Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

On the dual emission of *p*-dimethylaminobenzonitrile and its photophysical implications

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Using the Abe's approach (60) we have evaluated the changes undergone by the **DMABN** on electronic photoexcitation in its dipole moments and isotropic polarizability. This approach is given by the equation :

$$[(\mu_i)^2 - (\mu_0)^2] + (\alpha_i) \cdot \mathbf{A} = \mathbf{B}$$

Where μ_i and μ_0 are the dipole moments of the chromophore in the excited and ground states, respectively, which are involved in the electronic transition, and α_i is the isotropic polarizability of the excited electronic state. of its slope we can obtain the isotropic polarizability for the chromophore, and of its ordinate at the origin we can obtain the dipole moment for the excited electronic state.

Where

$$\mathbf{A} = 3 \times [(2(\varepsilon^s - (n^s)^2)(\varepsilon^s + (n^s)^2)) / \varepsilon^s ((n^s)^2 + 2)^2 + ((n^s)^2 - 1) / ((n^s)^2 + 2)]^{-1} \times [kt \times ((\varepsilon^s - (n^s)^2) (2\varepsilon^s + (n^s)^2) / \varepsilon^s ((n^s)^2 + 2)^2 + 0.5 ((n^s)^2 - 1) / ((n^s)^2 + 2))) (I^s(I - hc\nu)) / (I^s + I - hc\nu)]$$

and

$$\mathbf{B} = 3 \times [(2(\varepsilon^s - (n^s)^2)(\varepsilon^s + (n^s)^2)) / \varepsilon^s ((n^s)^2 + 2)^2 + ((n^s)^2 - 1) / ((n^s)^2 + 2)]^{-1} \times [kt \times ((\varepsilon^s - (n^s)^2) (2\varepsilon^s + (n^s)^2) / \varepsilon^s ((n^s)^2 + 2)^2 + 0.5 ((n^s)^2 - 1) / ((n^s)^2 + 2))) \times (I^s \times I / I^s +)) (\alpha_0) - 8.351 \times 10^{-42} \times (\rho^s/M^s)^{1/3} \times \Delta\nu \times (((M/\rho)^{1/3} + (M^s/\rho^s)^{1/3})^{-4} + ((M/\rho)^{1/3} + 3(M^s/\rho^s)^{1/3})^{-4} + ((M/\rho)^{1/3} + 5 (M^s/\rho^s)^{1/3})^{-4})^{-1}]$$

The notations s will refer to solvent.

The values of **A** and **B** can be calculated from observed values of : molecular weight (M), densities (ρ), refraction index (n), dielectric constant(ε), ionization potential(I) and electronic transition energies(ν), which are gathered in the following Table:

Solvent	n	ε	M	ρ	IP	T
CLB343	1.3713	5.601	92.57	0.830	10.84	343.0
CLB333	1.3770	5.979	92.57	0.841	10.84	333.0
CLB323	1.3827	6.357	92.57	0.852	10.84	323.0
CLB313	1.3884	6.735	92.57	0.863	10.84	313.0
CLB303	1.3941	7.113	92.57	0.873	10.84	303.0
CLB293	1.3998	7.491	92.57	0.884	10.84	293.0
CLB273	1.4112	8.247	92.57	0.906	10.84	273.0
CLB263	1.4169	8.625	92.57	0.917	10.84	263.0
CLB253	1.4226	9.003	92.57	0.927	10.84	253.0
CLB243	1.4283	9.381	92.57	0.938	10.84	243.0
CLB233	1.4340	9.759	92.57	0.949	10.84	233.0
CLB223	1.4397	10.137	92.57	0.960	10.84	223.0
CLB213	1.4454	10.515	92.57	0.971	10.84	213.0
CLB203	1.4511	10.839	92.57	0.981	10.84	203.0
CLB193	1.4568	11.271	92.57	0.992	10.84	193.0
CLB183	1.4625	11.649	92.57	1.003	10.84	183.0
CLB173	1.4682	12.027	92.57	1.014	10.84	173.0
CLB163	1.4739	12.405	92.57	1.024	10.84	163.0
CLB153	1.4796	12.783	92.57	1.035	10.84	153.0