ELECTRONIC ABSORPTION, FLUORESCENCE AND POLARISATION SPECTRA OF α,β-DIAMINO-9,10-ANTHRAQUINONES AND THEIR INTERPRETATION BY THE METHOD OF CONFIGURATION ANALYSIS*

Miloš NEPRAŠ[a], Miloš TITZ[a], Jürgen FABIAN[b] and Bohuslav GAŠ[a]

[a] *Research Institute of Organic Syntheses,*
532 18 Pardubice - Rybitví, Czechoslovakia and
[b] *Department of Chemistry,*
Technical University of Dresden, Dresden, German Democratic Republic

Received August 25th, 1981

Dedicated to Professor Dr J. Klikorka on the occasion of his 60th birthday.

On the basis of measurement of absorption frequency-dependent polarisation spectra of fluorescence (APF) and dichroism on oriented polyvinyl alcohol sheets, interpretation has been carried out of absorption spectra of α,β-diamino-9,10-anthraquinones in the wavelength range 250 to 600 nm. Character of the excited states has been investigated by the method of configuration analysis (PPP–CA).

In the Parts X to XII of this series[1–3] electronic absorption spectra of 1- and 2-amino-9,10-anthraquinones, α,α′- and β,β′-diamino-9,10-anthraquinones were interpreted on the basis of the PPP method in the approximation with variable values of β^c and γ integrals with the help of APF spectra and measurement of dichroism on oriented polyvinyl alcohol sheets. Character of the excited states was determined by the method of configuration analysis, that of electronic transitions was determined from changes of LCI π-electronic charges during $S_0 \rightarrow S_n$ excitation[4].

The present paper deals with interpretation of electronic spectra and investigation of character of the excited states of α,β-diamino-9,10-anthraquinones by the same experimental and theoretical methods as those used in the previous communications[1–3].

EXPERIMENTAL

The theoretical $\pi\pi^*$ electronic spectra were obtained by the PPP method with the so called β-parameters ($b(\text{C}{=}\text{O}) = 0{\cdot}7$; $b(\text{C}{-}\text{NH}_2) = 0{\cdot}7$; for details see ref.[1]). The substances investigated

---

[*] Part XIII in the series on Electronic Structure and Properties of Polynuclear Aromatic Ketones and Quinones; Part XII: This Journal *47*, 2594 (1982).

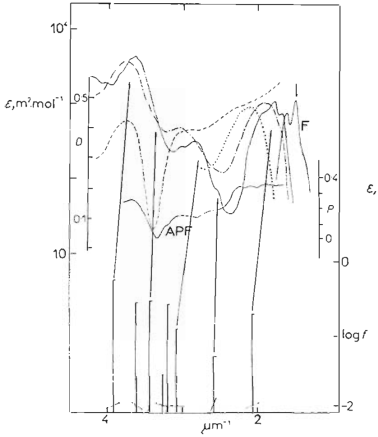


FIG. 1

Electronic spectrum of 1,2-diamino-9,10-anthraquinone: (———) the absorption spectrum in ethanol–methanol mixture 4 : 1 at 88 K; (F—) the fluorescence spectrum in ethanol–methanol mixture 4 : 1 at 77 K (the small arrow denotes the wave number of fluorescence at which the excitation spectrum was measured); (APF—) the absorption frequency-dependent polarisation spectrum of fluorescence in ethanol–methanol mixture 4 : 1 at 77 K; (-·-·-·) the absorption spectrum on oriented polyvinyl alcohol sheet; (·······) the absorption spectrum in benzene; (-----) the dichroic curve on oriented polyvinyl alcohol sheet; *D* degree of dichroism; *P* degree of fluorescence polarisation; the vertical lines denote the theoretical transitions calculated by the PPP method, the short lines denote directions of the transition moments with respect to *y*-axis, the arrows denote assignment of individual transitions to the corresponding absorption bands

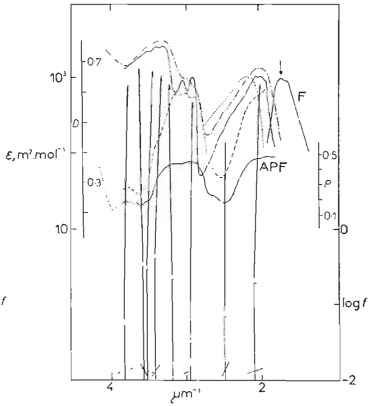


FIG. 2

Electronic spectrum of 1,6-diamino-9,10-anthraquinone (for explanation of symbols see Fig. 1)

TABLE I

Theoretical spectral characteristics of the first eight singlet $\pi\pi^*$ transitions calculated by the PPP method with variable β^c and γ integrals and the parameters given in Table I of ref.[1]; the y-axis is perpendicular to connecting line of C=O bonds

n	$\Delta^1 E_n(S_0 \rightarrow S_n)$		log f	$\sphericalangle$ (**M**, y)	The first two main configurations
	eV	μm^{-1}			
			1,2-Diamino-9,10-anthraquinone		
1	2·552	2·059	−0·685	201°	1,1′ (83·4); 2,1′ (11·0)
2	3·198	2·580	−1·259	252°	2,1′ (67·0); 3,1′ (13·1)
3	3·811	3·075	−0·891	180°	4,1′ (84·5)
4	3·950	3·187	−0·561	85°	3,1′ (45·9); 5,1′ (33·2)
5	4·034	3·254	−1·500	344°	1,2′ (71·2); 1,4′ (13·1)
6	4·252	3·430	−0·517	84°	2,2′ (21·9); 3,1′ (21·8)
7	4·482	3·616	−0·538	323°	5,1′ (32·6); 2,2′ (22·8)
8	4·865	3·925	−0·237	25°	1,3′ (49·7); 2,2′ (25·1)
			1,3-Diamino-9,10-anthraquinone		
1	2·575	2·078	−0·786	1°	1,1′ (88·4)
2	3·151	2·543	−1·032	101°	2,1′ (86·1)
3	3·771	3·042	−0·935	309°	5,1′ (62·0); 1,2′ (11·5)
4	3·814	3·077	−0·995	22°	4,1′ (76·6)
5	4·009	3·235	−0·791	296°	3,1′ (42·0); 1,2′ (40·1)
6	4·294	3·464	−0·277	74°	3,1′ (35·6); 1,2′ (29·1)
7	4·445	3·586	−0·505	183°	2,3′ (53·8); 2,4′ (17·0)
8	4·821	3·890	−0·434	143°	1,3′ (58·6); 3,2′ (12·4)
			1,6-Diamino-9,10-anthraquinone		
1	2·587	2·087	−0·703	16°	1,1′ (90·0)
2	3·080	2·485	−1·148	63°	2,1′ (85·7)
3	3·657	2·950	−1·517	22°	4,1′ (70·0); 1,2′ (8·9)
4	3·952	3·188	−0·660	268°	3,1′ (49·2); 2,2′ (15·0)
5	4·236	3·418	−0·382	55°	1,2′ (65·2); 3,1′ (8·2)
6	4·363	3·520	−0·522	340°	2,2′ (44·6); 5,1′ (19·6)
7	4·429	3·573	−0·480	117°	5,1′ (48·2); 3,1′ (28·2)
8	4·735	3·821	−1·274	198°	1,3′ (51·0); 3,2′ (18·2)
			1,7-Diamino-9,10-anthraquinone		
1	2·609	2·105	−0·791	10°	1,1′ (91·1)
2	3·068	2·475	−0·882	134°	2,1′ (84·5)
3	3·683	2·972	−1·816	150°	4,1′ (73·1); 2,2′ (10·7)
4	3·981	3·212	−0·538	275°	3,1′ (53·6); 1,2′ (17·9)
5	4·230	3·413	−0·562	95°	1,2′ (56·9); 5,1′ (13·5)
6	4·355	3·514	−0·349	13°	2,2′ (56·3); 4,1′ (19·6)
7	4·451	3·591	−0·713	246°	5,1′ (65·2); 3,1′ (17·4)
8	4·737	3·822	−1·096	310°	1,3′ (57·8); 3,2′ (14·0)

TABLE II

Results of configuration analysis (PPP–CA) for α,β-diamino-9,10-anthraquinones with 1-amino-9,10-anthraquinone as the reference system (the S_n^0 excited states), NB means non-bonding configuration of the ground state of the system (1-amino-9,10-anthraquinone + NH_2 group); r_M is the index expressing suitability of the chosen fragmentation ($r_M \leqq 100\%$)

$\tilde{\nu}$, μm^{-1}	log f		% NB	S_1^0	S_2^0	S_3^0	S_4^0	S_5^0	S_6^0	S_7^0	S_8^0	% CT	% r_M
		1,2-Diamino-9,10-anthraquinone											
—	—	S_0	91	0	0	0	0	0	0	1	0	7	98
2·059	−0·685	S_1	0	80	2	0	0	0	0	1	0	9	92
2·580	−1·259	S_2	1	9	45	0	0	3	0	2	0	32	91
3·075	−0·891	S_3	0	0	1	87	0	0	2	0	0	1	91
3·187	−0·561	S_4	0	0	17	1	53	8	3	0	0	8	91
3·254	−1·500	S_5	0	1	7	2	17	2	22	4	0	32	92
3·430	−0·517	S_6	0	0	0	0	4	58	2	7	0	17	90
3·616	−0·538	S_7	1	1	11	0	11	3	0	30	0	27	89
3·925	−0·237	S_8	1	0	0	0	2	1	2	24	18	22	91
		1,3-Diamino-9,10-anthraquinone											
—	—	S_0	90	0	0	0	0	0	0	0	0	8	98
2·078	−0·786	S_1	0	84	1	0	0	1	0	0	0	5	92
2·543	−1·032	S_2	1	6	33	0	0	7	1	0	0	42	91
3·042	−0·935	S_3	0	1	46	13	0	11	2	0	0	18	91
3·077	−0·995	S_4	0	0	4	75	0	6	1	0	0	4	91
3·235	−0·791	S_5	0	0	0	0	80	3	0	1	0	4	91
3·464	−0·277	S_6	1	0	1	0	1	36	41	0	0	7	89
3·586	−0·505	S_7	1	0	3	0	5	0	5	33	1	33	91
3·890	−0·434	S_8	1	0	0	0	2	4	0	37	8	24	90
		1,6-Diamino-9,10-anthraquinone											
—	—	S_0	90	0	0	0	0	0	0	0	0	8	98
2·087	−0·703	S_1	0	86	1	1	1	0	0	0	0	3	91
2·485	−1·148	S_2	1	4	21	18	3	2	0	0	0	40	91
2·950	−1·517	S_3	0	0	52	28	0	1	1	0	0	8	91
3·188	−0·660	S_4	0	0	9	13	50	12	0	0	0	6	91
3·418	−0·382	S_5	1	0	2	1	27	22	14	0	6	14	90
3·520	−0·522	S_6	1	0	0	9	1	7	5	2	28	31	91
3·573	−0·480	S_7	1	0	4	14	3	26	2	0	0	31	84
3·821	−1·274	S_8	0	0	0	0	0	3	9	74	0	2	90

TABLE II
(*Continued*)

$\tilde{\nu}$, μm^{-1}	log f		% NB	S_1^0	S_2^0	S_3^0	S_4^0	S_5^0	S_6^0	S_7^0	S_8^0	% CT	% r_M
		1,7-Diamino-9,10-anthraquinone											
—	—	S_0	90	0	0	0	0	0	0	0	0	8	98
2·105	−0·791	S_1	0	90	0	0	0	0	0	0	0	0	91
2·475	−0·882	S_2	1	0	28	8	7	1	1	0	0	45	91
2·972	−1·816	S_3	0	0	30	52	0	0	0	0	0	9	91
3·212	−0·538	S_4	0	0	15	7	45	18	0	0	1	5	91
3·413	−0·562	S_5	0	0	1	0	31	36	8	0	2	8	90
3·514	−0·349	S_6	1	0	0	6	0	8	1	1	32	35	91
3·591	−0·713	S_7	1	0	6	9	5	6	26	1	1	27	85
3·822	−1·096	S_8	0	0	0	0	0	2	10	76	0	1	91

were synthetized and purified by known procedures. Their purity was checked by TLC and by excitation fluorescence spectra.

RESULTS AND DISCUSSION

On the basis of the APF spectrum and dichroism it is possible to assign several transitions to absorption bands in the spectra, however, the interpretation is made difficult by low symmetry of the systems investigated.

Fig. 1 gives the absorption, fluorescence, APF spectrum and dichroic curve along with theoretical electronic spectrum for 1,2-diamino-9,10-anthraquinone; scheme A. The first transition at 2·06 μm^{-1} can be assigned unambiguously to the longest-wave band in the spectrum. The second transition corresponds to the shoulder at 2·5 μm^{-1}. In the region 2·5 to 3·2 μm^{-1} there is a broad absorption band; this band could be connected with the transition at 3·07 μm^{-1} in the theoretical spectrum. In the region of 3·4 μm^{-1} the APF curve and, especially, the D curve exhibit a marked minimum indicating the presence of a band in this region (this band is not seen in the absorption spectrum) with polarisation almost perpendicular to the first band of the spectrum. We assign the transition at 3·43 μm^{-1} to this band. The transition at 3·92 μm^{-1} (parallel polarisation with the first transition) is assigned to intensive band with the maximum at 3·7 μm^{-1} on the basis of the polarisation curves. Assignment of the other transitions is doubtful.

Fig. 2 gives electronic absorption and polarisation spectra of 1,6-diamino-9,10-anthraquinone; scheme B. A clean-cut shape of the absorption spectrum and character of the polarisation curves allow assignment of all eight transitions in the way given

TABLE III

Results of configuration analysis (PPP–CA) for α,β-diamino-9,10-anthraquinones with 2-amino-9,10-anthraquinone as the reference system (the S_n^0 excited states), NB means non-bonding configuration of the ground state of the system (2-amino-9,10-anthraquinone + NH_2 group); r_M is the index expressing suitability of the chosen fragmentation ($r_M \leqq 100\%$)

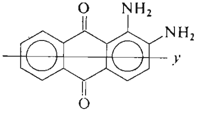
$\tilde{\nu}$, μm^{-1}	log f		% NB	S_1^0	S_2^0	S_3^0	S_4^0	S_5^0	S_6^0	S_7^0	S_8^0	% CT	% r_M
1,2-Diamino-9,10-anthraquinone													
—	—	S_0	88	0	0	0	0	2	0	0	0	9	97
2·059	−0·685	S_1	2	19	17	0	1	1	0	0	0	48	90
2·580	−1·259	S_2	1	63	17	0	1	0	1	0	0	5	89
3·075	−0·891	S_3	0	0	1	85	1	0	0	0	0	1	89
3·187	−0·561	S_4	1	0	18	2	57	0	0	1	1	7	89
3·254	−1·500	S_5	1	2	11	0	0	24	11	2	3	30	91
3·430	−0·517	S_6	1	0	10	0	16	0	24	6	7	20	89
3·616	−0·538	S_7	0	0	0	0	0	47	17	4	3	17	90
3·925	−0·237	S_8	0	0	1	0	2	8	0	31	0	24	90
1,3-Diamino-9,10-anthraquinone													
—	—	S_0	87	0	0	0	0	0	0	0	0	10	98
2·078	−0·786	S_1	2	23	8	0	2	1	4	0	0	49	89
2·543	−1·032	S_2	0	60	10	0	3	1	4	0	0	11	89
3·042	−0·935	S_3	0	1	59	4	8	1	7	0	0	7	88
3·077	−0·995	S_4	0	0	3	83	1	0	0	0	0	1	88
3·235	−0·791	S_5	2	1	0	0	47	2	9	0	1	21	89
3·464	−0·277	S_6	1	0	3	0	12	24	17	1	2	21	89
3·586	−0·505	S_7	1	0	1	0	3	51	0	3	4	20	90
3·890	−0·434	S_8	0	0	0	0	1	5	0	10	6	25	89
1,6-Diamino-9,10-anthraquinone													
—	—	S_0	87	0	0	0	0	0	0	0	0	10	98
2·087	−0·703	S_1	2	10	1	23	0	0	0	0	0	52	89
2·485	−1·148	S_2	0	77	0	6	0	0	0	0	0	4	88
2·950	−1·517	S_3	0	0	81	4	1	0	0	0	0	2	88
3·188	−0·660	S_4	1	0	1	1	68	0	0	0	0	12	88
3·418	−0·382	S_5	2	0	1	0	16	15	0	2	1	31	89
3·520	−0·522	S_6	0	0	0	0	2	68	6	1	0	6	88
3·573	−0·480	S_7	0	0	0	2	0	4	79	0	0	2	88
3·821	−1·274	S_8	0	0	0	1	0	0	0	31	7	42	91

TABLE III
(*Continued*)

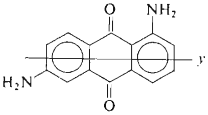
$\tilde{\nu}$, μm^{-1}	log f		% NB	S_1^0	S_2^0	S_3^0	S_4^0	S_5^0	S_6^0	S_7^0	S_8^0	% CT	% r_M
1,7-Diamino-9,10-anthraquinone													
—	—	S_0	87	0	0	0	0	0	0	0	0	10	97
2·105	−0·791	S_1	3	0	6	25	0	0	0	0	0	54	89
2·475	−0·882	S_2	0	87	0	1	0	0	0	0	0	0	88
2·972	−1·816	S_3	0	0	77	9	0	0	0	0	0	2	88
3·212	−0·538	S_4	1	0	1	0	64	0	2	1	0	15	89
3·413	−0·562	S_5	2	0	1	2	20	3	1	2	1	33	89
3·514	−0·349	S_6	0	0	0	0	0	83	2	0	0	1	88
3·591	−0·713	S_7	0	0	1	5	0	0	72	0	0	7	88
3·822	−1·096	S_8	0	0	0	1	0	0	0	31	8	40	90

in Fig. 2. Usefulness of measurement results of dichroism for interpretation of the spectrum can be demonstrated by the example of local maximum of the dichroism curve at 3·75 μm^{-1}. This maximum corresponds to the minimum at the absorption curve and indicates quite unambiguously an overlapped band to which we assign the eighth transition in theoretical spectrum (parallel polarisation with the first transition).

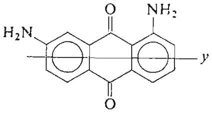
Course of absorption spectrum of 1,7-diamino-9,10-anthraquinone (Fig. 3; scheme C) is very similar to that of 1,6-isomer, however, a less clean-cut character of the polarisation spectra allows only assignment of the first four transitions with certainty. To complete the series, we also give theoretical data on 1,3-diamino-9,10-anthraquinone, even though the experimental spectrum is missing.



A



B



C

Table I gives theoretical spectral characteristics of the first eight $\pi\pi^*$ electronic transitions for α,β-diamino-9,10-anthraquinones. From the given results it follows that the theoretical spectra calculated by the PPP method agree very well with the experimental spectra.

For determination of character of the excited states we used the method of configuration analysis (PPP–CA). For α,β-diamino-9,10-anthraquinones two possibilities were considered with regard to choice of reference system: either 1-amino-9,10-anthraquinone with the second amino group entering β position or 2-amino-9,10-anthraquinone with the second amino group entering α position. The results are given in Tables II and III. The correlations obtained from the configuration analysis are seen in Fig. 4. The transitions were connected, if participation of the reference

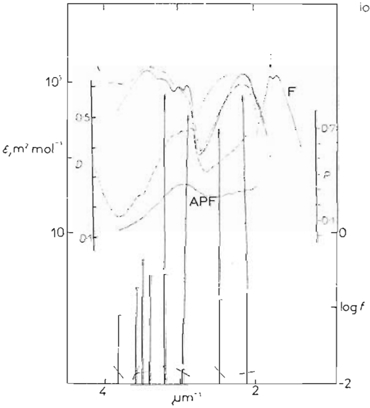


FIG. 3

Electronic spectrum of 1,7-diamino-9,10-anthraquinone (for explanation of symbols see Fig. 1)

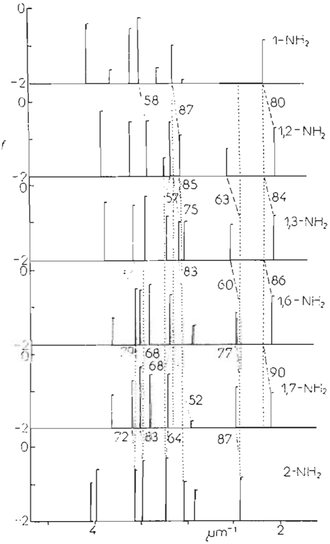
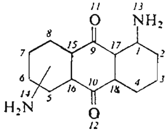


FIG. 4

Correlation graph of the singlet excited states constructed on the basis of PPP–CA results for α,β-diamino-9,10-anthraquinones with 1- and 2-amino-9,10-anthraquinones as the reference systems

TABLE IV

The character of transitions of α,β-diamino-9,10-anthraquinones determined from changes of LCI π-electron charges at the subsystems during $S_0 \rightarrow S_n$ transition; amino groups and 9,10-anthraquinone were used as the subsystems. Numbering of the centres follows the scheme:



Transition	Character	%	Δq_a [a]	Δq_{CT} [b]	Δq_{LE} [c]	The main centres	Δq_μ
			1,2-Diamino-9,10-anthraquinone				
$S_0 \rightarrow S_1$	CT(1,2-NH_2→9,10-AQ)	82	0·72	0·59	—	acceptor	9 (0·19); 11 (0·14); 12 (0·10); 10 (0·09)
	LE(9,10-AQ)	18		—	0·13	donor	13 (—0·51)
$S_0 \rightarrow S_2$	CT(1,2-NH_2→9,10-AQ)	63	0·65	0·41	—	acceptor	9 (0·16); 11 (0·14); 12 (0·12); 10 (0·12)
	LE(9,10-AQ)	37		—	0·24	donor	14 (—0·37); 3 (—0·12)
$S_0 \rightarrow S_3$	CT(1,2-NH_2→9,10-AQ)	1	0·45	0·004	—	acceptor	10 (0·12); 9 (0·12)
	LE(9,10-AQ)	99		—	0·45	donor	8 (—0·21); 5 (—0·21)
$S_0 \rightarrow S_4$	CT(1,2-NH_2→9,10-AQ)	27	0·63	0·17	—	acceptor	9 (0·17); 10 (0·11)
	LE(9,10-AQ)	73		—	0·46	donor	14 (—0·12); 7 (—0·12); 15 (—0·12); 6 (—0·11)
			1,3-Diamino-9,10-anthraquinone				
$S_0 \rightarrow S_1$	CT(1,3-NH_2→9,10-AQ)	77	0·73	0·56	—	acceptor	9 (0·15); 12 (0·12); 11 (0·11); 10 (0·11)
	LE(9,10-AQ)	23		—	0·17	donor	13 (—0·53)
$S_0 \rightarrow S_2$	CT(1,3-NH_2→9,10-AQ)	79	0·71	0·57	—	acceptor	12 (0·15); 10 (0·15); 9 (0·12); 11 (0·12)
	LE(9,10-AQ)	21		—	0·15	donor	14 (—0·47); 2 (—0·14); 13 (—0·10)
$S_0 \rightarrow S_3$	CT(1,3-NH_2→9,10-AQ)	37	0·59	0·22	—	acceptor	10 (0·15); 12 (0·13); 9 (0·12); 11 (0·11)
	LE(9,10-AQ)	63		—	0·37	donor	14 (—0·16); 16 (—0·13); 7 (—0·13)
$S_0 \rightarrow S_4$	CT(1,3-NH_2→9,10-AQ)	4	0·51	0·02	—	acceptor	10 (0·13); 9 (0·10)
	LE(9,10-AQ)	96		—	0·49	donor	8 (—0·19); 5 (—0·16)

				1,6-Diamino-9,10-anthraquinone			
$S_0 \to S_1$	CT(1,6-$NH_2 \to$9,10-AQ)	81	0·71	0·58	—	acceptor	9 (0·16); 11 (0·13); 12 (0·11); 10 (0·11)
	LE(9,10-AQ)	19		—	0·13	donor	13 (−0·56)
$S_0 \to S_2$	CT(1,6-$NH_2 \to$9,10-AQ)	74	0·62	0·46	—	acceptor	10 (0·16); 12(0·16); 9 (0·11)
	LE(9,10-AQ)	26		—	0·16	donor	14 (−0·44)
$S_0 \to S_3$	CT(1,6-$NH_2 \to$9,10-AQ)	17	0·56	0·09	—	acceptor	10 (0·13); 9 (0·13); 12 (0·11)
	LE(9,10-AQ)	83		—	0·47	donor	16 (−0·10); 7 (−0·08); 14 (−0·08)
$S_0 \to S_4$	CT(1,6-$NH_2 \to$9,10-AQ)	44	0·44	0·19	—	acceptor	9 (0·14); 10 (0·09)
	LE(9,10-QA)	56		—	0·25	donor	13 (−0·13); 12(−0·08); 14 (−0·06)
				1,7-Diamino-9,10-anthraquinone			
$S_0 \to S_1$	CT(1,7-$NH_2 \to$9,10AQ)	77	0·74	0·57	—	acceptor	9 (0·19); 11 (0·14); 12 (0·11); 10 (0·10)
	LE(9,10-AQ)	23		—	0·17	donor	13 (−0·57)
$S_0 \to S_1$	CT(1,7-$NH_2 \to$9,10-AQ)	73	0·66	0·48	—	acceptor	9 (0·16); 11 (0·15); 10 (0·11); 12 (0·09)
	LE(9,10-AQ)	27		—	0·17	donor	14 (−0·49)
$S_0 \to S_3$	CT(1,7-$NH_2 \to$9,10-AQ)	16	0·54	0·09	—	acceptor	10 (0·13); 9 (0·13); 11 (0·09); 12 (0·09)
	LE(9,10-AQ)	84		—	0·45	donor	15 (−0·10); 13 (−0·10); 14 (−0·08); 8 (−0·08)
$S_0 \to S_4$	CT(1,7-$NH_2 \to$9,10-AQ)	43	0·47	0·20	—	acceptor	10 (0·14); 9 (0·12)
	LE(9,10-AQ)	57		—	0·27		13 (−0·16); 17 (−0·07); 11 (−0·07)

---

[a] The total redistribution of π-electron charge (CT migration + LE redistribution); [b] migration of the total amount of π-electron charge during CT transition; [c] redistribution of the total amount of π-electron charge during LE.

configuration exceeded 50% and the respective transition had the value $\log f > -1$. An important point follows from the graph; if 1-amino-9,10-anthraquinone is considered as the reference system, then the first excited state of α,β-diamino-9,10-anthraquinones is the local excited state of the reference system, whereas the second exited state has a relative "high" contribution of CT configuration, and transition to this state has a distinct CT character; if 2-amino-9,10-anthraquinone is considered as the reference system, then the first excited state has a relatively high contribution of CT configuration, and the transition to the first excited state can be classified as a CT transition, whereas the second excited state is a local excited state of 2-amino-9,10-anthraquinone.

However, what is the nature of the local excited states of 1- and 2-amino-9,10-anthraquinone? From the results[1] of configuration analysis of the monoaminoanthraquinones it follows that the first excited state of these compounds has a significant CT character with charge transfer from amino group to 9,10-anthraquinone. Considering the fragmentation to 9,10-anthraquinone and two amino groups, the above conclusion means that the first excited state of α,β-diamino-9,10-anthraquinones has a predominant character of CT state with charge transfer from α-amino group, and the second excited state has a predominant character of CT state with charge transfer from β-amino group. This result is confirmed by the character of transitions and the amount of transferred charge determined from changes of the LCI π-electron charges during the $S_0 \rightarrow S_n$ transition in the case of fragmentation to 9,10-anthraquinone and two amino groups (Table IV). Thus in contrast to α,α'- and β,β'-diamino-9,10-anthraquinones (refs[2,3]), it is impossible to speak about "splitting" of the first band of the reference system in the case of α,β-diamino-9,10-anthraquinones. The data of Table IV also show that the main acceptor centres in the first two transitions are the both carbonyl groups, and the third transition is a very "pure" anthraquinone transition.

REFERENCES

1. Nepraš M., Fabian J., Titz M., Gaš B.: This Journal *47*, 2569 (1982).
2. Nepraš M., Gaš B., Fabian J., Titz M.: This Journal *47*, 2583 (1982).
3. Nepraš M., Titz M., Gaš B., Fabian J.: This Journal *47*, 2594 (1982).
4. Nepraš M., Titz M.: Int. J. Quantum Chem. *16*, 543 (1979).

Translated by J. Panchartek.