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Molecular Complexes of Quinones: I. π–π Complexes of *p*-Chloranil with Benzene and Its Derivatives

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Abstract—The relation between the position of the charge transfer band of molecular complexes formed by *p*-chloranil with benzene derivatives and ionization potentials of the donor molecule was analyzed. Electronic absorption spectra of *p*-chloranil complexes with donor molecules possessing degenerate molecular orbitals were examined. Unlike complexes with other acceptors, such as 1,3,5-trinitrobenzene and 1,3-dinitrobenzenea, molecular complexes of *p*-chloranil with analogous donors were classed within a single group.

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In the preceding publications I have assigned molecular complexes formed by some acceptors, namely 1,3,5-trinitrobenzene [1], 1,3-dinitrobenzene [2], and iodine [3] to different groups and substantiated [4] the necessity of classification of molecular complexes into groups with account taken of their structure rather than (as it is usually performed) by the type of interacting orbitals. The present publication deals with molecular complexes of a strong π-acceptor, tetrachloro-1,4-benzoquinone (chloranil), which were examined in terms of the same approach, i.e., by analyzing [5] linear (1) or hyperbolic correlation (2) between the charge-transfer band energy ($h\nu$) and adiabatic ionization potential of the donor molecule (IP).

$$h\nu = aIP + b; \quad (1)$$

$$h\nu = IP - C_1 + C_2/(IP - C_1). \quad (2)$$

Here, a, b, C_1, and C_2 are empirical parameters.

The relation between the positions of charge-transfer band maxima of molecular complexes derived from chloranil and various benzene derivatives and ionization potentials of donor molecules was studied. The set of donor molecules included benzene, its methyl- and some alkyl-substituted derivatives, substituted styrenes, alkoxybenzene, secondary and tertiary *N*-alkylanilines, diphenyl sulfide, and halo (fluoro, chloro, bromo) benzenes and their derivatives (Table 1). The data for the corresponding complexes were obtained in the present work or taken from available literature. Phenols and primary amines capable of hydrogen bonding are intended to be discussed separately. In keeping with published data, the complexes under study have a composition of 1 : 1. By analogy with charge-transfer complexes formed by other acceptors [1–3], I class the examined chloranil complexes as *p-chloroanil complexes of the benzene group*, for the benzene aromatic system is the base donor unit. Substituents in donor molecules do not affect the structure of complexes via additional intermolecular interactions with the acceptor molecule, so that only π–π interaction is intrinsic thereto. The benzene and quinone rings in these complexes are almost parallel but are displaced with respect to each other [34]. All complexes conform to linear relations like (1) involving both adiabatic (IP_a) and vertical (IP_v) ionization potentials of donor components. In the first case, the correlation is better (Table 2). For example, the dispersion (the range of deviations of the experimental data from the calculated linear dependence) for the IP_a dependence is smaller by factors of 3 (in CCl_4) and 2 (in $CHCl_3$) than that for the IP_v dependence.

Hyperbolic dependence was calculated for complexes in chloroform solution with respect to adiabatic potentials. Nonlinearity is observed only in the region of $IP < 7$ eV (see figure). The corresponding coefficients are $C_1 = 5.651\pm0.022$ and $C_2 = 0.602\pm0.060$ ($c^2 = 0.00346$; $n = 32$). The number of experimental data for $IP < 7$ eV is limited; therefore, the error in the determination of C_2 is as large as 10%. The hyperbolic dependence is characterized by two asymptotes. One asymptote is parallel to the $h\nu$ axis,

Table 1. Parameters of the electronic absorption spectra of *p*-chloranil complexes and ionization potentials of donor components

Donor	Charge transfer band maximum, λ_{max}, nm		Ionization potential of donor [6–9], eV		
	$CHCl_3$	CCl_4	IP_a	IP_v	orbital
Benzene ($\lambda_1 + \lambda_2$)	345 [10]	339 [11] 340^a 340 [12] 342 [13] 347^b [14]	9.241	9.241	$\pi(\mathrm{b}_1)+\pi(\mathrm{a}_2)$
Toluene	365^a	370 [11] 371 [15] 372 [16] 375 [12]	8.82	8.85	$\pi(b_1)$
Ethylbenzene	–	375 [12]	8.76	8.77	$\pi(b_1)$
n-Propylbenzene	–	376 [12]	(8.83)	8.73	$\pi(b_1)$
Isopropylbenzene	–	372^b[12]	8.69	8.71	$\pi(b_1)$
n-Butylbenzene		378 [12]	(8.81)	8.69	$\pi(b_1)$
4-Isopropyltoluene, λ_1	–	433 [12]	(8.33)	8.29	$\pi(b_1)$
4-Isopropyltoluene, λ_2	–	350 [12]	(9.11)		$\pi(a_2)$
o-Xylene	389^a	403 [11] 405 [12]	8.56	8.57	$\pi(b_1)$
m-Xylene	389^a	403 [15] 404 [11] 405 [12] 410^a	8.56	8.55	$\pi(b_1)$
p-Xylene, λ_1	407^a	425 [11] 429 [12] 429 [16]	8.44	8.44	$\pi(b_1)$
p-Xylene, λ_2		350 [12]	(9.11)	9.14	$\pi(a_2)$
Mesitylene ($\lambda_1 + \lambda_2$)	415^a	425^a 426 [17] 429 [15] 429 [12] 440^b [18]	8.40	8.42	$\pi(b_1) + \pi(a_2)$
1,2,4-Trimethylbenzene	–	427^a	8.27	8.27	$\pi(b_1)$
Durene, λ_1	–	440^b [19] 472^a 475 [18] 484 [15] 488 [12] 488 [17]	8.025	8.07	$\pi(b_1)$
Durene, λ_2	–	420 [12]	8.57	8.68	$\pi(a_2)$
1,2,3,4-Tetramethylbenzene, λ_1	–	486 [12]	(7.97)	8.18	$\pi(b_1)$
1,2,3,4-Tetramethylbenzene, λ_2		420 [12]	(8.43)		$\pi(a_2)$
Pentamethylbenzene	–	490 [15] 493 [17]	7.92	7.92	$\pi(b_1)$
Hexamethylbenzene, $\lambda_1 + \lambda_2$	515 [20] 517 [19]	510 [18] 516 [20] 517 [15] 518 [21] 519 [19] 521 [12] 521 [17]	7.85	7.85	$\pi(b_1) + \pi(a_2)$

Table 1. (Contd.)

Donor	Charge transfer band maximum, λ_{max}, nm		Ionization potential of donor [6–9], eV		
	$CHCl_3$	CCl_4	IP_a	IP_v	orbital
Hexaethylbenzene	–	470[b] [12]	–	7.71	$\pi(b_1)$
Styrene, λ_1	–	423 [16]	8.42	8.48	$\pi(b_1)$
		428 [12]			
Styrene, λ_2	–	349 [12]	9.13	9.28	$\pi(a_2)$
4-Methylstyrene	–	466 [16]	(8.09)	8.20	$\pi(b_1)$
α-Methylstyrene	442[a]	448[a]	8.20	8.50	$\pi(b_1)$
β-Methylstyrene, λ_1	–	471 [12]	8.20	8.37	$\pi(b_1)$
β-Methylstyrene, λ_2	–	365 [12]	(8.94)	9.14	$\pi(a_2)$
β-Bromostyrene, λ_1	–	411 [12]	(8.05)	–	$\pi(b_1)$
β-Bromostyrene, λ_2	–	365 [12]	(8.94)	–	$\pi(a_2)$
4-Methoxystyrene	–	521 [16]	(7.77)	–	$\pi(b_1)$
4-Dimethylaminobenzylideneaniline	436 [22]	–	(8.26)	–	$\pi(b_1)$
Anisole, λ_1	440[a]	448[a]	8.22	8.42	$\pi(b_1)$
	437 [23]	448 [11]			
	460[b] [10]	452 [12]			
		459 [24]			
Anisole, λ_2	337[a]		(9.20)	9.21	$\pi(a_2)$
		342 [11]	(9.21)		
		343[a]	(9.19)		
		345 [12]	(9.17)		
4-Methylanisole	–	485 [16]	(7.97)	8.14	$\pi(b_1)$
Phenethole (ethoxybenzene)	455[a]	459[a]	8.13	–	$\pi(b_1)$
1,2-Dimethoxybenzene	510[b] [10]	510[b] [11]	7.61	8.24	$\pi(b_1)$
1,3-Dimethoxybenzene, λ_1	–	500 [12]		8.14	$\pi(b_1)$
1,3-Dimethoxybenzene, λ_2	–	430 [12]		8.72	$\pi(a_2)$
1,4-Dimethoxybenzene, λ_1	–	545 [11]	7.532	7.90	$\pi(b_1)$
		549 [12]			
1,4-Dimethoxybenzene, λ_2	–	345 [11]	(9.17)	9.25	$\pi(a_2)$
		350 [12]	(9.11)		
Diphenyl ether	457 [23]	–	8.10	8.35	$\pi(b_1)$
4,4'-Ditolyl ether	484[a]	–	(7.94)	–	$\pi(b_1)$
4-Dimethylaminobenzaldehyde	604[a]	–[c]	7.36	7.70	$\pi(b_1)$
4,4'-Bis(dimethylamino)benzophenone	640[a]	–[c]	7.25	–	$\pi(b_1)$
Diphenylamine, λ_1	642[a]	646[a]	7.25	7.44	$\pi(b_1)$
	652 [25]	652 [26]			
	660 [27]	652 [28]			
Diphenylamine, λ_2	380[a]	390[a]	8.75	9.00	$\pi(a_2)$
N-Methylaniline	590 [25]	590 [26]	7.34	7.65	$\pi(b_1)$
		595 [29]			
N-Ethylaniline	605 [30]	–	–	7.67	$\pi(b_1)$
N,*N*-Dimethylaniline, λ_1	654[a]	676[a]	7.14	7.45	$\pi(b_1)$
	667 [23]	668 [31]			
	667 [30]				
	675 [25]				
N,*N*-Dimethylaniline, λ_2	385[a]	381[a]	8.70	9.00	$\pi(a_2)$
N,*N*-Diethylaniline, λ_1	744[a]	730[a]	6.95	7.20	$\pi(b_1)$

Table 1. (Contd.)

Donor	Charge transfer band maximum, λ_{max}, nm		Ionization potential of donor [6–9], eV		
	$CHCl_3$	CCl_4	IP_a	IP_v	orbital
N,*N*-Diethylaniline, λ_2	392^a	391^a	8.60	8.90	$\pi(a_2)$
N,*N*,4-Trimethylaniline	680 [23]	–	6.96	7.25	$\pi(b_1)$
4-Bromo-*N*,*N*-dimethylaniline	674^a 680 [23]	–	(7.13) (7.11)	–	$\pi(b_1)$
4-Methoxy-*N*,*N*-dimethylaniline	730 [32] 735 [23]	–	6.70	7.22	$\pi(b_1)$
Bis(4-tolyl)amine	740 [27]	–	$(6.62)^d$	–	$\pi(b_1)$
Bis(4-methoxyphenyl)amine	800 [27]	–	$(6.81)^d$	–	$\pi(b_1)$
Bis(4-bromophenyl)amine	630 [27]	–			$\pi(b_1)$
Bis(4-methoxyphenyl)methylamine	750 [27]	–			$\pi(b_1)$
Diphenyl sulfide	–	512^a	7.80	7.88	$\pi(b_1)$
N-Methylphenothiazine	686 [28]	–	(7.09)	7.15	$\pi(b_1)$
N-Ethylphenothiazine	670 [28]	–	(7.14)		$\pi(b_1)$
N-Propylphenothiazine	675 [28]	–	(7.13)		$\pi(b_1)$
N-Acetylphenothiazine	662 [28]	–	(7.17)		$\pi(b_1)$
N-Acetyl-3,7-dibromophenothiazine	656 [28]	–	(7.19)		$\pi(b_1)$
3,7-Dichloro-*N*-methylphenothiazine	715 [28]	–	(7.01)		$\pi(b_1)$
3,7-Dibromo-*N*-methylphenothiazine	710 [28]	–	(7.02)		
Fluorobenzene	346^a	345^a	9.11	9.11	$\pi(b_1)$
2-Fluorotoluene	362^a	362^a	8.92	8.93	$\pi(b_1)$
Chlorobenzene	–	308 [12]	(9.67)	9.69	$\pi(a_2)$
2-Chlorotoluene	–	357 [12]	(9.03)	8.97	$\pi(b_1)$
3-Chlorotoluene	–	355 [12]	(9.05)	–	$\pi(b_1)$
4-Chlorotoluene	–	388 [16] 395 [12]	8.70	8.75	$\pi(b_1)$
4-Chlorostyrene	–	425 [16]	(8.39)	–	$\pi(b_1)$
Bromobenzene		307 [12]	(9.68)	9.67	$\pi(a_2)$
3-Bromotoluene		355 [12]		8.77	$\pi(b_1)$
4-Bromotoluene		402 [12]	(8.58)	8.69	$\pi(b_1)$
Benzaldehyde diphenylhydrazone	648 [33]	–	(7.21)	–	$\pi(b_1)$
4-Bromobenzaldehyde diphenylhydrazone	609 [33]	–	(7.35)	–	$\pi(b_1)$
4-Methoxybenzaldehyde diphenylhydrazone	645 [33]	–	(7.22)	–	$\pi(b_1)$
4-Chlorobenzaldehyde diphenylhydrazone	609 [33]	–	(7.35)	–	$\pi(b_1)$
2-Iodobenzaldehyde diphenylhydrazone	597 [33]	–	(7.40)	–	$\pi(b_1)$

[a] Data of this work. [b] The value was not included in correlation analysis since it strongly deviated from the calculated linear dependence (1) and was not confirmed by other authors; the complexes with isopropylbenzene and hexaethylbenzene fall out from the calculated linear dependence (1) for steric reasons (for comments, see text). [c] The complex or donor is insoluble. [d] Calculated by the hyperbolic equation.

and it crosses the IP_a axis at $IP_a = 5.651$. The other asymptote is described by the equation $h\nu = IP_a - 5.651$. The asymptotes intersect at an angle of 45°; the intersection point has the following coordinates: $IP_a = 5.651$, $h\nu = 0$ (it lies on the hyperbola major axis). The vertex has the coordinates: $\lambda_{max} = 798.9$ nm, $IP_a = 6.427$ eV. It should be noted that the point corresponding to the chloranil complex with *N*,*N*,*N*′,*N*′-tetramethylbenzene-1,4-diamine should be located on the ascending branch of dependence (2), for IP_a of the donor molecule (6.18 eV) is lower than the minimum at the IP_a axis. Charge-transfer band of that complex was not detected because of its poor solubility in the solvents used (the complex is unstable in solution [35]) and structural variation [36]. Its absorption maximum in cyclohexane [37], acetonitrile, and acetonitrile–carbon tetrachloride [38] is observed at λ 843 nm.

A second charge-transfer band was detected for chloranil complexes with *N*,*N*-dialkylanilines and diphenylamine, and their maxima were also involved in correlation analysis. Second charge-transfer band was observed previously in the spectra of chloranil complexes with anisoles [11], heterocyclic compounds [39], and substituted carbazoles [40]. Fukuzumi and Kochi [12] assigned absorption bands observed for chloranil complexes with chloro- and bromobenzenes to second charge-transfer bands, for the corresponding $h\nu$ values conformed better to linear relation (1) with IP_a^2 than with IP_a^1. All second charge-transfer bands of chloranil complexes fit well correlation (1) with adiabatic ionization potentials. An attempt was made previously to correlate charge-transfer bands of tetracyanoethylene complexes due to transitions from different π-orbitals of benzoid systems in terms of a single linear equation [41].

Some CT bands of polymethoxy-substituted benzenes do not fit well correlation (1) because of steric interactions between CH_3O groups in the donor molecules [42]. The data for such complexes [11, 15, 43] are not given in Table 1. One methoxy group in *ortho*-substituted benzenes is oriented orthogonally to the aromatic ring, which creates steric hindrances to the complexation with *p*-chloranil. Analogous effect was noted for the complex with hexaethylbenzene [42] (Table 1) and some other alkylbenzenes with bulky alkyl groups [44], as well as with benzocycloalkenes [45] (the data are not given in Table 1). Such complexes were not classed with the benzene group and were included into the group of sterically hindered benzene complexes. Analogous group was distinguished previously among iodine complexes [3].

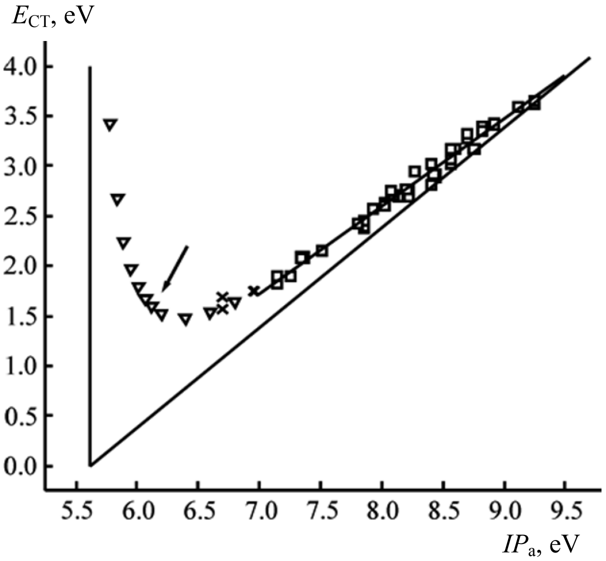
The spectra of chloranil complexes with benzene, mesitylene, and hexamethylbenzene deserve separate consideration. Molecules of these donors have two energy-degenerate but structurally different highest occupied molecular orbitals (HOMO) π(b_1) and π(a_2) [9]. Therefore, their first and second ionization potentials should be equal, and one-electron transitions from these two orbitals should give two CT bands with equal intensities. However, only one CT band is observed in the electronic spectrum, i.e. complexation of chloranil with highly symmetric donors does not remove degeneracy of the two HOMOs, as it occurs upon introduction of a substituent into benzene ring. No separate CT bands due to transitions from degenerate orbitals were observed in the spectra of tetracyanoethylene complexes [46]. Complexes of this very strong π-acceptor with a large number of unsymmetrical benzene derivatives displayed two bands corresponding to transitions from the π(b_1) and π (a_2) levels, but only one band was present in the spectra of its complexes with benzene and highly symmetric benzene derivatives possessing a symmetry axis of third or higher order. According to [4], interaction of molecular iodine with aromatic π(b_1) and π(a_2) orbitals having different symmetries gives rise to two CT bands with different λ_{max} values. Analogous pattern is also observed for complexes with compounds having degenerate orbitals. This is the result of formation of complexes with different structures via complexation at structurally different orbitals of the donor component.

Table 2. Correlation analysis of equation (1) for *p*-chloranil complexes

Parameter	Solvent	IP_a	IP_v
Coefficient *a*	CCl_4^a	0.8665	0.9942
	$CHCl_3$	0.8521	–
	$CHCl_3^b$	0.8890	0.9842
Mean-square deviation of *a*, s_a^2	CCl_4^a	0.0000999	0.000378
	$CHCl_3$	0.000284	–
Coefficient *b*	$CHCl_3^b$	0.000182	0.000766
	CCl_4^a	–4.3534	–5.0804
	$CHCl_3$	–4.1895	–
Mean-square deviation of *b*, s_b^2	$CHCl_3^b$	–4.4985	–5.4131
	CCl_4^a	0.00686	0.0271
Correlation coefficient *r*	$CHCl_3$	0.0178	–
	$CHCl_3^b$	0.0118	0.0504
Range	CCl_4^a	0.9959	0.9829
	$CHCl_3$	0.9942	–
	$CHCl_3^b$	0.9970	0.9872
Dispersion S^2	CCl_4^a	0.1717	0.5619
	$CHCl_3$	0.2885	–
	$CHCl_3^b$	0.1989	0.4510
Sample volume *n*	CCl_4^a	0.002190	0.01151
	$CHCl_3$	0.005141	–
	$CHCl_3^b$	0.002354	0.01632
	CCl_4^a	64	85
	$CHCl_3$	3228	–
	$CHCl_3^b$		35

[a] The linear dependence was calculated for $IP_a \geq 7$ eV; it was not analyzed throughout the IP_a range, for only one chloranil complex (with *N*,*N*-diethylaniline) has $IP_a < 7$ eV. [b] The dependence was calculated for $IP_a \geq 7$ eV.

Unlike other acceptors, 1,3,5-trinitrobenzene and 1,3-dinitrobenzene [1, 2], molecular complexes of chloranil with analogous benzene derivatives cannot be divided into particular groups. For example, *p*-xylene group typical of 1,3,5-trinitrobenzene and 1,3-dinitrobenzene complexes cannot be distinguished. 1,3,5-Trinitrobenzene and 1,3-dinitrobenzene are weaker acceptors than chloranil [5, 47]. A stronger (i.e., more



Plot of the CT band energies E_{CT} for chloranil complexes with benzene derivatives in chloroform versus adiabatic ionization potentials IP_a of donor molecules; *squares* denote experimental data for $IP_a > 7$ eV (approximated by a linear dependence in the region $7 < IP_a < 9.5$ eV); *crosses* denote experimental data for $IP_a < 7$ eV; *triangles* denote calculated values for $IP_a < 7$ eV (hyperbolic dependence). Arrow indicates possible location of the point for the chloranil complex with *N*,*N*,*N*′,*N*′-tetramethylbenzene-1,4-diamine on the ascending branch of the hyperbolic dependence.

reactive) acceptor is less selective. A common feature for the complexes derived from the above acceptors is that their particular groups comprise donor compounds of different chemical natures (alkyl- and halobenzenes, N-substituted anilines, anisoles). This indicates reduced contribution of atoms as structure-forming elements in the generation of supramolecular entities.

The first adiabatic ionization potentials of donor molecules (Table 1) were calculated on the basis of the obtained correlations (Table 2) and CT band maxima of some complexes. The calculations were performed using linear correlation (1) for λ_{max} values measured in CCl_4. Linear equation (1) was also used to correlate the data for the complexes with $\lambda_{max} < 725$ nm in $CHCl_3$, while hyperbolic correlation (2) was applied to those characterized by $\lambda_{max} > 725$ nm in $CHCl_3$. The coefficient C_2 in Eq. (2) was decreased by the mean-square deviation $s(C_2)$ ($C_2 = 0.542$) for $\lambda_{max} > 800$ nm. The coefficient C_2 was determined with an error of 10% because of small number of experimental data in the region $IP < 7$ eV. The C_2 value strongly affects the position of the minimum of (2) at the $h\nu$ axis: it changes from 841 nm for $C_2 - s(C_2)$ to 761 nm for $C_2 + s(C_2)$. It was impossible to calculate IP from C_2 and $C_2 + s(C_2)$ in the region $\lambda_{max} > 800$ nm ($h\nu < 1.55$ eV); in this case, $h\nu$ values appear below the calculated minimum of hyperbolic dependence (2) (see figure). Variation of C_1 within its mean-square deviation changes the position of that minimum on the IP axis by no more than 0.02 eV, whereas the position on the $h\nu$ axis remains unchanged. Calculation of IP_a from the positions of CT band maxima by Eq. (2) gives two values corresponding to the left and right branches of the hyperbola. Table contains IP_a values pertaining to the right branch. For instance, calculation by Eq. (2) for bis(4-tolyl)amine gives IP_a values of 6.067 and 6.846 eV. Introduction of a methyl group reduces the adiabatic ionization potential from 7.70 eV for aniline to 7.24 eV for 4-methylaniline ($\Delta = 0.46$ eV). Therefore, it might be expected that IP_a of diphenylamine (7.25 eV) will decrease by approximately the same value, so that IP_a for bis(4-tolyl)amine will be ~6.79 eV, which is better consistent with the value 6.846 eV rather than 6.067 eV.

The calculated IP_a values are given in Table 1 in parentheses, and they were not included in correlation analysis. These IP_a values are very consistent with the corresponding IP_v values and IP_a of analogous compounds (Table 1). For example, the difference $IP_v - IP_a$ for anisole is 0.2 eV, and the calculated difference for 4-methylanisole is 0.18 eV. The second vertical ionization potential of anisole is equal to 9.21 eV. Its adiabatic ionization potential should be the same or very similar, for substituent does not affect the energy of the second HOMO of benzene. The calculated IP_a^2 values of anisole either coincide with or very similar to IP_v^2.

EXPERIMENTAL

Chloroform and carbon tetrachloride (both of analytical grade) were dried over calcium chloride and distilled under atmospheric pressure. *p*-Chloranil (tetrachloro-1,4-benzoquinone, analytical grade) was purified by recrystallization from carbon tetrachloride; its concentration in solutions of CT complexes was 0.005 M or 0.01 to 0.005 M for complexes with *N*,*N*-dialkylanilines. The donor components: benzene (analytical grade), toluene (ultrapure), *o*-xylene, *m*-xylene, *p*-xylene, mesitylene, 1,2,4-trimethylbenzene, durene, anisole, ethoxybenzene, 4,4′-ditolyl ether, diphenylamine, 4,4′-bis(dimethylamino)benzophenone, 4-dimethylaminobenzaldehyde, 4-bromo-*N*,*N*-dimethylaniline, fluorobenzene, and 2-fluorotoluene (all of analytical grade) were used without additional purification. α-Methylstyrene, *N*,*N*-dimethylaniline, *N*,*N*-diethylaniline, and diphenyl sulfide (all of analytical grade) were purified by vacuum distillation.

Rge electronic absorption spectra of CT complexes were recorded at room temperature on an SF-46 spectrophotometer through a step of 1 to 5 nm using quartz or glass cells with a cell path length of 1 cm. The spectra were measured against the corresponding solvent. To reveal second CT bands of complexes with aromatic amines, the reference cell was charged with a solution of the corresponding donor or acceptor at the same concentration as in the working cell. Correlation analysis was performed as described in [1].

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