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Spectrophotometric Studies of Complexation of Safranine T and Safranine O with [60]- and [70]Fullerenes and Other Electron Acceptors

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The electron donor−acceptor (EDA) interactions of the dye, namely, Safranine T (ST) and Safranine O (SO) with [60]- and [70]fullerenes and some other electron acceptors (e.g., 2,3-dichloro-5,6-dicyano-*p*-benzoquinone, *o*-chloranil, and *p*-chloranil) were studied in 1,4-dioxan medium using the absorption spectroscopic technique. An absorption band due to a charge transfer (CT) transition is observed in the visible region for all of the complexes studied. The experimental CT transition energies ($h\nu_{CT}$'s) are well-correlated (through Mulliken's equation) with the vertical electron affinities of the acceptors. From an analysis of this correlation, vertical ionization potentials of ST and SO have been determined. The influences of ST and SO on the absorption spectrum of [60]- and [70]fullerenes are studied. The experimental results were explained using a theoretical model that takes into account the interaction between electronic subsystems of ST and SO with [60]- and [70]fullerenes. Oscillator strengths, transition dipole strengths, and resonance energies of the EDA complexes have been estimated. Formation constants of the complexes were determined in terms of the Benesi−Hildebrand equation. The magnitudes of the formation constants indicate that SO binds more strongly than ST with [60]- and [70]fullerenes.

1. Introduction

Since the discovery and establishment of bulk preparation of fullerenes, in particular, [60]- and [70]fullerenes,[1,2] a great deal of work has been done on these two novel π-systems.[3−6] In contrast to planar π-electron acceptors, fullerenes possess a number of characteristic features, namely, spherical shape, unique electronic structure, high symmetry, and polarizability.[7] These extraordinary properties[7] of fullerenes have attracted the attention of physicists,[8] chemists,[9] material scientists,[10] and, now, biologists[11] also. Most of the chemical investigations of fullerenes are directed toward their chemical transformations.[12−14] Our investigations, on the other hand, are directed toward the possible effects of charge transfer (CT) interactions of [60]- and [70]fullerenes with organic dye molecules. CT interactions in fullerene-conducting polymers and other fullerene-based compounds is currently of immense technological importance, because these materials can be utilized in xerography, energy phototransducers, and molecular switches.[15] Beside this, an understanding of CT interaction between fullerenes and various organic species could be useful[16] for the studies on optical, nonlinear optical, and superconducting properties of fullerenes and their derivatives. Though interactions of [60]- and [70]fullerenes with amines,[17] aromatic hydrocarbons,[18] and tetrathiafulvelenes[19] have now been widely studied, no such investigation has been done on their complexation with any organic dye molecules similar to those used in optical spectroscopic investigations. In the present study, we examine the electron donor−acceptor (EDA) interaction of [60]- and [70]fullerenes with two organic dye molecules, namely, Safranine T (3,6-diamino-2,7-dimethylphenyl phenazinium chloride) and Safranine O (3,7-diamino-2,8-dimethylphenyl phenazinium chloride). The CT absorption bands are located in each case, and some important molecular parameters have been determined from the trends in such bands. The concept of CT interaction also offers a platform for explaining the interactions between electronic subsystems of dye molecules (i.e., ST and SO) and fullerenes and, hence, widens the scope of the present investigation on molecular interactions of [60]- and [70]fullerenes with various electron donors.

2. Materials and Methods

[60]Fullerene was obtained from Sigma, U.S.A. [70]Fullerene was collected from Lancaster, U.K. *o*-Chloranil was collected from Sigma. *p*-Chloranil (from Fluka, Switzerland) was further purified by sublimation just before use. The other acceptor, 2,3-dichloro-5,6-dicyano-*p*-benzoquinone (DDQ), was collected from Sigma and used without further purification. ST (Fluka, Switzerland) and SO (Lancaster, U.K.) were used without further purification. The solvent, 1,4-dioxan, was of UV spectroscopic grade. All spectral measurements were carried out at 304 K on a UV-2101 PC model spectrophotometer fitted with TB-85 thermal bath.

3. Results and Discussions

3.1. Observation of CT bands. To obtain the CT bands, the spectrum of each of the solutions (in 1,4-dioxan) containing the [60]- and [70]fullerenes, *o*-chloranil, *p*-chloranil, and DDQ as acceptors and the donors (i.e., ST and SO) individually was recorded against the pristine acceptor solution as reference. Some typical CT absorption bands are shown in Figures 1 and 2. When the mixture of donor and acceptor solutions gives rise to a spectrum (the spectral pattern should be different from the spectra of the components) having multiple peaks, it is custom-

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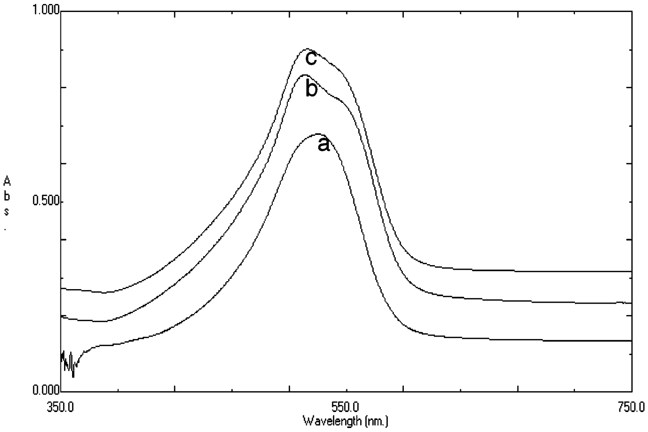

Figure 1. CT absorption spectra of (a) DDQ (3.348×10^{-4} mol·dm^{-3}) + ST (2.256×10^{-4} mol·dm^{-3}), (b) [70]fullerene (1.190×10^{-5} mol·dm^{-3}) + ST (1.520×10^{-3} mol·dm^{-3}), and (c) *o*-chloranil (2.642×10^{-6} mol·dm^{-3}) + ST (1.520×10^{-3} mol·dm^{-3}) against pristine acceptor solution as reference.

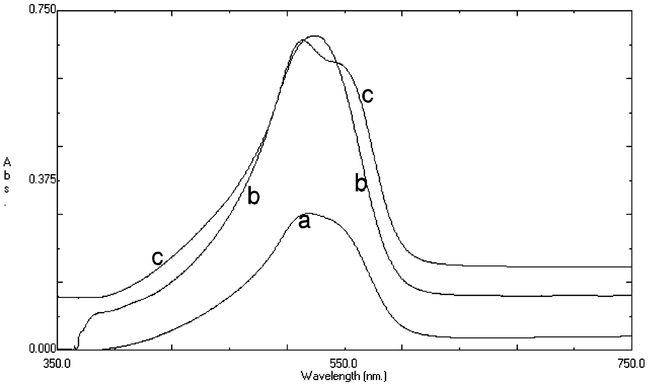

Figure 2. CT absorption spectra of (a) *o*-chloranil (2.642×10^{-6} mol·dm^{-3}) + SO (3.808×10^{-4} mol·dm^{-3}), (b) DDQ (3.348×10^{-4} mol·dm^{-3}) + SO (5.701×10^{-4} mol·dm^{-3}), and (c) [60]fullerene (6.250×10^{-5} mol·dm^{-3}) + SO (1.235×10^{-4} mol·dm^{-3}) against pristine acceptor solution as reference.

ary to identify the longest wavelength peak as the charge transfer (CT) peak. In Figure 2c, the shoulder region lies in the longer wavelength side. For this reason, the shoulder region of the peak has been considered as the CT peak. Some typical CT absorption spectra of the mixtures of [60]fullerene with varying concentrations of ST are shown in Figure 3. Figure 3 shows clearly that [60]fullerene does not absorb strongly in the region where the CT band appears. The absorption spectra were analyzed by fitting to the Gaussian function $y = y_0 + [A/(w\sqrt{(\pi/2)}]\exp[-2(x-x_c)^2/w^2]$, where x and y denote wavelength and absorbance, respectively, and the results are illustrated in Table 1. One such Gaussian analysis plot has been shown in Figure 4. The energies corresponding to the maxima of the CT bands are given in Table 2.

3.2. Determination of Vertical Ionization Potentials (I_D^v's) of Safranine T and Safranine O. For complexes with neutral ground state, a CT band corresponds to a transfer of an electron from a donor (D) to an acceptor (A) molecule with the absorption of a quantum given by the expression:

$$D^{\delta+}\cdots A^{\delta-} \xrightarrow{h\nu_{CT}} D^{(1-\delta)+}A^{(1-\delta)-}$$

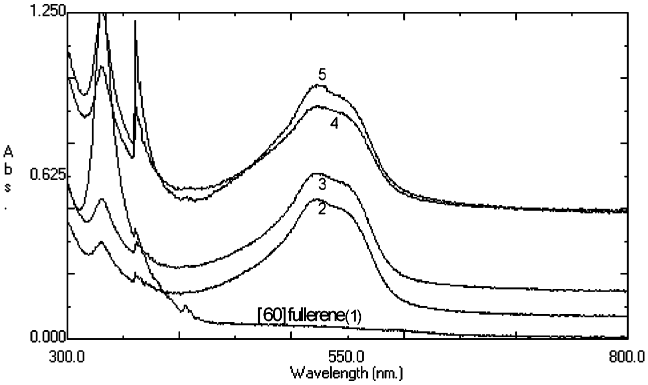

Figure 3. Absorption spectra of (1) [60]fullerene (2.778×10^{-5} mol·dm^{-3}), (2) [60]fullerene (2.778×10^{-5} mol·dm^{-3}) + ST (0.000 356 mol·dm^{-3}), (3) [60]fullerene (2.778×10^{-5} mol·dm^{-3}) + ST (0.000 427 mol·dm^{-3}), (4) [60]fullerene (2.778×10^{-5} mol·dm^{-3}) + ST (0.000 713 mol·dm^{-3}), and (5) [60]fullerene (2.778×10^{-5} mol·dm^{-3}) + ST (0.000 855 mol·dm^{-3}) in 1,4-dioxan against the solvent as reference.

The relationship between the energy ($h\nu_{CT}$) of the lowest-energy intermolecular CT band and the E_A^v of the acceptor for a series of complexes with a common donor species has been the source of much discussion. According to Mulliken's theory,[20] the ground state of the complex is a resonance hybrid of a "no-bond" state (D···A) and a "dative state" (D^+A^-) with the former predominating; the excited state is a resonance hybrid of the same two structures with the dative one predominating. CT transition energies in these complexes are related to the vertical ionization potentials (I_D^v's) of the donors by the following relationship

$$h\nu_{CT} = I_D^{\ v} - C_1 + C_2/(I_D^{\ v} - C_1) \tag{1}$$

Here,

$$C_1 = E_A^{\ v} + G_1 + G_0 \tag{2}$$

where E_A^v is the vertical electron affinity of the acceptor, G_0 is the sum of several energy terms (like dipole−dipole, van der Waals interaction, etc.) in the no-bond state, and G_1 is the sum of a number of energy terms in the dative state. In most cases, G_0 is small and can be neglected, while G_1 is largely the electrostatic energy of attraction between D^+ and A^-. The term C_2 in eq 1 is related to the resonance energy of interaction between the no-bond and dative forms in the ground and excited states, and for a given acceptor, it may be supposed constant.[20] A rearrangement of eq 1 yields

$$2C_1 + h\nu_{CT} = C_1(C_1 + h\nu_{CT})/I_D^{\ v} + C_2/I_D^{\ v} + I_D^{\ v} \tag{3}$$

The vertical electron affinities of [60]fullerene, [70]fullerene, *o*-chloranil, *p*-chloranil, and DDQ were collected from references.[21−24] By neglecting G_0 and taking the typical D−A distance in π-type EDA complexes to be 3.5 Å, the major part of G_1 is estimated to be $e^2/4\pi\epsilon_0 r = 4.13$ eV. By using these values, C_1 is obtained from eq 2 for each of the acceptors. A plot of $2C_1 + h\nu_{CT}$ versus $C_1(C_1 + h\nu_{CT})$ for a given donor and various acceptors yields a slope of $1/I_D^v$, from which the values of I_D^v have been obtained for Safranine T and Safranine O. Both ST and SO produce similar values of I_D^v (i.e., 7.56 eV). This is because, although ST and SO are structurally different, they have the same molecular formula. For this reason, they have the same I_D^v value. The following linear regression equation has been obtained with the present data with a correlation coefficient of 0.99 (Figure 5)

$$2C_1 + h\nu_{CT} = (0.1323 \pm 0.003)[C_1(C_1 + h\nu_{CT})] + (7.67 \pm 0.18) \tag{4}$$

TABLE 1: Gaussian Curve Analysis for the CT Spectra of ST and SO with [60]- and [70]Fullerenes and Some Other Electron Acceptors[a]

system	area of the curve (A), nm	width of the curve (w), nm	center of the curve (x_c), nm	y_0
[60]fullerene−ST	39.06 ± 5.30	56.39 ± 3.80	544.2 ± 0.64	0.027 ± 0.038
[60]fullerene−SO	6.26 ± 5.30	29.61 ± 11.02	543.2 ± 1.08	0.47 ± 0.08
[70]fullerene−ST	13.56 ± 6.94	35.24 ± 8.69	542.7 ± 1.20	0.47 ± 0.084
[70]fullerene−SO	36.52 ± 5.77	50.20 ± 4.00	544.3 ± 0.72	0.19 ± 0.05
o-chloranil−ST	49.10 ± 3.96	68.46 ± 3.30	526.5 ± 1.00	0.33 ± 0.012
o-chloranil−SO	21.82 ± 1.45	66.22 ± 3.21	526.7 ± 1.01	0.04 ± 0.008
p-chloranil−ST	31.33 ± 2.04	48.52 ± 1.92	544.8 ± 0.58	0.14 ± 0.01
p-chloranil−SO	20.13 ± 1.04	45.65 ± 1.52	545.4 ± 0.52	0.24 ± 0.007
DDQ−ST	38.88 ± 2.21	60.90 ± 2.65	524.8 ± 0.90	0.17 ± 0.012
DDQ−SO	44.48 ± 2.46	63.34 ± 2.70	524.5 ± 0.92	0.13 ± 0.013

[a] e.g., DDQ, *o*-chloranil, and *p*-chloranil. Temperature = 304 K.

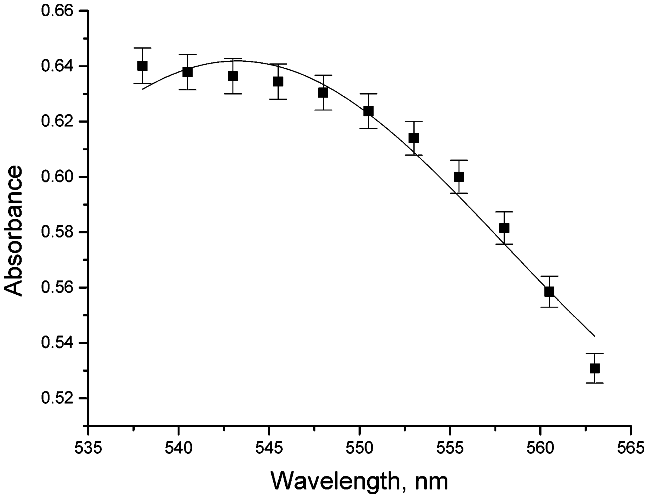

Figure 4. Gaussian analysis curve of the shoulder region of the CT band for [60]fullerene/SO system.

3.3. Theoretical Model in Favor of Electric Dipole−Dipole Interaction between the Fullerene Molecules and Donors (i.e., ST & SO). Consider the interaction of [60]fullerene and SO. The interaction between the dipole−dipole transitions of [60]fullerene and SO can be represented in the form

$$H = \sum_{i=1}^{N_{\max}} (d_{[60]\text{fullerene}}\, \sigma_x^{[60]\text{fullerene}}\, d^i_{\text{SO}}\, \sigma_{x,i}^{\text{SO}})(1 - 3\cos^2\theta_i)/\epsilon_\infty r_i^3 \tag{5}$$

where $d_{[60]\text{fullerene}}$ and $d^i_{[\text{SO}]}$ are dipole moments of the corresponding transitions in [60]fullerene and the ith SO molecule, $\sigma_x^{[60]\text{fullerene}}$ and $\sigma_{x,i}^{\text{SO}}$ are the corresponding Pauly matrices, r_i is the distance between the [60]fullerene and SO molecules, and ϵ_∞ in eq 5 is the high-frequency dielectric constant. The reconstruction of the resulting spectrum, taking into account eq 5, is determined by mixing of the states of the [60]fullerene molecule and the surrounding SO molecules. For one [60]fullerene−SO pair, eq 5 gives

$$E_\pm^{\,i} = (E_{[60]\text{fullerene}} + E_{\text{SO}})/2 \pm \{[(E_{[60]\text{fullerene}} - E_{\text{SO}})/2]^2 + |V_i|^2\}^{1/2} \tag{6}$$

where $E_{[60]\text{fullerene}}$ and E_{SO} are the energies of dipole transitions for [60]fullerene and SO, respectively, and $V_i = [d_{[60]\text{fullerene}}\, d^i_{\text{SO}}(1 - 3\cos^2\theta_i)]\,\epsilon_\infty^{-1}\, r_i^{-3}$ is the matrix element of the state mixing.

The final expression has the form

$$\epsilon_- = \epsilon_-^{(0)} - (|V_i|N^{1/2})/2 \tag{7}$$

where V is the amplitude of the nondiagonal flip-flop dipole−dipole matrix element for [60]fullerene and of the dipole transitions in neighboring SO molecules and N is the number of neighboring SO molecules. Such a dependence of the absorption band edge is valid only under the condition $N < N_{\text{thr}}$, where N_{thr} is the maximum number of SO molecules that can take part in the dipole−dipole flip-flop interaction with [60]fullerene. A further increase in the concentration of SO does not increase the number of these molecules in the nearest environment of [60]fullerene. Figure 6 shows that the dependences are saturated when the concentrations of donor (i.e., SO) exceeds 0.001 M, in agreement with the theory. This mechanism also allows us to explain the formation of the donor−acceptor complex in the system under study.

3.4. Determination of Oscillator (f's) and Transition Dipole Strengths (μ_{EN}'s). From the CT absorption spectra, we can extract an oscillator strength. The oscillator strength f is estimated using the formula

$$f = 4.32 \times 10^{-9} \int \epsilon_{\text{CT}}\, d\nu \tag{8}$$

where $\int \epsilon_{\text{CT}}\, d\nu$ is the area under the curve of the extinction coefficient of the absorption band in question versus the frequency. The integral is to be formed from zero to infinity. To a first approximation

$$f = 4.32 \times 10^{-9}\, \epsilon_{\max}\, \Delta\nu_{1/2} \tag{9}$$

where $\epsilon_{\max}$ is the maximum extinction coefficient of the band and $\Delta\nu_{1/2}$ is the half-width (i.e., the width of the band at one-half the maximum extinction. The observed oscillator strengths of the CT bands are summarized in Table 2. Variation of oscillator strengths with the vertical electron affinity values of the acceptors produces a parabolic-type plot (Figure 7). It can be said that any other function would fit the experimental data as well as the parabolic plot.

The extinction coefficient is related to the transition dipole by

$$\mu_{\text{EN}} = 0.0952\, [\epsilon_{\max}\, \Delta\nu_{1/2}/\Delta\nu]^{1/2} \tag{10}$$

where $\Delta\nu \approx \bar{\nu}$ at $\epsilon_{\max}$ and μ_{EN} is defined as $-e \int \psi_{\text{ex}} \sum_i r_i \psi_{\text{g}}\, d\tau$. Values of μ_{EN} for the complexes of ST and SO with different electron acceptors (e.g., [60]- and [70]fullerenes, *o*-chloranil, *p*-chloranil, and DDQ) are given in Table 2.

TABLE 2: CT Absorption Maxima and Transition Energies of the Complexes of ST and SO with [60]- and [70]Fullerenes and Some Other Electron Acceptors;[a] Degrees of Charge Transfer (α's), Oscillator Strengths (f's), Transition Dipole Strengths (μ_{EN}'s) and Resonance Energies (R_N's) of the Complexes of ST and SO with Acceptors

	λ_{CT}, nm		$h\nu_{CT}$, eV		$10^3 \times f$		μ_{EN} (Debye)		$\|R_N\|$, eV		10^5 α	
acceptor	ST	SO	ST	SO	ST	SO	ST	SO	ST	SO	ST	SO
[60]fullerene	544.2	543.2	2.279	2.283	6.62	2.470	15.694	13.22	0.463	0.415	3.22	3.22
[70]fullerene	542.7	544.3	2.285	2.278	7.69	10.307	21.394	20.75	0.536	0.529	3.38	3.38
o-chloranil	526.5	526.7	2.355	2.354	0.273	0.265	2.899	2.899	0.052	0.052	3.53	3.53
p-chloranil	544.8	545.4	2.276	2.274	0.451	0.424	4.417	4.417	0.106	0.106	2.80	2.80
DDQ	524.8	524.5	2.363	2.364	0.292	0.303	3.098	3.098	0.059	0.059	3.77	3.77

[a] e.g., DDQ, *o*-chloranil, and *p*-chloranil. Temperature = 304 K.

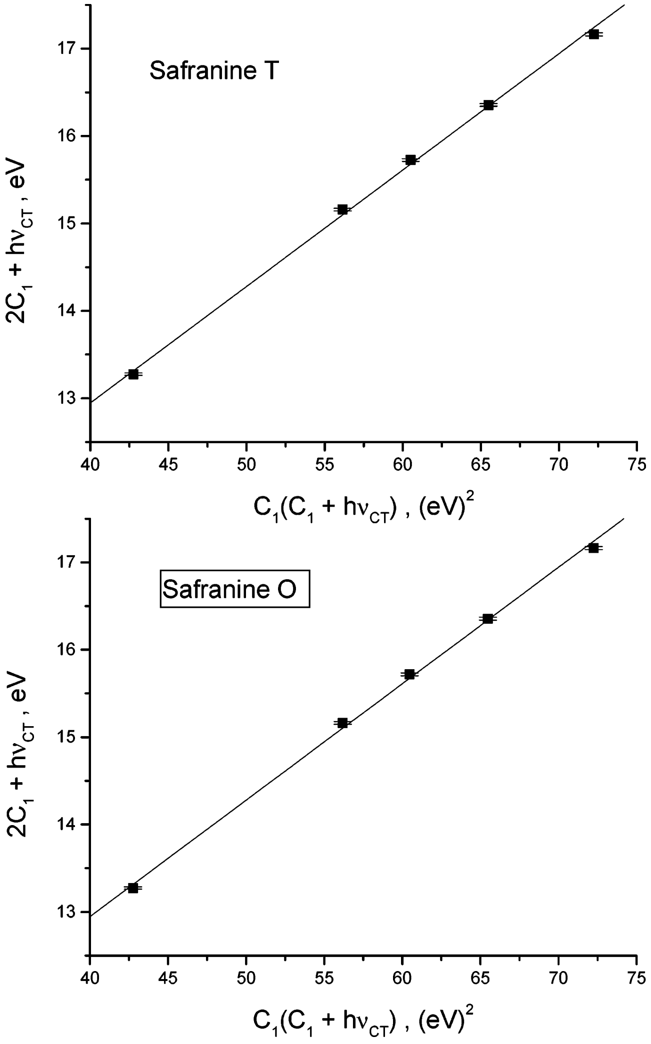

Figure 5. Plot of $2C_1 + h\nu_{CT}$ vs $C_1(C_1 + h\nu_{CT})$ for Safranine T and Safranine O.

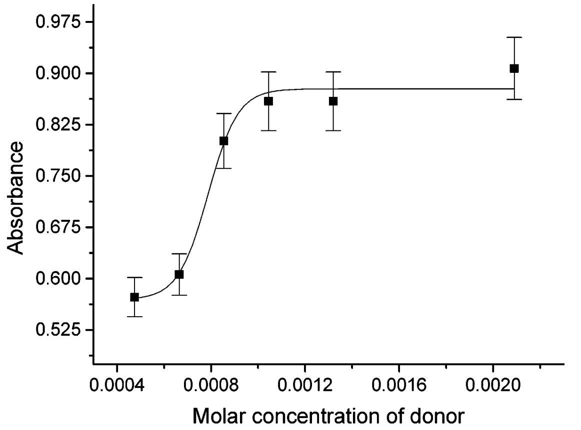

Figure 6. Absorbance data of [60]fullerene/SO system against molar concentration of donor.

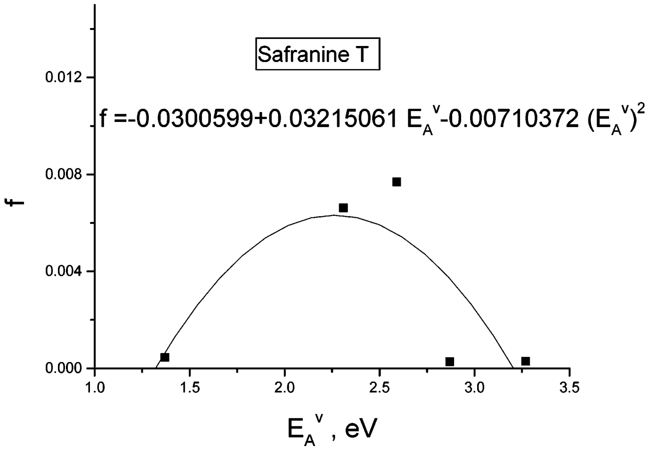

Figure 7. Variation of f vs E_A^v of the acceptors.

3.5. Determination of Resonance Energy (R_N). Briegleb and Czekalla[25] theoretically derived the relationship

$$\epsilon_{max} = 7.7 \times 10^4/[h\nu_{CT}/|R_N| - 3.5] \qquad (11)$$

where ϵ_{max} is the molar extinction coefficient of the complex at the maximum of the CT absorption, ν_{CT} is the frequency of the CT peak, and R_N is the resonance energy of the complex in the ground state, which obviously is a contributing factor to the stability constant of the complex (a ground-state property). The values of R_N for the complexes under study have been given in Table 2.

3.6. Degrees of Charge Transfer (α's). In a Mulliken two-state model,[20] the ground-state (ψ_g) and excited-state (ψ_{ex}) wavefunctions of the CT complexes are described by a linear combination of dative $\psi(D^0, A^0)$ and ionic $\psi(D^+, A^-)$ states

$$\psi_g = \{\surd(1 - \alpha)\}\, \psi(D^0, A^0) + (\surd\alpha)\, \psi(D^+, A^-) \qquad (12)$$

$$\psi_{ex} = \{\surd(1 - \alpha)\}\, \psi(D^+, A^-) - (\surd\alpha)\, \psi(D^0, A^0) \qquad (13)$$

where α is the degree of charge transfer. The function $\psi(D^+, A^-)$ differs from $\psi(D^0, A^0)$ by the promotion of an electron from the donor to the acceptor. α is given by[20]

$$\alpha = (C_2/2)/[(I_D^v - E_A^v + C_1)^2 + C_2/2] \qquad (14)$$

The values of α (calculated by using eq 14 and given in Table 2) are small and indicate that very little charge transfer occurs in the ground state. The dependence of α on E_A^v of the acceptors is shown in Figure 8. It is found that α increases with increasing electron affinity of the acceptors, as expected.

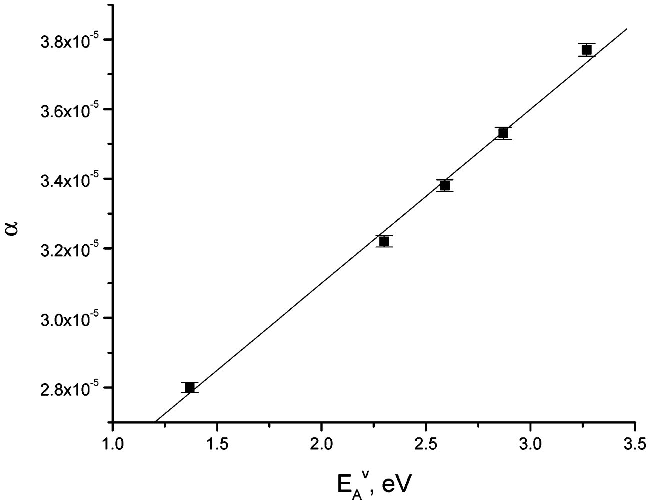

Figure 8. Degrees of charge transfer (α's) of the complexes of ST with different acceptors as a function of E_A^v of the respective acceptors.

TABLE 3: Data for Spectrophotometric Determination of Stoichiometry, Formation Constants (*K*'s), and Molar Absorptivities (ε's) of the [60]Fullerene·ST and [60]Fullerene·SO Complexes[a]

donor	10^4 donor concentration (mol·dm^{-3})	10^5 $[A]_0$ (mol·dm^{-3})	absorbance at λ_{CT}	K (dm^3·mol^{-1})	ϵ (dm^3·mol^{-1}·cm^{-1})
ST	2.49	2.778	0.502	1412 ± 17	54 354 ± 4890
	3.56		0.501		
	4.27		0.601		
	6.06		0.680		
	7.13		0.866		
	8.55		0.929		
	10.30		0.913		
SO	4.75		0.573	2410 ± 255	
	6.65		0.606		
	8.55		0.801		
	10.45		0.859		
	13.20		0.859		
	20.91		0.907		

[a] Temperature = 304 K.

TABLE 4 Data for Spectrophotometric Determination of Stoichiometry, Formation Constants (*K*'s) and Molar Absorptivities (ε's) of the [70]Fullerene·ST and [70]Fullerene·SO Complexes[a]

donor	10^4 donor concentration (mol·dm^{-3})	10^5 $[A]_0$ (mol·dm^{-3})	absorbance at λ_{CT}	K (dm^3·mol^{-1})	ϵ (dm^3·mol^{-1}·cm^{-1})
ST	5.70	1.701	1.313	2030 ± 570	98 100 ± 7430
	6.84		1.013		
	7.98		1.197		
	12.54		1.235		
	17.10		1.561		
SO	4.56		0.946	3075 ± 1110	
	8.14		1.261		
	10.26		1.622		
	18.24		1.495		
	22.17		1.517		

[a] Temperature = 304 K.

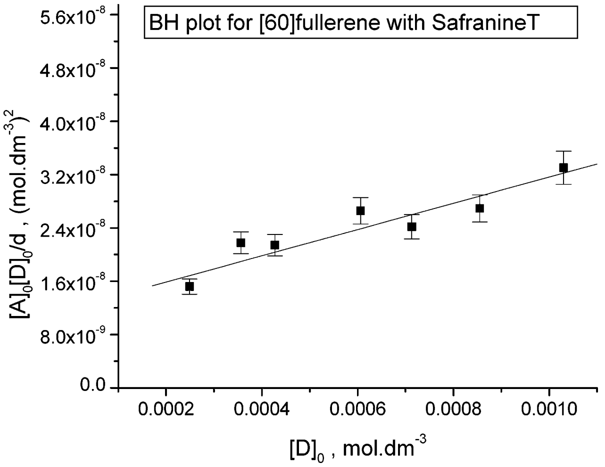

Figure 9. Benesi–Hildebrand plot for the complex of [60]fullerene with Safranine T at 304 K.

3.7. Determination of Formation Constants. The formation constants of the [60]fullerene/ST, [60]fullerene/SO, [70]fullerene/ST, and [70]fullerene/SO complexes were determined using the Benesi–Hildebrand (BH)[26] equation in the form

$$[A]_0[D]_0/d = [D]_0/\epsilon + 1/K\epsilon \qquad (15)$$

Here, $[A]_0$ and $[D]_0$ are the initial concentrations of the acceptor and donor respectively and d is the absorbance of the donor–acceptor mixture at λ_{CT}; d_A^0 and d_D^0 are the absorbances of the acceptor and donor solutions with the same molar concentrations as in the mixture at the same wavelength (i.e., λ_{CT}). The quantity ϵ is the molar absorptivity of the complex at λ_{CT}. K is the formation constant of the complex. Equation 15 is valid[26] under the condition $[D]_0 \gg [A]_0$ for a 1:1 donor–acceptor complex. The intensity in the visible portion of the absorption band (see Figure 3) increases systematically with gradual addition of ST and SO. Thus, it is definitely established in this work that the systematic increase in intensity of the broad 400–700 nm absorption band (resulting from a forbidden singlet–singlet transition in [60]- and [70]fullerenes[27,28]) is due to the 1:1 molecular complex formation between fullerenes and the dye molecules. Experimental data are given in Tables 3–4. In all cases, very good linear plots according to eq 15 are obtained, one typical case being shown in Figure 9. The correlation coefficients of all such plots were >0.95. It is observed that with the same donor in a given solvent the formation constant of a [70]fullerene complex is usually higher than that of a [60]fullerene complex. This was also observed in some of our earlier work.[29,30] For example, in CCl_4 medium, K = 0.67 , 1.67 , 10.24, and 6.8 dm^3·mol^{-1} for complexes of [60]fullerene with naphthalene, phenanthrene, anthracene, and pyrene, respectively, while for the corresponding [70]fullerene complexes, K = 10.6, 59.2 , 489.7, and 64.6 dm^3·mol^{-1}, respectively. This trend in formation constant values can be accounted for by the fact that [70]fullerene has a higher electron affinity value (i.e., 2.73 eV) than that of [60]fullerene (i.e., 2.65 eV).[31,32] It is also observed that SO binds more tightly with [60]- and [70]fullerenes than ST. The observed diminution in K values for [60]fullerene/ST and [70]fullerene/ST most certainly is a reflection of the increased hindrance to a coplanar arrangement of the two rings of the donor ST. In interpreting this observation, it has been assumed that the acceptor would interact strongly with only one ring of the dye molecule ST. Apparently, the second ring, when it is forced to lie far out of the plane of the donor ring, provides interference in donor–acceptor interaction. It is presumed that under these circumstances the acceptor molecule is forced out of a favorable parallel orientation with respect to the donor ring, or if a parallel configuration is maintained, then it is forced to lie so far away from the donor ring that effective interaction cannot occur to such an extent.

4. Conclusions

Ground-state complex formation of Safranine T and Safranine O with [60]- and [70]fullerenes and some other elctron acceptors have been established. CT bands could be located in all cases. The $h\nu_{CT}-E_A^v$ dependences have been utilized to obtain the I_D^v values of Safranine T and Safranine O. Oscillator strengths, transition dipole strengths, resonance energies, and degrees of charge transfer of the complexes have been estimated. The very low values of degree of charge transfer and oscillator strength indicate that the CT complexes studied here have almost neutral character in their ground states. The formation constants are in the order Safranine O > Safranine T. This trend in the formation constants values suggests that the arrangement of aromatic ring and the positions of different functional groups in the present dye molecules govern the EDA interaction processes with [60]- and [70]fullerenes.

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