. The calculated degree of fluorescence polarization of BPO vapor when fluorescent and absorptive transition moments coincide and are oriented along the B- or C-axis is 4.3% and 10.6%, respectively. The experimental value is 8.2%, which is indicative of the transition moment direction along the C-axis.



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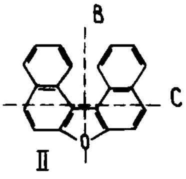
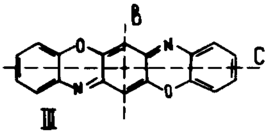
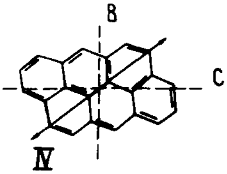


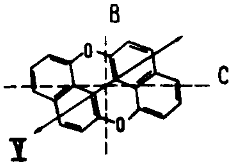
II



III



IV



V

The fluorescent transition dipole moments of molecules (II) and (III) are oriented along the B- or C-axis due to molecular symmetry. The calculated degree of fluorescence polarization of substance II diluted vapors when the dipole moments are oriented along the B- or C-axis is 4.9% and 9.6%, respectively. Low fluorescence polarization of isotropic rigid solution (ether + isopentane + ethanol, 5:5:2, 90° K) (32%)

shows that the fluorescent transition is composed of two orthogonal partial transition moments. According to this, the recalculated values of polarization [8] are 4.5% and 6.2%. So, the experimental value 5.5% is indicative of orientation along the C-axis.

The calculated 10.6% (C), 4.3% (B) and experimental 10.7% degree of polarization of triphendioxazine vapor fluorescence indicate the C-axis transition moment orientation.

The lower symmetry of planar anthanthrene (IV) and perixanthenoxanthene (V) molecules allows any orientation of the transition dipole moment. Molecules IV and V have the same coefficients r_A, r_B and r_C due to practically equal ratios of the principal inertia moments. The observed value of fluorescence polarization of substance IV vapors is low (2.5%), giving the transition moment orientation ±42° and ±64° to the C-axis. The direction of the fluorescent transition dipole moment is 43° as calculated from the atomic function density data [10]. Similarly, the measured degree of substance V fluorescence polarization is 4%, corresponding to the moment orientation ±34° and ±76° to the C-axis. Due to the similarity between the π--electron structures and the spectra of these molecules and the planar configuration of 1,1'-dinaphthyle [10,11], substance V has preferably orientation 34°.

The polarization spectra of compounds I, II and V confirm the identity of the long-wave absorptive and fluorescent transition dipole moments and constant orientation within the corresponding bands (Fig.2).

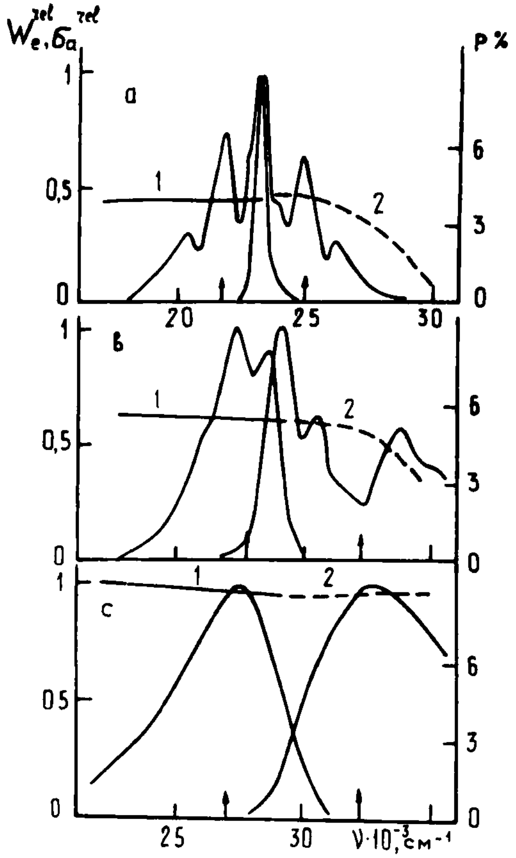


FIG. 2. The polarization spectra of fluorescence (1) and absorption (2) of perixanthenoxanthene (a), dinaphtho [2,1-b; 1',2'-d] furan (b) and BPO (c) vapors. The arrows mark the excitation and observation wavelengths.

Circular Polarized Luminescence

The circular polarized luminescence of the optically active molecules in condensed phase is a well studied phenomenon. It is known to be determined by the scalar product of the magnetic $\vec{\mu}_m$ and electric $\vec{\mu}_e$ dipole moments of the electronic transition. The circular polarized luminescence is measured by the dissymmetry factor

$$g = 2\,\frac{W_L - W_R}{W_L + W_R}\,, \tag{6}$$

where W_L and W_R are the left- and right-hand polarized components of the luminescence intensity. When rotational relaxation is introduced by second-rank orientation correlation functions, the dissymmetry factor is expressed in the form [6]

$$g(t) = \frac{4\sigma_{em}\int_0^\infty W_a(t-t')e^{-t'/\tau}((\vec{e}\ \vec{m}) + K(\eta)C_2(\vec{\mu}_a,\vec{\mu}_e,\vec{\mu}_m;t'))dt'}{\sigma_e\int_0^\infty W_a(t-t')e^{-t'/\tau}(1+K(\eta)C_2(\vec{\mu}_a,\vec{\mu}_e;t'))dt'}\,, \tag{7}$$

where W_a is the exciting light intensity, $\sigma_{em} = i\mu_e\mu_m$, $\sigma_e = \mu_e^2$, $e = \frac{\vec{\mu}_e}{\mu_e}$, $m = \frac{\vec{\mu}_m}{\mu_m}$, $K(\eta)$ is the parameter determined by experiment geometry, $C_2(\vec{\mu}_a,\vec{\mu}_e,\vec{\mu}_m;t')$ and $C_2(\vec{\mu}_a,\vec{\mu}_e;t')$ are the second-rank orientation correlation functions, The factor $K(\eta)$ for the linearly polarized exciting radiation with the angle η between the electric vector of exciting light and the observation direction is

$$K(\eta) = \frac{1}{5}\,(3\cos^2\eta - 1) \tag{8}$$

The form of the expression for the dissymmetry factor is as for the isotropic distribution of excited molecules.

$$g = \frac{4\sigma_{em}}{\sigma_e}\,(\vec{e}\cdot\vec{m}) \tag{9}$$

when $3\cos^2\eta = 1$.

For the stationary collisionless conditions the dissymmetry factor (7) becomes

$$g = \frac{4\sigma_{em}}{\sigma_e} \frac{((\vec{e}\cdot\vec{m}) + K(n)C_2(\vec{\mu}_a,\vec{\mu}_e,\vec{\mu}_m))}{(1 + K(n)C_2(\vec{\mu}_a,\vec{\mu}_e))} . \qquad (10)$$

Here, $C_2(\vec{\mu}_a,\vec{\mu}_e,\vec{\mu}_m)$ and $C_2(\vec{\mu}_a,\vec{\mu}_e)$ are the stationary components of the orientation correlation functions:

$$\begin{aligned} 2C_2(\vec{\mu}_a,\vec{\mu}_e,\vec{\mu}_m) = {} & G_A^2((\alpha_1^2-\beta_1^2)(\alpha_2\alpha_m-\gamma_2\gamma_m)+(\alpha_2\alpha_m-\beta_2\beta_m)(\alpha_1^2-\gamma_1^2))+ \\ & + G_B^2((\beta_1^2-\alpha_1^2)(\beta_2\beta_m-\gamma_2\gamma_m)+(\beta_2\beta_m-\alpha_2\alpha_m)(\beta_1^2-\gamma_1^2)) + \qquad (11) \\ & + G_C^2((\gamma_1^2-\alpha_1^2)(\gamma_2\gamma_m-\beta_2\beta_m) + (\gamma_2\gamma_m-\alpha_2\alpha_m)(\gamma_1^2-\beta_1^2)) , \end{aligned}$$

where α_m,β_m , γ_m are the direction cosines of the magnetic transition dipole moment. $C_2(\vec{\mu}_a,\vec{\mu}_e)$ is obtained from $C_2(\vec{\mu}_a,\vec{\mu}_e,\vec{\mu}_m)$ if $\alpha_2=\alpha_m$, $\beta_2=\beta_m$, $\gamma_2=\gamma_m$, G_A^2, G_B^2, G_C^2 are given in (5). One can see from this expression that circular polarized luminescence for free molecules depends not only on the value of electric and magnetic transition dipole moments and on the angle between them, but also on their intramolecular orientation.

It is interesting that relations (10) and (11) result in a dissymmetry factor of the form (9) when $\alpha_1^2 = \beta_1^2 = \gamma_1^2$ or $\alpha_2\alpha_m = \beta_2\beta_m = \gamma_2\gamma_m$ or both.

Two-Photon Excited Luminescence

The intensity of an arbitrary linearly polarized component of two-photon excited luminescence of isotropic nonrigid media W is presented as a function of seven independent molecular parameters M_s [13] which are transformed as unreducible second-rank tensors (contrary to rigid media [12])

$$W(t) = \sum_{s=1}^{7} P_s M_s \quad , \tag{12}$$

where P_s are coefficients introduced only by the experiment geometry

$$P_1 = 1, \quad P_2 = \frac{3}{2} E_{pq}^{11}(\vec{\lambda}\cdot\vec{\varkappa}), \quad P_3 = \frac{2}{5} E_{pq}^{22}(3(\vec{\lambda}\cdot\vec{\varkappa})^2 - 1),$$

$$P_4 = \frac{2}{5} E_{pq}^{20}(3(\vec{\lambda}\cdot\vec{\nu})^2 - 1), \quad P_5 = \frac{2}{5} E_{pq}^{02}(3(\vec{\varkappa}\cdot\vec{\nu})^2 - 1), \tag{13}$$

$$P_6 = \frac{2}{5} E_{pq}^{11}((\vec{\lambda}\cdot\vec{\varkappa})(\vec{\varkappa}\cdot\vec{\nu}) - \frac{1}{3}(\vec{\lambda}\cdot\vec{\varkappa})), \quad P_7 = \frac{8}{35} E_{pq}^{22}(3(\vec{\xi}\cdot\vec{\nu})^2 - 1),$$

$$E_{pq}^{J_1 J_2} = (-1)^{p+q} C_{1p1-p}^{J_1 0} C_{1q1-q}^{J_2 0} / C_{1010}^{J_1 0} C_{1010}^{J_2 0}, \quad J_1,\ J_2 \neq 1 ;$$

$$E_{pq}^{11} = (-1)^{p+q} C_{1p1-p}^{10} C_{1q1-q}^{10} \quad .$$

Since C_{1p1q}^{J0} are the Clebsch-Cordon coefficients, p and q are equal to 0, 1 and -1 for the linear, right- and left-hand circular polarization of exciting light, $\vec{\lambda}$, , $\vec{\nu}$ are unit vectors of exciting and emitted photons polarization, respectively (for circularly polarized light, $\vec{\lambda}$ and $\vec{\varkappa}$ are oriented along the wave vector), $\vec{\xi}$ is a vector produced by components ξ_i :

$$\xi_i^2 = (\vec{\lambda}\cdot\vec{\varkappa})\lambda_i \varkappa_i + |\vec{\lambda}\times\vec{\varkappa}|_i^2 \quad . \tag{14}$$

In (12), the first three molecular parameters

$$M_1 = \delta_G, \quad M_2 = \delta_F - \delta_H, \quad M_3 = \frac{3}{4}(\delta_F - \delta_H) - \frac{1}{2}\delta_G \tag{15}$$

are functions consisting of McClain parameters of absorption anisotropy δ_F, δ_G, δ_H |12|. The other M_s are the orientational correlation functions of the unreducible second-rank tensors composed of the two-photon absorption tensors T_{ij} [12] and of the vector of emitting oscillator $\vec{\mu}_e$ [13]. For the stationary limit they have the form

$$M_4 = C_2(T^{20},\vec{\mu}_e), \qquad M_5 = C_2(T^{02},\vec{\mu}_e),$$

$$M_6 = C_2(T^{11},\vec{\mu}_e), \qquad M_7 = C_2(T^{22},\vec{\mu}_e) \qquad (16)$$

with

$$C_2(T^{J_1J_2},\vec{\mu}_e) = G^2_{oo}S^2_o(T^{J_1J_2})S^2_o(\vec{\mu}_e)+G^2_{22}S^2_{20}(T^{J_1J_2})S^2_{20}(\vec{\mu}_e)+$$

$$+ G^2_{20}(S^2_{20}(T^{J_1J_2})S^2_o(\vec{\mu}_e) + S^2_o(T^{J_1J_2})S^2_{20}(\vec{\mu}_e)), \qquad (17)$$

where symmetrized second-rank tensors $S^2_{mo}(T^{J_1J_2})$ are the functions of the components of two-photon absorption tensor

$$T^{J_1J_2} = \sum_{m,n,i,k=-1}^{1} C^{J_1 0}_{1m1i} C^{J_2 0}_{1n1k} T_{mn} T_{ik},$$

and $S^2_{mo}(\vec{\mu}_e)$ are the functions of orientation of the transition dipole moment of emission [13].

$$G^2_{oo} = G^2_C, \qquad G^2_{22} = \frac{1}{3}(2G^2_A+2G^2_B-G^2_C), \qquad G^2_{20} = \frac{1}{3^{1/2}}(G^2_B-G^2_A).$$

It can be seen from relationships (12) to (17) that the polarization indicatrix for a given direction of two-photon excited luminescence has a rather complex form. Since the coefficients at M_s in (12) depend on the experiment geometry, one can find them by seven experiments of different geometries.

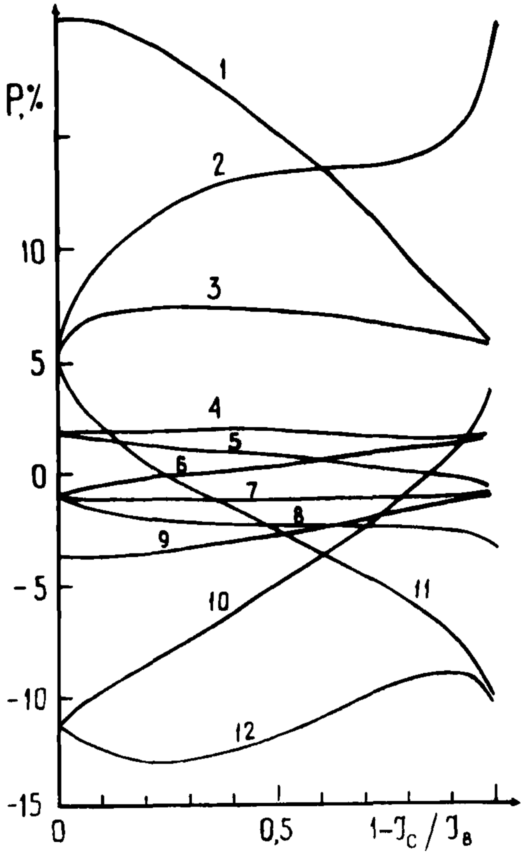


FIG. 3. The polarization degree of two-photon excited luminescence of planar rigid molecules in a vapor phase as a function of the inertia parameter $1-I_C/I_B$ when the first (i) and second (j) absorptive and luminescent (k) transition dipole moments are directed along the main inertia axes (ijk): 1=AAA; 2=CCC; 3=BBB; 4=ABA=BCC; 5=ACA=BCB; 6=ABB=ACC; 7=ACB; 8=ABC; 9=CBA; 10=AAB=BBA; 11=BBC=CCB; 12=AAC=CCA.

So, with the aid of the above relationships the degree of luminescence polarization can be calculated provided that the intramolecular components of the two-photon absorption tensor and the direction of the luminescent transition moment are known. Fig. 3 shows polarization of two-photon excited luminescence of planar molecules as a function of the inertia parameter $1-I_C/I_B$ when the transition dipole moments are oriented along the principal inertia axes and the exciting photons are equal and polarized linearly and in parallel.

The parallel transition dipole moments (AAA) result in the highest polarization degree (20%). The highest negative value (-13%) is predicted for parallel absorptive transition moments oriented along the A-axis and the luminescent transition moment oriented along the C-axis or v.v. (AAC=CCA). When the orientation of absorptive transition dipole moments is orthogonal the polarization is between -3.5% and 2%.

CONCLUSIONS

We have shown that polarization of complex molecule luminescence in diluted vapors depends not only on the mutual orientation of the transition dipole moments but on its intramolecular orientation and on the principal inertia moments relation, too. In the stationary approach the dependences are represented by three products of the same inertia factors for all the kinds of luminescence described and simple linear functions of intramolecular components of the transition dipole moments.

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