# SPECTRAL CHARACTERISTICS, STRUCTURE, AND
PROPERTIES OF PHENANTHRIDONE DERIVATIVES

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On the basis of IR and electronic spectra and quantum-chemical calculations, a conclusion has been drawn regarding the structure of phenanthridone and its derivatives: It has been confirmed that in the crystalline state and in solutions, phenanthridones exist primarily in the lactam form. An interpretation is given for the long-wave bands in the electronic absorption spectra. Certain spectral criteria are proposed for determining the positions of substituents in the phenyl rings of phenanthridones, and the direction of aromatic substitution of the lactim and cationic forms of phenanthridone have been evaluated. Acid association constants of phenanthridone and its derivatives have been determined.

The chemical and physical properties of phenanthridones (I) should be determined by their lactam—lactim tautomerism. It was shown in [1-5] that in the crystalline state and in solutions in organic solvents, I exists primarily in the lactam form. Depending on the pH of the medium, we can expect a transition to the lactim form and the corresponding ions:

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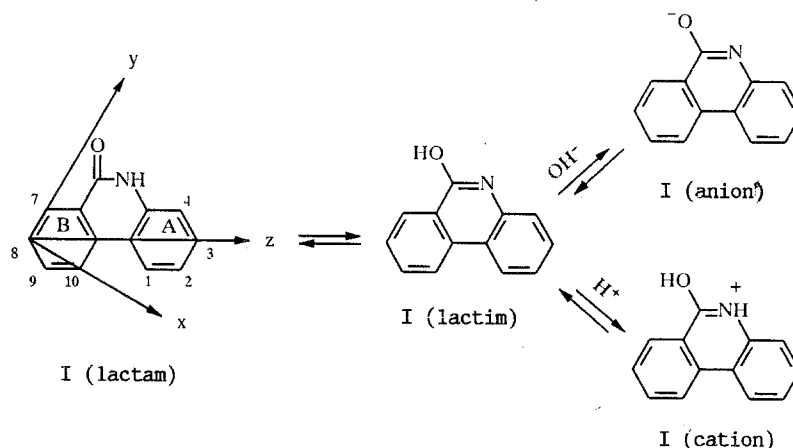
Since studies of the chemical reactions of I are carried out in a number of different media (for example, nitration in strong acids), the possible existence of the above forms must be taken into account. Data for the lactam form I are reported in the literature [1-8]: In [3], the discussion deals with the bands of stretching vibrations of carbonyl groups $\nu_{NC=O}$ in IR absorption spectra; electronic absorption and luminescence spectra are examined in [3, 5]; and the results of quantum-chemical calculations for the lactam form I are presented in [5].

Here we are reporting on a study of the influence of the pH of the medium and the type of substituent on the structure of the phenanthridone. In these studies we utilized information on infrared and electronic absorption spectra and calculations by the Pariser—Parr—Pople (PPP) method.

Stability. In evaluating the relative stabilities of the lactam, lactim, and ionic forms of phenanthridone and its derivatives, we used the results of a quantum-chemical calculation in which different parametrizations were used for the ground state and electronically excited states. It can be seen from Table 1 that the heat of atomization of the lactam tautomer of I is

TABLE 1. Energy Characteristics of Phenanthridone and Its Derivatives

Compound	Energy of π-bonds E_π, eV (and E_π/n, eV)	Energy of σ-bond E_σ, eV	HOMO/LUMO energy ratio E_n/E_m, eV	Heat of atomization ΔH^*, eV	Solvation coefficient M	Dipole moment μ_π, D
I, lactam	23,57 (1,47)	62,33	-9,406/-2,238	125,60	2,434	3,212
I, lactim	22,25 (1,39)	62,34	-8,692/-1,958	124,53	0,928	3,567
I, cation	23,60 (1,48)	62,38	-9,236/-2,174	125,58	1,950	3,481
I, anion	23,30 (1,46)	62,33	-8,498/-1,874	121,14	0,884	3,924
2-NO$_2$-I	27,18 (1,35)	65,71	-9,859/-3,524	128,15	5,918	1,499
4-NO$_2$-I	27,22 (1,35)	65,71	-9,619/-3,681	128,20	5,969	6,082
9-NO$_2$-I	27,12 (1,36)	65,71	-9,569/-3,651	128,10	5,860	4,963
N-Me-2-NO$_2$-I	27,91 (1,40)	65,70	-9,441/-3,524	128,67	6,565	1,775
2,4,7,9-(NO$_2$)$_4$-I	37,33 (1,17)	75,79	-10,519/-4,508	149,59	16,553	1,969
N-Me-I	24,35 (1,35)	62,33	-8,998/-2,123	126,38	2,886	3,481
2-Cl-I	24,52 (1,36)	62,40	-8,839/-2,069	125,19	2,480	5,389
4-Cl-I	24,48 (1,36)	62,40	-9,069/-2,052	125,14	2,467	3,639
9-Cl-I	24,56 (1,36)	62,41	-9,108/-2,006	125,24	2,534	4,330
2-(OMe)-I	24,94 (1,23)	66,37	-8,553/-2,809	131,02	2,620	6,288

TABLE 2. Indexes of Reactivity of Lactim and Cationic Forms of Phenanthridone

Atom No.	I, lactim			I, cation		
	Q_r	q_r^+	q_r^-	Q_r	q_r^+	q_r^-
1	-0,001	0,026	0,105	0,013	0,006	0,258
2	-0,025	0,301	0,087	-0,013	0,303	0,006
3	0,004	0,035	0,022	0,016	0,138	0,216
4	-0,019	0,152	0,137	-0,045	0,034	0,082
7	-0,006	0,085	0,228	0,045	0,049	0,018
8	-0,010	0,062	0,007	0,001	0,176	0,179
9	0,012	0,030	0,472	0,019	0,005	0,186
10	0,000	0,113	0,112	-0,007	0,139	0,014

Note. Q_r is the total π-charge on the atoms; q_r^+ is the electron density on the atoms on the HOMO; q_r^- is the possible electron density in the LUMO.

1.07 eV greater than for the lactim form, indicating higher stability of the lactam form of phenanthridone in the gas phase. The higher value of the solvation coefficient for the lactam form suggests that in the condensed state and in solutions, the lactam form will also be preferred; this conclusion is in complete agreement with experiment. Both the cation and the anion have π-energies close to that of the lactam tautomer, which is to say that they are more stable than the lactim form. From a comparison of the energies of the π bonds per π electron of the system (ratio $E_{\pi/n}$ in Table 1), it can be seen that the introduction of various substituents into the phenanthridone molecule (NO$_2$, Cl, OCH$_3$) lowers the value of $E_{\pi/n}$, i.e., lowers the stability of the molecule as a result of π delocalization.

Reactivity. Electrophilic substitution (nitration) of I proceeds in a strongly acidic medium, in which the protonated form is the most probable. It has been established that the nitro group substitutes first at positions 2 and 4, and then at positions 8 and 10 [9].

For an evaluation of the direction of aromatic substitution, we calculated certain indexes of reactivity of I (Table 2): the electron density on the atoms of the highest occupied molecular orbital (HOMO, Ψ_n) q_r^+; the possible electron density on the lowest unoccupied molecular orbital (LUMO, Ψ_m) q_r^-; and the total π charge on the carbon atoms Q_r. In this case, electrophilic substitution should take place primarily on the atom having the greatest negative charge Q_r or electron density q_r^+. An analysis of these factors showed that satisfactory agreement is observed for the cationic and neutral forms of the lactim tautomer. For the lactim form, on the basis of the index q_r^+, we found the order of substitution $C_{(2)} > C_{(4)} > C_{(10)}$; and on the basis of the index Q_r we found the order $C_{(2)} > C_{(4)} > C_{(8)}$. For the cationic form of the lactim I, on the basis of the index Q_r, we found the order $C_{(4)} > C_{(2)} > C_{(10)} > C_{(8)}$, and on the basis of the index q_r^+ the order $C_{(2)} > C_{(8)} > C_{(10)}$.

TABLE 3. Electronic Absorption Spectra of Phenanthridone and Its Derivatives (experimental data)

| Substituent in molecule of I	Solvent	λ_{max} (log ε)
—	C₂H₅OH	207 (3,89), 224 (4,43), 231 (4,48), 237 (4,46), 250 (4,13), 258 (4,21), 270 (4,01), 296 (3,67), 306 (3,76), 321 (3,94), 338 (3,91)
	C₂H₅OH/NaOH	211 (4,62), 231 (4,52), 238 (4,50), 250 (4,28), 258 (4,30), 270 (4,19), 296 (3,94), 306 (3,99), 321 (4,07), 338 (4,03)
	H₂SO₄	215 (4,23), 241 (3,81), 251 (4,31), 259 (4,17), 306 (3,64), 341 (3,87), 352 (2,92)
7-COOH	C₂H₅OH	207 (4,34), 225 (4,39), 233 (4,43), 238 (4,44), 261 (4,23), 312 (4,05), 327 (3,99), 342 (4,07)
	C₂H₅OH/NaOH	208 (4,59), 233 (4,45), 238 (4,48), 261 (4,22), 302 (3,97), 312 (3,97), 327 (4,07), 342 (4,01)
	H₂SO₄	205 (3,51), 218 (3,64), 244 (4,19), 258 (4,19), 340 (3,67), 352 (3,87)
1-COOH	C₂H₅OH	207 (4,20), 234 (4,45), 262 (4,23), 301 (3,83), 325 (3,96), 338 (3,56)
	C₂H₅OH/NaOH	209 (4,61), 235 (4,47), 244 (4,45), 265 (4,32), 301 (4,04), 325 (4,06), 338 (4,07)
	H₂SO₄	226 (4,42), 252 (4,18), 339 (3,64)
1-COOH-9-NH₂	C₂H₅OH	207 (4,28), 226 (4,40), 243 (4,38), 271 (4,30), 320 (4,14)
	C₂H₅OH/NaOH	210 (4,62), 242 (4,45), 274 (4,37), 312 (4,09)
	H₂SO₄	223 (4,25), 254 (4,14), 338 (3,81), 348 (3,85)
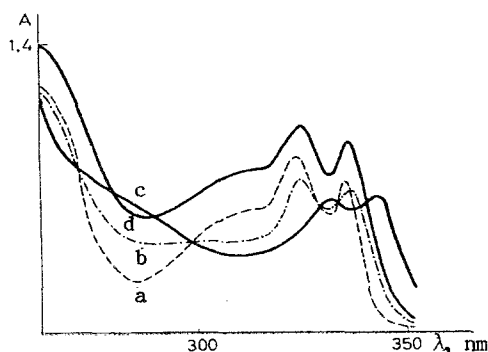
Fig. 1. Electronic absorption spectra of phenanthridone in various media, $C = 5 \cdot 10^{-5}$ M: a) ethanol; b) ethanol—H_2SO_4 (25% solution); c) ethanol—H_2SO_4 (50% solution); d) ethanol—NaOH.

Thus, electrophilic substitution is described satisfactorily by the distribution of π-electron density on the atoms in the HOMO of the neutral and protonated forms of I. Also listed in Table 2 are values of q_r^{+} for nucleophilic substitution of the phenanthridone molecule.

A calculation of values of Q_r and q_r^{+} for the 2-NO₂, 4-NO₂, and 8-NO₂ derivatives of the lactim form of I showed the following: In the 2-nitro derivative, positions 4 and 10 have the largest populations; in the 4-nitro derivative, these are positions 2 and 10; and in the 8-nitro derivative, positions 2 and 4. These data can be used to estimate the preferred direction of subsequent attack of the electrophile.

Electronic Structure and Absorption Spectra. Experimental and calculated electronic spectra and characteristic of the tautomers of I and its derivatives are in satisfactory agreement with each other (Tables 3 and 4 and Fig. 1). For the long-wave band in the spectrum of N-methylphenanthridone, 74% pertains to the transition from the HOMO (Ψ_n) to the LUMO (Ψ_m). The transition is polarized 28.6° relative to the x axis and is accompanied by transfer of π charge from ring A and the nitrogen atom to the C=O group and ring B. In the spectrum that is experimentally observed in ethanol, the long-wave absorption band of phenanthridone is characterized by fine structure with a 1400 cm⁻¹ difference between the vibrational components.

TABLE 4. Electronic Absorption Spectra of Phenanthridone and Its Derivatives (calculated data)

| Compound	λ_{max}, nm	Oscillator strength F	Polarization ϕ, deg	Eigenvectors of ICI
I, lactam	338,3	0,166	28,62	0,86 $(\psi_n \to \psi_m)$
	302,2	0,155	-55,33	0,85 $(\psi_n \to \psi_{m+1})$
	287,4	0,017	-67,90	0,59 $(\psi_n \to \psi_{m+2})$;
				0,49 $(\psi_{n-1} \to \psi_m)$
I, lactim	346,4	0,150	26,70	0,63 $(\psi_n \to \psi_m)$
				0,53 $(\psi_n \to \psi_{m+1})$;
	306,4	0,170	-15,01	0,66 $(\psi_n \to \psi_m)$;
				0,62 $(\psi_n \to \psi_{m+1})$
I, cation	326,5	0,180	18,95	0,81 $(\psi_n \to \psi_m)$
	295,4	0,060	-87,36	0,63 $(\psi_n \to \psi_{m+1})$;
				0,49 $(\psi_{n-2} \to \psi_m)$
I, anion	350,2	0,182	24,92	0,67 $(\psi_n \to \psi_m)$
				0,51 $(\psi_n \to \psi_{m+1})$
	315,2	0,206	-23,04	0,68 $(\psi_n \to \psi_{m+1})$
				0,63 $(\psi_n \to \psi_m)$
2-NO$_2$-I	355,0	0,25	-28,17	0,87 $(\psi_n \to \psi_m)$
	323,3	0,18	-33,94	0,71 $(\psi_{n-1} \to \psi_m)$
				0,50 $(\psi_n \to \psi_{m+1})$
4-NO$_2$-I	407,1	0,23	27,91	0,92 $(\psi_n \to \psi_m)$
	318,9	0,20	-77,08	0,77 $(\psi_{n-1} \to \psi_m)$
				0,36 $(\psi_{n-2} \to \psi_m)$
9-NO$_2$-I	376,2	0,14	-2,77	0,87 $(\psi_n \to \psi_m)$
	311,3	0,06	33,76	0,75 $(\psi_n \to \psi_{m+1})$
				0,37 $(\psi_{n-2} \to \psi_m)$
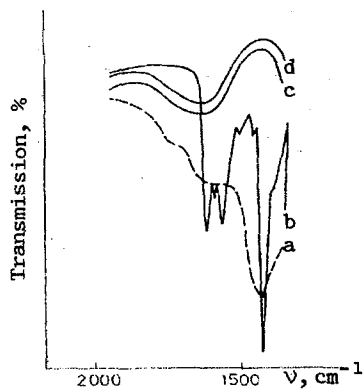
Fig. 2. IR absorption spectra: *a*) Na-phenanthridone; *b*) phenanthridone; *c*) concentrated H$_2$SO$_4$; *d*) phenanthridone in concentrated H$_2$SO$_4$.

The second calculated transition (λ 302 nm) is 72% due to the transition $\Psi_n \to \Psi_{m+1}$. The transition is localized on the benzene rings. In the experimental spectrum, it overlaps a low-intensity transition at 287 nm ($\Psi_n \to \Psi_{m+2}$) and is manifested in the form of an asymmetric shoulder with $\lambda_{max} = 296$ nm on the long-wave side of the absorption band.

The most intense transition in the calculated spectrum of the molecule of I is that with $\lambda = 260$ nm. The direction of electron transfer is almost perpendicular to the long-wave transition; it is 45% due to $\Psi_{n-1} \to \Psi_{m+1}$ and 22% to the $\Psi_n \to \Psi_m$ configurations. Assignments of the other bands in the electronic spectrum of phenanthridone are given in Table 4.

A calculation of electronic spectra of the lactim form of I shows that conversion to the lactim should lead to a bathochromic shift of the long-wave absorption band by about 5 nm. The band polarized 26.7° relative to the x axis is a superposition of a number of bands due to electronic transitions, of which the most important is the $\Psi_n \to \Psi_m$ transition (40%).

In the electronic absorption spectra of solutions of I in the fixed N-methyl form, in an ethanol—H$_2$SO$_4$ mixture, an isobestic point is observed, characterizing the presence of two compounds in the solution — the neutral lactam form and the protonated form (see Fig. 1). Evidence in favor of the protonated form may be found in the disappearance of the band of stretching vibrations of the NC=O group in the IR spectrum of compound I in concentrated H$_2$SO$_4$ (Fig. 2). This behavior is explained by the property of α-pyridone ∪ α-quinolone systems to be protonated at the oxygen atom of the lactam group [13]:

TABLE 5. Absorption Band Maxima (cm⁻¹) in IR Spectra of Phenanthridone and Its Derivatives in the Crystalline State (in KBr tablets)

Compound	$\nu_{NH\ldots O=CN}$	ν_{CH}	$\nu_{NC=O}$	ν_{C-C}	ν_{NO_2}	δ_{CH}
I	3180 3110 2940 2900 2860	3050	1677* 1667 1633	1610 1590	—	799 793s 722m 760vs 733vs
4-NO₂-I	3308 3108 2860	3090m 3075w 3045	1689* 1673	1618vs 1590m 1498vs	1540vs 1350vs 1330m 1295	774s 756s 746s
2-NO₂-I	3175 3130 2980 2970 2905 2880	3095 3050 3031	1693	1614 1497	1533s 1339vs	802 782s 752 742 724
2,4-(NO₂)₂-I	3332vs 3260	3112s 3070 3060sh	1692sh 1683	1618vs 1505vs	1560 1520vs 1332 1305vs	798 792 767 757 742 731
8-NO₂-I	3220 3110 2980 2900 2870	3040	1687* 1666	1620 1578w 1495 1480sh	1533s 1341s	803 757vs 739
2,4,8,10-(NO₂)₄-I	3230		1721* 1697	1622s 1593w 1490s	1550s 1535w 1350s 1335	801vs 774s 744vs 728s
2,4,8-(NO₂)₃-I	3250	3080 3000sh	1696 1690sh	1621 1498 1485sh	1551 1536sh 1345 1330sh	
1-COOH-I	3250 3200 2950	3010	1690**	1620 1520 1490 1460	1390s 1300 1280	990w 940w 800 750
10-COOH-I	3170 2990 2900 2850	3105 3010	1665**	1590 1495 1410	1520sh 1385 1270	1070 950 870 830 800 725
1-COOH-8-NH₂-I	3170 2860	3020	1680** 1600	1620 1600	1520 1500 1350 1260	1070 970 900w 850w 795m 750 710

*In CHCl₃ solution.
**Overlapped by ν_{OC-O} bands.
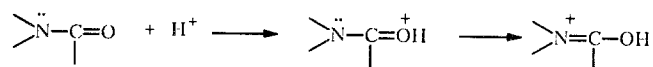
The long-wave absorption band in the electronic spectrum of the cationic form is shifted bathochromically by 10-14 nm (Fig. 1). This means that the molecule of I in an acid medium exists in a form that is protonated at the nitrogen atom.

In the electronic spectra of alkaline ethanol solutions of I, the long-wave band is shifted slightly, but becomes much more intense (Fig. 1), whereas in the fixed lactam form of the phenanthridone (N-methyl), no changes are observed when the change is made to alkaline solutions, since there is no mobile hydrogen atom in the molecule. In the IR spectra of the sodium

salt (Fig. 2), there is no carbonyl-group absorption band; this means that deprotonation of the phenanthridone takes place in caustic solutions.

Using the potentiometric method described by Albert and Serjeant [14], we determined the constants of acidic dissociation of I and its derivatives in 50% ethanol. For I, pKa = 7.16±0.16; for the derivatives, the values (pKa$_1$ and pKa$_2$, respectively) are as follows: for the 1-carboxyphenanthridone, 5.18±0.06 and 7.20±0.12; for the 10-carboxyphenanthridone, 5.25±0.04 and 7.69±0.09; for the 1-carboxy-8-NH$_2$-phenanthridone, 5.44±0.06 and 7.22±0.13.

The introduction of a substituent into the molecule of I (in particular, a nitro group) shifts the 342-nm absorption band toward longer wavelengths, the amount of the shift depending on the position of the substituent; the amount of the shift increases in the series of substitution at the atoms $C_{(2)} > C_{(3)} > C_{(4)}$. Medium-intensity transitions are related to electron transfer from the HOMO to the LOMO.

IR Absorption Spectra. In the IR absorption spectra of I and its derivatives (Table 5), we observe a band in the 1633—1721 cm^{-1} region corresponding to stretching vibrations of the NC=O grouping. In the spectrum of the unsubstituted I we observe two bands at approximately 1667 and 1635 cm^{-1}. These are 15-20 cm^{-1} higher than $\nu_{NC=O}$ in the spectrum of a related compound, 2-quinolone [15]. The splitting of the band may be related to participation of the carbonyl group in hydrogen bonding. In the IR spectrum of I in solution in CHCl$_3$, one band remains with $\nu_{NC=O}$ = 1675 cm^{-1}; this change can be explained by rupture of hydrogen bonds. The introduction of a nitro group into position 4 of I leads to an increase of the $\nu_{NC=O}$ frequency by 6 cm^{-1} (in the crystalline state). At the same time, a nitro group in position 2 increases $\nu_{NC=O}$ by 27 cm^{-1} in comparison with the unsubstituted I (see Table 5). In the IR spectra of nitro derivatives of I in solutions in CHCl$_3$, the value of $\nu_{NC=O}$ is increased by 17—25 cm^{-1}. A similar trend in the influence of halogen atoms and nitro groups on the $\nu_{NC=O}$ absorption band was noted by Pan and Fletcher [2, 16]. The influence of the nitro group on the vibration of bonds of the phenanthridone ring can be explained primarily by two effects: participation in donor—acceptor interactions, and effects of intermolecular hydrogen bonds.

Additional data on the character of the hydrogen bond can be obtained from an analysis of the NH stretching vibrations. It can be seen from Table 5 that in the IR spectra of the compounds that have a substituent in position 4 (NO$_2$, NH$_2$, Br), i.e., in the *peri* position relative to the NH group of the phenanthridone fragment, in the crystalline state we observe one narrow, intense band at 3332-3250 cm^{-1}. It was shown in [6] that the NO$_2$ group forms an intramolecular hydrogen bond with the NH group of the phenanthridone fragment. If there are none of the indicated substituents in the *peri* position relative to the NH group, we observe broad bands in the IR spectrum (half-width about 1000 cm^{-1}) with a set of absorption maxima. The center of gravity of these bands is at 3050-2980 cm^{-1}. The presence of this series of absorption maxima should be explained by Fermi resonance of the ν_{NH} vibration with the skeletal vibrations of the molecule [17].

The appearance of an intense absorption band in the 1702-1690 cm^{-1} region for the carboxy derivatives of I can be attributed to vibrations of the OC=O group. The band is largely overlapped by the $\nu_{NC=O}$ band of the lactam fragment of I. The absorption bands of the OH groups of the carboxyl fragment are superposed on the absorption bands of NH groups.

The bending vibrations δ_{CH} for the molecule of I and its derivatives are manifested in the IR spectra in the 1113-724 cm^{-1} region, with the intensities and positions of these bands depending largely on the position of the substituents in the benzene rings of I. An analysis of the IR absorption spectra provides us with grounds for proposing a spectral criterion in determining the number and position of unsubstituted CH groups and derivatives of I. For example, in the case of an isolated $C_{(1)}$H group, intense bands are manifested in the 774-767 cm^{-1} region, and also a band at 895-890 cm^{-1}, the intensity of which in the various substituted phenanthridones may vary from weak to very strong. The isolated $C_{(7)}$H group gives the following set of bands: 8.95 (m), 8.03, 735-724 (s) cm^{-1}.

When two adjacent CH groups are present in the molecule of I, the IR spectra are characterized by the following set of bands: 1263, 1113 (s), 782 (s) cm^{-1}. Three adjacent CH groups give absorption bands at 1271 (vs), 1061 (vs), and 746 (vs) cm^{-1}. In the case of an unsubstituted phenyl ring of the molecule of I (four adjacent CH groups), we observe bands at 760-752 and 735-733 cm^{-1}. It should be noted that the relationship we have found is not the same as that reported in [18] for derivatives of benzene.

Assignments of the other absorption frequencies in the IR spectra of I and its derivatives are given in Table 5.

EXPERIMENTAL

The phenanthridone and its derivatives were obtained by procedures described in [9, 10]. The purity and individuality of the compounds were monitored by thin-layer chromatography. The IR spectra were recorded in KBr tablets and in CCl$_4$

solutions in a Specord IR-75 spectrometer. Electronic absorption spectra in ethanol (at different levels of pH) and in concentrated H_2SO_4 were recorded in a Specord UV-Vis spectrophotometer. The quantum-chemical calculation of the molecule of phenanthridone and its derivatives were performed by means of the Pariser—Parr—Pople method [11], using a program given in [12].

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