ELECTRONIC STRUCTURE OF 2-HYDROXYAZABENZANTHRONES

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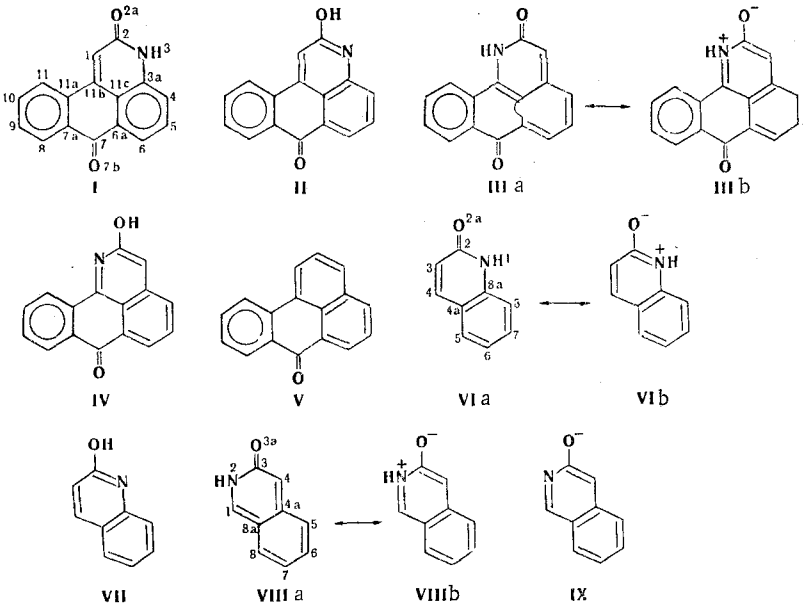
The structures of the tautomers of 2-hydroxyazabenzanthrones were investigated as compared with those of benzanthrone and the tautomers of 2-quinolone and 3-isoquinolone by a quantum-chemical method. In the lactam form of 2-hydroxy-3-azabenzanthrone the bonds in both extreme rings are equalized, and the heteroring is less aromatic than in 2-pyridone and 2-quinolone. In the lactam form of 2-hydroxy-1-azabenzanthrone and equality of the bonds in the extreme ring, as in benzanthrone, is disrupted, and the heterocyclic fragment is similar with respect to the distribution of the bonds and charges to the isolated 3-isoquinolone molecule. The data obtained are in good agreement with the chemical and spectral properties of 2-hydroxyazabenzanthrones.

2-Hydroxy-3-azabenzanthrone [anthrapyridone or 7H-dibenz[f,ij]isoquinoline-2,7(3H)-dione (I)] and 2-hydroxy-1-azabenzanthrone [2-hydroxy-7H-dibenzo[de,h]quinolin-7-one (IV)] compounds are important in the chemistry of dyes. The former find application as dyes of various types [1] and luminophores [2], while the latter are used in the synthesis of vat dyes and polycyclic pigments [3, 4]. The value of 2-hydroxyazabenzanthrones draws attention to a study of their properties and electronic structures.

Substantial differences in the tautomerism and acid–base and spectral properties of 2-hydroxyazabenzanthrones determined by different mutual orientations of the annelated 2-pyridone/2-hydroxypyridine and anthrone rings were noted in [5-7]. In order to characterize the peculiarities of the electronic structures that are responsible for these differences we undertook a quantum-chemical analysis of the tautomers of 2-hydroxy-3-azabenzanthrone (I/II) and 2-hydroxy-1-azabenzanthrone (III/IV) as compared with benzanthrone (V) and the tautomers of 2-quinolone (VI/VII) and 3-isoquinolone (VIII/IX). The calculation was made by the Pariser–Parr–Pople (PPP) method by means of the program in [8] with allowance for the interaction of 25 singly excited configurations.



I II III a III b

IV V VI a VI b

VII VIII a VIIIb IX

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TABLE 1. Bond Orders in I-IX

Bond	Ground state					Excited state				
	I	II	III	IV	V	I	II	III	IV	V
1—2	0,357	0,547	0,485	0,530	0,584	0,418	0,525	0,450	0,511	0,667
2—2a	0,789	0,263	0,680	0,474	—	0,740	0,452	0,737	0,584	—
2—3	0,382	0,708	0,476	0,632	0,746	0,446	0,547	0,433	0,486	0,609
3—3a	0,303	0,514	0,683	0,576	0,530	0,545	0,574	0,615	0,591	0,536
3a—11c	0,615	0,569	0,481	0,546	0,567	0,446	0,420	0,502	0,501	0,551
3a—4	0,617	0,521	0,453	0,502	0,520	0,540	0,498	0,501	0,516	0,551
4—5	0,688	0,750	0,794	0,763	0,755	0,660	0,701	0,715	0,692	0,688
5—6	0,640	0,579	0,526	0,565	0,573	0,579	0,564	0,601	0,612	0,630
6—6a	0,662	0,707	0,737	0,714	0,715	0,599	0,687	0,601	0,601	0,630
6a—11c	0,578	0,515	0,465	0,505	0,511	0,520	0,555	0,530	0,537	0,547
6a—7	0,299	0,312	0,328	0,318	0,303	0,387	0,374	0,377	0,388	0,366
7—7a	0,303	0,302	0,316	0,313	0,302	0,354	0,356	0,361	0,370	0,368
7—7b	0,834	0,827	0,823	0,827	0,837	0,741	0,745	0,757	0,731	0,741
7a—11a	0,599	0,602	0,593	0,600	0,604	0,574	0,544	0,548	0,370	0,506
7a—8	0,643	0,639	0,634	0,638	0,638	0,626	0,632	0,627	0,629	0,634
8—9	0,664	0,668	0,672	0,669	0,671	0,678	0,657	0,675	0,667	0,635
9—10	0,661	0,658	0,652	0,657	0,656	0,645	0,625	0,626	0,624	0,608
10—11	0,666	0,671	0,677	0,672	0,674	0,682	0,692	0,698	0,695	0,693
11—11a	0,638	0,671	0,626	0,635	0,634	0,682	0,582	0,586	0,695	0,693
11a—11b	0,323	0,322	0,343	0,323	0,322	0,371	0,412	0,427	0,426	0,469
11b—11c	0,368	0,499	0,611	0,524	0,511	0,495	0,451	0,497	0,453	0,445
11b—1	0,823	0,721	0,563	0,676	0,708	0,660	0,638	0,539	0,600	0,552
	VI	VII	VIII	IX		VI	VII	VIII	IX	
1—2	0,529	0,656	0,614	0,730		0,466	0,531	0,496	0,594	
2—2a	0,712	0,495	—	—		0,729	0,552	—	—	
2—3	0,377	0,473	0,471	0,506		0,398	0,443	0,434	0,445	
3—3a	—	—	0,674	0,471		—	—	0,719	0,580	
3—4	0,855	0,797	0,496	0,652		0,673	0,647	0,463	0,518	
4—4a	0,423	0,494	0,676	0,567		0,523	0,510	0,558	0,545	
4a—8a	0,579	0,565	0,483	0,548		0,424	0,384	0,498	0,434	
4a—5	0,581	0,542	0,456	0,509		0,505	0,530	0,532	0,543	
5—6	0,717	0,748	0,803	0,767		0,653	0,647	0,685	0,643	
6—7	0,608	0,575	0,508	0,556		0,560	0,534	0,589	0,566	
7—8	0,720	0,751	0,799	0,763		0,623	0,654	0,687	0,668	
8—8a	0,566	0,530	0,468	0,521		0,539	0,508	0,529	0,512	
8a—1			0,674	0,471				0,719	0,580	

The validity of regarding the tautomers of 2-hydroxyazabenzanthrones as electronic analogs of benzanthrone follows from the data on the aromatic character of the 2-pyridone and 2-hydroxypyridine rings [9]. Their aromatic character is confirmed by determinations of the exaltation [10] and nonlocal component [11] of the magnetic susceptibility due to the ring currents. It follows from a study of the tautomerism [12] and basicities in the gas phase [13] that the resonance energies of 2-pyridones amounts to only 0.26 to 0.30 eV, i.e., one fifth of the resonance energy of benzene less than that of 2-hydroxypyridines. X-ray diffraction measurements for 2-pyridones [14, 15] indicate equality of the bonds, while studies of the integral intensities in the IR spectra [16] and of complexing reactions [17] indicate the increased population of the C—O bond, which corresponds to the contribution of aromatic oxidopyridinium structures corresponding to the Hückel rule. Within the framework of structural criteria, the 2-pyridone ring is more aromatic, the greater the equality of the bonds in it and the higher the charges of opposite sign on the heteroatoms.

The benzanthrone molecule (V) can be regarded as consisting of two aromatic fragments, viz., benzene and naphthalene fragments connected by single bonds. In fact, it is apparent from a calculation of the bond orders (Table 1) that in benzanthrone in the ground state the bonds in the benzene fragment are almost completely delocalized, whereas in the naphthalene fragment they are distributed in the same way as in naphthalene itself: The 11b—1, 2—3, 4—5, and 6—6a bonds, which correspond to the α—β bonds of naphthalene, have increased orders, whereas the remaining bonds have decreased orders. The greater effect of the carbonyl group on the 6 and 4 positions in the naphthalene fragment that are conjugated with it and to which nucleophilic attack is directed in benzanthrone is explained by fixation of the bonds [18]. The benzanthrone structure is clearly reflected by structural formula V, in which the circle, which symbolizes the aromatic sextet π electrons, emphasizes delocalization of the bonds, while the alternation of the single and double bonds indicates partial localization character.

TABLE 2. Charges on the Atoms in I-IX

Atom	Ground state					Excited state				
	I	II	III	IV	V	I	II	III	IV	V
1	0,002	−0,028	0,541	−0,282	0,017	−0,076	−0,147	0,517	−0,273	−0,032
2	0,251	0,061	0,121	0,088	0,000	0,152	0,191	0,132	0,167	0,064
2a	−0,476	0,151	−0,577	0,210	—	−0,340	0,195	−0,294	0,359	—
3	0,200	−0,270	−0,009	−0,109	0,012	0,590	−0,272	0,052	0,034	0,066
3a	0,014	0,069	0,016	0,032	−0,004	0,033	0,142	0,007	0,029	−0,002
4	−0,007	0,021	0,034	0,013	0,026	−0,067	−0,034	−0,037	−0,047	−0,029
5	0,018	0,007	0,011	0,008	0,000	0,006	−0,009	−0,015	−0,034	−0,019
6	0,040	0,052	0,070	0,047	0,061	0,125	0,131	0,021	0,066	0,038
6a	−0,012	−0,024	−0,023	−0,014	−0,024	−0,075	−0,054	−0,051	−0,054	−0,027
7	0,284	0,282	0,256	0,265	0,270	0,205	0,200	0,195	0,171	0,171
7a	−0,017	−0,014	−0,010	−0,014	−0,023	−0,041	0,041	0,038	−0,040	−0,048
7b	−0,406	−0,413	−0,398	−0,399	−0,399	−0,500	−0,485	−0,464	−0,489	−0,472
8	0,046	0,044	0,051	0,042	0,043	0,040	0,050	0,051	0,043	0,062
9	0,010	0,005	0,015	0,005	0,000	−0,009	0,021	0,003	0,010	0,055
10	0,022	0,017	0,024	0,015	0,017	0,010	−0,006	0,007	−0,027	−0,025
11	0,010	0,001	−0,013	0,012	−0,004	−0,006	0,017	−0,014	0,029	0,077
11a	0,007	0,007	−0,015	0,009	0,014	−0,024	−0,002	0,053	−0,024	0,010
11b	0,042	0,044	−0,027	0,012	−0,007	−0,051	−0,012	−0,051	0,094	0,069
11c	−0,027	−0,016	−0,059	−0,038	0,004	0,033	0,017	0,031	0,071	0,041
	VI	VII	VIII	IX		VI	VII	VIII	IX	
1	0,469	−0,334	−0,020	0,134		0,621	−0,319	−0,201	0,016	
2	0,154	0,119	0,561	−0,280		0,135	0,131	0,502	−0,383	
2a	−0,542	0,223	—	—		−0,349	0,317	—	—	
3	−0,009	−0,070	0,116	0,083		−0,120	−0,114	0,116	0,150	
3a	—	—	−0,582	0,208		—	—	−0,242	0,363	
4	0,031	0,053	−0,046	−0,125		−0,109	−0,093	−0,022	−0,022	
4a	−0,049	−0,039	0,023	0,037		0,003	0,069	−0,018	−0,008	
5	0,118	0,03	−0,000	−0,017		−0,115	−0,083	−0,032	−0,031	
6	−0,014	−0,022	0,016	0,011		0,080	0,072	−0,057	−0,110	
7	−0,022	0,007	−0,006	−0,020		−0,076	−0,058	0,023	0,071	
8	−0,050	−0,016	0,000	0,012		−0,074	−0,047	−0,071	−0,068	
8a	−0,030	0,077	−0,061	−0,044		0,003	0,124	0,003	0,022	

In analogy with benzanthrone, in 2-hydroxy-3-azabenzanthrone tautomers I/II one can isolate a 2-quinolone/2-hydroxyquinoline fragment, and in 2-hydroxy-1-azabenzanthrone tautomers III/IV one can isolate a 3-isoquinolone/3-hydroxyisoquinoline fragment. A comparison with the corresponding isolated VI/VII and VIII/IX molecules gives some idea as to how inclusion of a heterocyclic fragment in the 2-hydroxyazabenzanthrone system affects the electronic structure.

In the case of lactim tautomers II and IV annelation does not qualitatively change the distribution of bonds and charges as compared with 2-hydroxyquinoline (VII) and 3-hydroxyisoquinoline (IX) (Tables 1 and 2). One can only note a certain equalization of the adjacent 11b—1 and 1—2 bonds in the heteroring and a decrease in the 6—6a and 6a—11c bond orders as compared with the analogous bonds in VII and IX. As in benzanthrone (V), a chain of bonds of alternating increased and decreased multiplicity is localized in the extreme ring of lactim tautomers II and IV that is adjacent to the heteroring. The calculation also shows that the monoprotonated forms of 2-hydroxyazabenzanthrones that contain a 2-hydroxypyridinium ring are similar with respect to the distribution of the bonds in the anthrone ring to lactim tautomers that contain a 2-hydroxypyridine ring.

The effect of annelation is more unusual in the case of lactam tautomers. In contrast to benzanthrone (V) and 2-quinolone (VI), in the lactam form of 2-hydroxy-3-azabenzanthrone (anthrapyridone) (I) in the ground state the equality of the bonds in the extreme ring adjacent to the heteroring is not disrupted. In the heteroring, however, equality of the bonds is virtually absent (Table 1), and the charges of opposite sign on the nitrogen and oxygen atoms are considerably lower than in 2-pyridone [19] and 2-quinolone (Table 2). This constitutes evidence for the low degree of aromatic character of the heteroring and the insignificant contribution of dipolar structures of the VIa type to the structure of the heterocyclic fragment of anthrapyridone. The anthrapyridone molecule is actually 9,10-anthraquinone-9-methide, in which both extreme rings have equalized bonds, as in anthrone [20] and in 9,10-anthraquinone [21], the 11b—1 bond is a double bond, and the amide bridge is connected to the carbon atoms in the 1 and 3a positions by single bonds. Formula VI [sic]

with symbols of equality of the bonds, viz., the circles in both extreme rings, reflects these structural peculiarities.

A diene chain that includes 4—5 and 6—6a bonds with increased multiplicity is localized in the lactam form of 2-hydroxy-1-azabenzanthrone (III) in the ground state in the extreme ring adjacent to the heteroring, as in benzanthrone (V) and 3-isoquinolone (VIII). Delocalization of the bonds and separation of the charges on the heteroatoms are greater in the heteroring than in 2-pyridone [19] and are close to what is observed in 3-isoquinolone (VIII) (Tables 1 and 2), and this corresponds to the significant contribution, in addition to structure IIIa, of dipolar structure IIIb.

Thus the different modes of peri-annelation of the 2-pyridone ring with the anthrone ring lead to different results. The equality of the bonds in both extreme rings that is characteristic for anthrone is retained in the lactam form of 2-hydroxy-3-azabenzanthrone (anthrapyridone) (I), and the aromatic character of the heteroring is decreased, while in the lactam form of 2-hydroxy-1-azabenzanthrone III the equality of the bonds in one of the extreme rings is disrupted, and the aromatic character of the heteroring is increased. The inclusion of a 2-quinolone ring as a fragment in the anthrapyridone (I) molecule leads to redistribution of the bonds and charges as compared with the isolated VI molecule as a consequence of the increased energic stability of the 9,10-anthraquinoid structure. The inclusion of a 3-isoquinolone ring in the energically less favorable 1,10-anthraquinoid structure of the lactam form of 2-hydroxy-1-azabenzanthrone III does not change the parameters of the heterocyclic fragment as compared with the isolated VIII molecule.

As the tautomers of 2-hydroxyazabenzanthrones I-IV pass to the first excited state, the equality of the bonds increases, and the π-electron density is shifted from the lactam or lactim grouping toward the keto carbonyl group (Tables 1 and 2). The longest-wave band, which is of the $S_{\pi\pi^*}$ type and is primarily due to transfer of an electron from the upper occupied molecular orbital (UOMO) to the lower vacant molecular orbital (LVMO), corresponds to this transition in the electronic spectra. The remaining transitions are complex (Table 3). The satisfactory agreement between the calculated and experimental spectra constitutes evidence in favor of the correctness of the selection of the computational parameters.

It is apparent from Table 4 that the longer-wave absorption of lactam tautomers I and III as compared with lactim tautomers II and IV is due to a decrease in the energy of the LVMO, whereas the longer-wave absorption of the tautomers of 2-hydroxy-1-azabenzanthrone III and IV as compared with the corresponding tautomers of 2-hydroxy-1-azabenzanthrone I and II is due to an increase in the energy of the UOMO. As applied to the chemical properties, this means that the lactam tautomers are stronger oxidizing agents than the lactim tautomers, while the 2-hydroxy-1-azabenzanthrones have higher polarizabilities of the π system than the 2-hydroxy-3-azabenzanthrones. A decrease in the energy of the transition from the introduction of an amino group in the 1 or 6 position of anthrapyridone I occurs with a simultaneous increase in the levels of the energies of the LVMO and UOMO due to a large increase in the latter (Table 4). Charge transfer during excitation in the amino derivatives is not realized from the lactam or lactim grouping but rather from the amino group in the ring.

The peculiarities of the fine structure of 2-hydroxyazabenzanthrones revealed on the basis of the calculation are in good agreement with their properties. Structure Ia with a p-quinonemethide grouping that includes the 1 position explains why anthrapyridone undergoes nucleophilic substitution of hydrogen in this position [22], while in benzanthrone such reactions are directed to the 6 and 4 positions [18]. Reactions with attack by the nucleophile at the methylidyne group are typical for p-quinonemethides [23]. It follows from the reactivity indexes calculated by the Hückel MO method that the 1 position is most vulnerable to both nucleophilic and electrophilic attack [19].

The contribution of dipolar structure IIIb is in agreement with the observed [7] pronounced effect of carboxylic acids on the stabilization of the lactam form of 2-hydroxy-1-azabenzanthrones, since the greater separation of charges in the heteroring increases the proton-acceptor character of the oxygen atom and the proton-donor character of the NH bond of the lactam grouping, thereby facilitating solvation due to hydrogen bonds with the formation of cyclic associates [24].

The similarity in the distribution of the bonds in the monoprotonated forms of 2-hydroxyazabenzanthrones and in benzanthrone confirms the conclusion regarding the similarity

TABLE 3. Calculated and Experimental Electronic Spectra of 2-Hydroxyazabenzanthrones

Compound	Calculated spectrum			Exptl. spectrum	
	λ_{max}, nm	oscillator force	wts. of the excited configurations, % (MO No.)	λ_{max}, nm	log ε
I	397,3	0,211	81 (10—11), 6 (9—11)	398*	3,92
	347,1	0,341	69 (9—11), 10 (8—11)	350	4,30
	315,4	0,100	62 (8—11), 10 (7—11)		
	308,3	0,553	69 (7—11), 10 (10—12)	310	4,27
	265,3	0,708	32 (10—13), 23 (10—12)		
	261,0	0,586	17 (10—13), 17 (9—12)	260	4,06
	252,9	0,045	34 (10—13), 21 (9—12)		
	246,9	0,145	31 (10—14), 22 (9—12)		
	239,7	0,104	28 (9—14), 30 (10—14)		
	230,9	0,642	45 (6—11), 11 (9—13)	230	4,76
II	368,6	0,290	68 (10—11), 23 (9—11)	356†	4,19
	339,2	0,399	50 (9—11), 30 (10—11)	315	3,98
	307,4	0,051	62 (8—11), 13 (7—11)		
	305,0	0,031	42 (7—11), 24 (8—11)	270	3,85
	256,5	0,245	57 (10—12), 10 (7—11)		
	248,4	0,080	35 (10—13), 25 (9—12)		
	246,1	0,629	31 (10—14), 19 (10—13)	250	4,32
	240,8	0,095	12 (10—13), 9 (10—14)		
	233,0	0,627	28 (8—12), 20 (9—14)		
III	489,8	0,463	98 (10—11)	515‡	3,86
	320,2	0,022	50 (10—12), 26 (8—11)	455	3,75
	310,0	0,049	28 (10—12), 19 (9—11)	320	3,40
	290,2	0,094	41 (8—11), 22 (10—14)		
	287,0	0,103	38 (7—11), 30 (10—13)	290	3,75
	282,8	0,181	49 (9—11), 18 (8—11)		
	270,7	0,088	24 (7—11), 22 (10—14)		
	244,8	0,878	36 (6—11), 29 (10—14)		
	233,1	0,546	69 (10—15)		
	226,0	0,477	36 (8—12), 25 (9—12)		
IV	405,0	0,444	92,3 (10—11)	450**	3,92
	308,1	0,107	38,4 (9—10), 21 (8—11)	425	3,88
	291,3	0,012	44 (7—11), 15 (8—11)	320	3,53
	287,6	0,010	62 (8—11), 6 (7—11)	295	3,92
	261,9	0,217	37 (10—12), 18 (9—12)		
	252,3	0,282	36 (10—13), 21 (9—12)		
	249,1	0,252	42 (10—14), 25 (6—11)		
	238,3	1,041	37 (6—11), 23 (10—13)		
	223,3	0,541	41 (8—12), 16 (9—13)		

*N-Methylanthrapyridone in ethanol. †2-Methoxy-3-azabenzanthrone in ethanol. ‡2-Hydroxy-1-azabenzanthrone in acetic acid. **2-Hydroxy-1-azabenzanthrone in ethanol.

TABLE 4. Energies of the UOMO and LVMO of 2-Hydroxyazabenzanthrones

Compound	$-E_{UOMO}$, eV	$-E_{LVMO}$, eV
I	3,42	9,28
II	3,20	9,24
III	3,64	8,58
IV	3,04	8,67
1-NH_2-1	3,00	8,30
6-NH_2-1	3,16	8,40

in their electronic structures that was drawn on the basis of a study of the protonation of amino derivatives [6, 7]. The lower level of the energy of the LVMO in the lactim tautomer is reflected in the polarographic reduction potentials of N- and O-methyl derivatives of 2-hydroxy-3-azabenzanthrone [25].

The direction of intramolecular charge transfer in the amino derivatives explains the effect of substituents in the 1 position on the spectra of 6-aminoanthrapyridones that was described in [26, 27]. Electron-donor substituents in the 1 position, by decreasing the

electron-acceptor character of the azabenzanthrone ring, hinder charge transfer from the 6-amino group and give rise to a hypsochromic shift, while electron-acceptor substituents, by increasing the electron-acceptor character of the ring, facilitate charge transfer and give rise to a bathochromic shift.

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