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Note

THE ENERGETICS OF SOME DONOR–ACCEPTOR SYSTEMS IN RELATION TO THE STRUCTURE OF THE DONORS

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In continuation of our research [1–5] on the energy parameters of various types of electron donor–acceptor systems, we have now calculated the energy parameters for some charge transfer complexes emplying the model of Sonnessa and Daisey [6] and an empirical formula reported earlier from our laboratory [5]. The aim of our present investigations is to correlate the energy parameters with the structure of the donors.

The computed values of energy parameters for some donor–acceptor systems are given in Tables 1 and 2. Inspection of these Tables reveals that there is little variation for any set of energy parameters. On the basis of these variations, the donors have been classified into groups A, B and C (Tables 1 and 2). A comparison of the energy terms of different groups shows the presence of some interesting trends in the calculated values of the energy parameters like those already reported in literature [1–6]. Further, on the basis of % charge transfer, i.e. F, the three sets of structures I, II and III (Fig. 1) are proposed and the effect of each set of structures

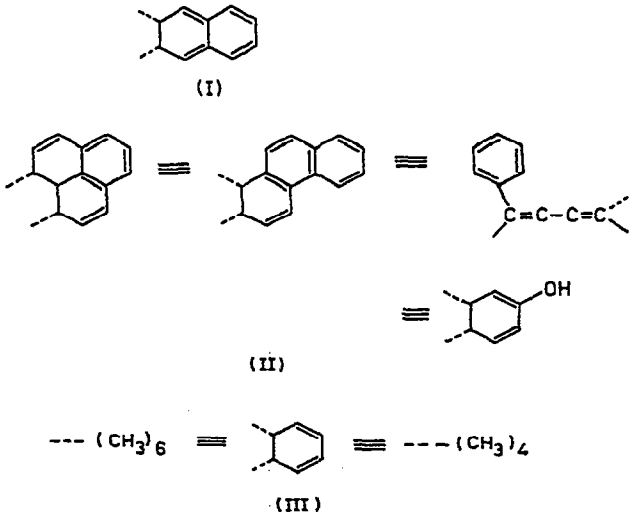

Fig. 1. Structure of the sets I, II and III.

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TABLE I

Experimental and theoretical energy parameters (in eV except a, b and F) for the CT complexes of benzotrifuroxan (BTF) with some donors

Donors	$h\nu_{CT}$ [a]	Δ	Energy parameters						
			$-X_0$	X_1	G_0	$-\Delta H^{\neq}_{calc.}$	a	b	F
Group A									
Anthracene	2.665	0.882	0.810	0.973	0.619	0.191	0.774	0.560	35.69
Azulene	2.689	0.937	0.792	0.960	0.608	0.184	0.781	0.552	34.78
Group B									
Pyrene	2.838	1.241	0.702	0.895	0.552	0.150	0.814	0.505	29.61
Chrysene	2.949	1.440	0.652	0.857	0.518	0.134	0.832	0.478	26.83
β-Naphthol	2.987	1.505	0.637	0.845	0.508	0.129	0.837	0.470	26.02
Group C									
Hexamethylbenzene	3.259	1.930	0.551	0.778	0.448	0.103	0.868	0.418	21.10
Naphthalene	3.396	2.127	0.517	0.752	0.423	0.094	0.880	0.396	19.17

[a] Ref. 7: $\beta_0 = -1.20$ eV; $S_{01} = 0.1$; $\neq$, predicted from the empirical formula.

TABLE 2

Experimental and theoretical energy parameters (in eV except a, b and F) for the CT complexes of benzotrifurazan (TFZ) with some donors

Donors	$h\nu_{CT}$ [a]	Δ	Energy parameters						
			$-X_0$	X_1	G_0	$-\Delta H^{\neq}_{calc.}$	a	b	F
Group A									
Azulene	2.677	0.910	0.801	0.966	0.609	0.192	0.774	0.559	35.58
Group B									
Pyrene	2.888	1.331	0.679	0.876	0.537	0.142	0.822	0.493	28.35
1,4-Diphenyl-butadiene	2.987	1.505	0.637	0.845	0.508	0.129	0.837	0.470	26.02
Chrysene	3.099	1.687	0.597	0.815	0.480	0.117	0.851	0.446	23.69
Group C									
Hexamethylbenzene	3.247	1.912	0.554	0.781	0.450	0.104	0.867	0.420	21.28
Phenanthrene	3.346	2.056	0.529	0.761	0.432	0.097	0.875	0.403	19.78
Durene	3.396	2.127	0.517	0.752	0.423	0.094	0.880	0.396	19.17

[a] Ref. 7: $\beta_0 = -1.20$ eV; $S_{01} = 0.1$; $\neq$, predicted from the empirical formula.

on the donating power of the benzene ring towards TFZ and BTF follows the trend: I > II > III.

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