method A to give 0.65 g (44%) of zinc TBP, which contained 0.053 g of pure product according to spectral analysis, total yield 36%.

D. A mixture of 0.25 g (0.42 mmole) of compound III, 0.09 g (0.41 mmole) of zinc acetate dihydrate, and 0.85 g (10.4 mmole) of sodium acetate was heated for 0.5 h in a current of nitrogen at 360°C; and after purification according to method A, 0.10 g of reaction product was obtained, containing 0.09 g (38%) of pure zinc IBP according to spectral analysis.

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MOLECULAR STRUCTURE OF N-MESITYL-6H-ANTHRA[9,1-bc]PYRROL-6-ONE

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The molecular and crystalline structure of 1-(2,4,6-trimethylphenyl)-6H-anthra-[9,1-bc]pyrrol-6-one was determined by the x-ray structural method. There is a larger uniformity of the bonds in the benzene ring of the isoindole fragment than in the N-substituted isoindoles; this derives from the electronic influence of the keto group. The structure of the whole molecule does not have marked 1,10-anthraquinoid character.

Pyrrolanthrone (6H-anthra[9,1-bc]pyrrol-6-ones, I) is a little-studied heterocyclic polycondensed system, the first stable examples of which [1-3] were obtained recently, as were the related systems of thiophenanthrone (II) [3] and furananthrone (III) [4]. Compounds of the type (I)-(III) are the benzoylene derivatives of isoindole, benzo[c]thiophene, and benzo[c]furan, and have the formal structure of 1,10-anthraquinonemethides. For the understanding of their properties [3, 4], it is important to know the extent of the localization of the ortho-quinoid structure in the benzoheterocyclic fragment, and of the 1,10-anthroquinoid structure in the whole molecule. The question is considered in the present paper taking as an example the pyrrolanthrone system (I) and its comparison with the isoindole system.

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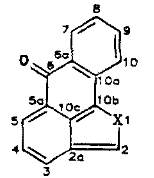
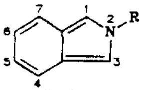
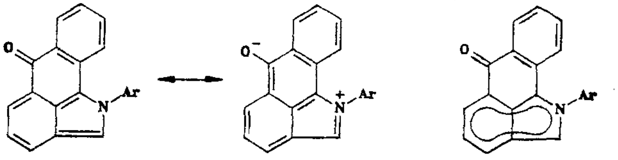
The electronic structure of isoindole has been the subject of lively discussion for many years (cf. [6, 7]). Conforming conclusions on the fact that isoindole is a single aromatic 10π-electron system with the appreciable localization of the bonds in the carbocyclic portion, similar to the localization in naphthalene, were recently reached on the basis of x-ray structural data for N-methylisoindole (IV) [8] and N-benzylisoindole (V) [9]. We carried out an x-ray structural investigation of the pyrrolanthrone derivative (VI) (Table 1 and Fig. 1) to evaluate the effect of the ring-fusion of the benzoylene residue in the transition from isoindole to pyrrolanthrone; (VI) contains the 2,4,6-trimethylphenyl (mesityl) grouping, the presence of which guarantees the stability of the compound, at the nitrogen atom [2, 3].



I-III



IV, V



VIa VIc VIb

I X=NR, II X=S, III X=O; IV R=Me, V R=CH_2Ph; VI Ar=2,4,6-$Me_3C_6H_2$

The polycondensed system is not completely plane. It consists of two planar fragments — the isoindole and the benzoylene — having the bend of the 2.8° angle along the $C_{(6)}\ldots C_{(10B)}$ line. The carbonyl oxygen atom deviates from the planes of these fragments by 0.043 and 0.064 Å (Table 1).

The examination of the bond lengths in the isoindole fragment of the pyrrolanthrone (VI) (Fig. 1) indicates that the alternation of the bonds, which is characteristic of the N-methyl- and N-benzylisoindoles (IV, V), is absent from the six-membered carbocycle. If the $C_{(4)}-C_{(5)}$ and $C_{(6)}-C_{(7)}$ bonds in N-methylisoindole are close to double bonds having the mean length 1.355(5) Å, and $C_{(5)}-C_{(6)}$ bond is lengthened to 1.424(8) Å [8], then the lengths of the corresponding bonds in the isoindole fragment of the pyrrolanthrone (VI) comprise 1.380(9), 1.405(8), and 1.382(9) Å; thus they are almost the same within the limits of experimental error. The bonds in the heterocycle of the pyrrolanthrone (VI) are close in length to the

TABLE 1. Coefficients of the Equations $A_x + B_y + C_z = D$ of the Plane Fragments and the Deviations Δ of the Atoms from the Planes

Plane	A	B	C	D	Δ, Å
P_1	0,377	0,852	−0,362	4,580	O −0,006; $N_{(1)}$ −0,028; $C_{(2)}$ −0,001; $C_{(2a)}$ 0,007; $C_{(3)}$ 0,060; $C_{(4)}$ 0,053; $C_{(5)}$ 0,004; $C_{(5a)}$ −0,045; $C_{(6)}$ −0,046; $C_{(6a)}$ −0,011; $C_{(7)}$ 0,012; $C_{(8)}$ 0,028; $C_{(9)}$ −0,041; $C_{(10)}$ 0,025; $C_{(10a)}$ −0,017; $C_{(10B)}$ − 0,035; $C_{(10c)}$ −0,032
P_2	0,755	−0,354	−0,552	3,343	$C_{(1')}$ 0,010; $C_{(2')}$ −0,012; $C_{(3')}$ 0,002; $C_{(4')}$ 0,010; $C_{(5')}$ −0,012; $C_{(6')}$ 0,002; $N^*_{(1)}$ −0,012; $C^*_{(2'')}$ −0,032; $C^*_{(4'')}$ 0,071; $C^*_{(6'')}$ −0,033
P_3	0,388	0,838	−0,383	4,597	$C_{(2a)}$ −0,009; $C_{(3)}$ 0,012; $C_{(4)}$ 0,009; $C_{(5)}$ −0,005; $C_{(5a)}$ −0,021; $C_{(6)}$ 0,015; $C_{(10B)}$ 0,012; $C_{(10c)}$ −0,013; O* 0,064; $N^*_{(1)}$ 0,002; $C^*_{(2)}$ −0,019
P_4	0,376	0,861	−0,343	4,523	$C_{(6)}$ −0,001; $C_{(6a)}$ 0,004; $C_{(7)}$ 0,005; $C_{(8)}$ − 0,007; $C_{(9)}$ 0,000; $C_{(10)}$ 0,007; $C_{(10a)}$ −0,007; $C_{(10B)}$ −0,001; O* 0,043; $N^*_{(1)}$ 0,010

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*Atoms not included in the calculation of the equation of the plane.

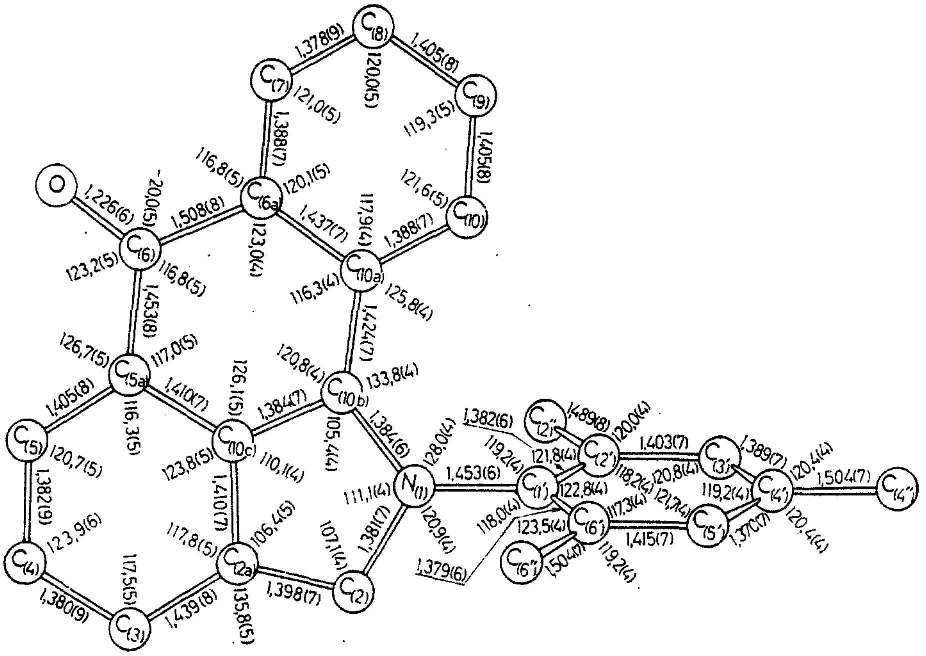

Fig. 1. The structure of the molecule of the pyrrolanthrone (VI).

bonds in pyrrole [10], and differ from the bonds in the isoindoles (IV, V) by the increase of the C—N interatomic distances.

Therefore, the six-membered ring in the isoindole fragment of pyrrolanthrone possesses greater uniformity of the bonds, and more aromaticity in the framework of structural criteria, than those in the molecules of the isoindoles (IV) and (V). In view of the absence of bond localization, the electronic structure of pyrrolanthrone is not adequately described by the formula of the 1,10-anthroquinonemethide (VIa). It may be more reliably given by the formula (VIb) with the symbolic expression of the generalized skeleton and the decet of π-electrons in the aromatic fragments.

However, the formula (VIb) does not contain any indication of the reasons for the bond leveling. In our opinion, at least one of them comprises the electron-acceptor influence of the carbonyl group. In the molecule of the pyrrolanthrone (VI), the C=O group, for which the bond length is 1.226(6) Å and is typical of ketones, is bound in a non-equivalent manner to the aromatic fragments. The $C_{(6)}-C_{(6a)}$ bond with the benzene ring is ordinary with the length of 1.508(8) Å, whereas the $C_{(5a)}-C_{(6)}$ bond with the isoindole fragment is shortened and had the length of 1.453(8) Å. This evidently expresses the more effective electronic interaction of the CO acceptor group with the fragment containing the heterocycle with the π-excess. The polarization of pyrrolanthrones in the basic state with an increase in the electron density on the keto group was previously determined from the decrease of the frequency ν_{CO} of the bond vibrations in the IR spectra [5].

The shift of the π-electron density from the heterocycle to the carbonyl group is equivalent to the contribution of the bipolar structure (VIc). The distribution of the bonds in the eight-membered chain of conjugation between the oxygen atom and the pyrrole nitrogen atom in the structures (VIa) and (VIc) are contrasting. the bonds represented as single in the formula (VIa) are double in the formula (VIc), and vice versa. The comparable contribution of these structures as the limiting ones is equivalent to the leveling of the bonds. Their combination expresses the features of the electronic structure of pyrrolanthrone.

The leveling effect of the bonds, which is determined by the polarization due to the influence of the keto group, should also appear in the heteroanalogs of pyrrolanthrone — thiophenanthrone (II) and furananthrone (III). The degree of the leveling, which depends on the π-donating characteristic of the heteroatom and the localization of the bonds in the corresponding benzo[c] heterocycle, should be the least in the furananthrone (III). This conforms with the ability of derivatives of the latter to enter into the addition reaction [4] and with the data of the chemical experiment not finding the manifestation of unsaturation in the systems of (I) and (II) [3].

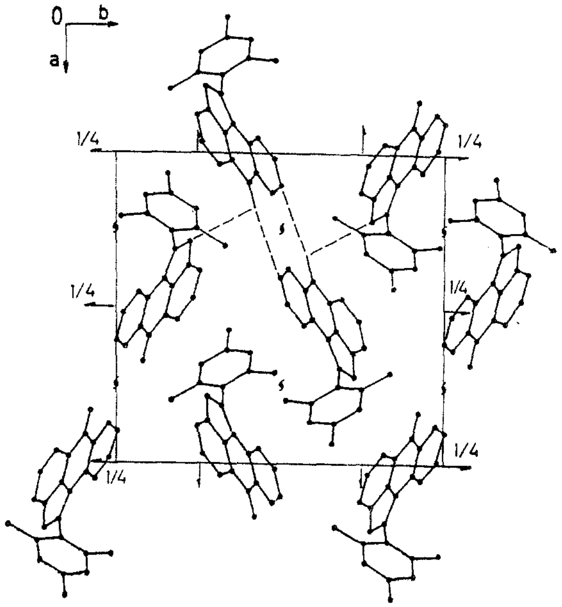

Fig. 2. The xy projection of the crystalline structure of the pyrrolanthrone (VI).

The steric stresses arising from the "tightening" of the 1 and 7 positions of isoindole by the six-membered carbocycle or the equivalent effect of the peri positions of the anthrone with the five-membered heterocycle, which are compensated by the deformation of the bond angles (Fig. 1), are a featured of the pyrrolanthrone system which is also determined by the ring-fusion. In the heterocycle of the isoindole fragment of the pyrrolanthrone (VI), the angle at the $C_{(10c)}$ atom is increased by 3°, and the angles at the $C_{(2a)}$ and $C_{(10B)}$ atoms is increased by 3°, and the angles at the $C_{(2a)}$ and $C_{(10B)}$ atoms are decreased by comparison with the isoindoles (IV) and (V). In the carbocycle of this fragment, the angles at the $C_{(4)}$ and $C_{(10c)}$ atoms increase by 2.5-4°, and the angles at the $C_{(2a)}$, $C_{(3)}$, and $C_{(5a)}$ atoms decrease by 1.5-2°. In the six-membered ring adjoining the isoindole fragment, the angles at the $C_{(6a)}$ and $C_{(10c)}$ atoms are increased to 123-126° and the angles at the $C_{(5a)}$ and $C_{(6)}$, and $C_{(10a)}$ atoms are decreased to 116-117°. In the anthrone nucleus, the mutually opposite "external" angles at the $C_{(6a)}$ and $C_{(10a)}$ atoms differ by 9°; those at the $C_{(5a)}$ and $C_{(10a)}$ atoms differ by 17°. The general picture of the deformation of the angles in the benzisoindole fragment is similar to that in the studied systems of acenaphthene [11] and benz [cd] indole [12, 13].

The other source of the steric stresses in the molecule of (VI) is the 2,4,6-trimethylphenyl (mesityl) substituent at the nitrogen atom; all the three bonds in it are situated in one plane (the sum of the bond angles is 360.0°). The plane of the mesityl residue is turned by 79.5° relative to the central plane of the pyrrolanthrone due to the steric repulsion between the atoms of the latter and the ortho-methyl groups. This turning completely excludes the conjugation between the π-systems of the polycyclic nucleus and the substituent. The $C_{(1')}-N$ bond corresponds in its length of 1.453(8) Å to the normal single $C_{(sp_2)}-N$ bond (1.452 Å [14]), and shows a 7° deviation toward the $C_{(2)}$ atom. The polarization of the pyrrolanthrone system increases the deficit of the electron density on the pyrrole nitrogen atom and strengthens its influence as a σ-acceptor; this appears as the increase of the endocyclic angle at the $C_{(1')}$ atom of the mesityl residue to 122.8(4)°. The electron-donating effect of the methyl groups causes a decrease in the corresponding angles of the benzene ring to 119.2-117.3(4)°.

The rotation of the plane of the mesityl grouping around the C-N bond does not completely remove the steric stresses. The observed contacts between the atoms of the ortho-disposed methyl groups and the nearest atoms of the nucleus comprise: $C_{(2'')} \ldots N$ 2.890(7) Å $C_{(6'')} \ldots N$ 2.876 Å, $C_{(2'')} \ldots C_{(10b)}$ 3.300(8) Å, $H_{(2'')} \ldots N$ 2.37 Å, and $H_{(6'')} \ldots C_{(2)}$ 2.52 Å. This is significantly less than the sum of the van der Waals radii of the C and N atoms (3.25 Å), the H and N atoms (2.75 Å), and the H and C atoms (2.90 Å), and the doubled van der Waals radius of the C atom (3.40 Å) [15].

The turned bulky mesityl grouping impedes the packing with the parallel disposition of the planes of neighboring molecules. Analysis of the crystal structure of the pyrrolanthrone (VI) shows the disposition of the molecules with the spacings exceeding the sums of the van

TABLE 2. Coordinates of the Atoms ($\times 10^4$; $\times 10^3$ for the H atoms) and Equivalent Isotropic Temperature Parameters (Å^2) V_{eq}^{iso} of the Non-hydrogen Atoms.

Atom	x	y	z	V_{eq}^{iso}	Atom	x	y	z
O	6708(3)	792(3)	−143(6)	8,4(2)	$H_{(2)}$	208	258	−77
$N_{(1)}$	3130(3)	1790(3)	−2027(4)	4,1(1)	$H_{(3)}$	313	296	208
$C_{(2)}$	2841(4)	2249(4)	−734(6)	4,9(2)	$H_{(4)}$	458	271	375
$C_{(2a)}$	3600(4)	2208(4)	308(6)	4,9(2)	$H_{(5)}$	606	165	230
$C_{(3)}$	3781(4)	2553(4)	1815(6)	6,1(2)	$H_{(7)}$	708	0	−292
$C_{(4)}$	4654(5)	2350(4)	2476(7)	7,1(2)	$H_{(8)}$	652	−28	−536
$C_{(5)}$	5358(4)	1842(4)	1774(7)	5,7(2)	$H_{(9)}$	510	7	−646
$C_{(5a)}$	5215(4)	1494(4)	300(6)	4,9(2)	$H_{(10)}$	377	82	−472
$C_{(6)}$	5901(4)	981(4)	−598(8)	5,4(2)	$H_{(3')}$	82	45	−494
$C_{(6a)}$	5602(3)	732(3)	−2197(6)	4,3(1)	$H_{(5')}$	188	313	−625
$C_{(7)}$	6264(3)	257(3)	−3067(8)	5,2(2)	$H_{(2''A)}$	162	−32	−276
$C_{(8)}$	6051(4)	−9(4)	−4535(8)	6,0(2)	$H_{(2''B)}$	268	−28	−261
$C_{(9)}$	5157(4)	210(4)	5181(7)	5,6(2)	$H_{(2''C)}$	224	21	−165
$C_{(10)}$	4486(4)	695(3)	−4312(6)	4,6(2)	$H_{(4''A)}$	29	213	−738
$C_{(10a)}$	4678(3)	956(3)	−2823(6)	3,8(1)	$H_{(4''B)}$	42	104	−750
$C_{(10B)}$	4047(3)	1447(3)	−1852(6)	3,6(1)	$H_{(4''C)}$	101	151	−817
$C_{(10C)}$	4329(3)	1697(3)	−397(6)	4,0(1)	$H_{(6''A)}$	298	379	−471
$C^{(1')}$	2510(3)	1730(3)	−3357(5)	3,6(1)	$H_{(6''B)}$	369	318	−407
$C^{(2')}$	1988(3)	952(3)	−3601(6)	3,7(1)	$H_{(6''C)}$	323	329	−291
$C^{(3')}$	1389(3)	912(3)	−4887(5)	3,8(1)				
$C^{(4')}$	1310(3)	1643(3)	−5870(5)	3,7(1)				
$C^{(5')}$	1816(3)	2414(3)	−5561(6)	3,9(1)				
$C^{(6')}$	2443(3)	2475(3)	−4294(5)	3,6(1)				
$C_{(2'')}$	2056(4)	164(4)	−2554(7)	6,1(2)				
$C_{(4'')}$	692(4)	1583(4)	−7274(6)	5,1(2)				
$C_{(6'')}$	2974(4)	3341(4)	−4009(7)	6,1(2)				

der Waals radii. The shortest contacts of the oxygen atom: O...C'$_{(2)}$ 3.395(7) Å and O...C$_{(8)}$ 3.374(6) Å (Fig. 2).

The data on the conformation and packing of the molecules of the pyrrolanthrone (VI) confirm the expressed concepts on the nature of the stabilizing influence of the bulky substituent at the nitrogen atom [3]. It consists of the prevention of the drawing together of the molecules with the parallel disposition of the aromatic systems with the spacings required for intermolecular charge transfer, and with the steric shielding of the most active position 2.

EXPERIMENTAL

1-(2,4,6-Trimethylphenyl)-6H-anthra[9,1-bc]pyrrol-6-one (VI). This compound was synthesized according to [3]; the monocrystal was obtained from the mixture of benzene-hexane. The crystals of (VI) are rhombic; $a = 13.9334(6)$, $b = 14.8334(8)$, and $c = 8.7612(8)$ Å; $V = 1811(1)$ Å^3; $d_{calc} = 1.238$ g/cm^3; $Z = 4$; the space group is $P2_12_12_1$.

The unit cell parameters and the intensities of the 1312 reflections were measured at 20°C on a Hilger-Watts automatic diffractometer (λCuK_α, graphite monochromator, $\theta/2\theta$-scanning, $\theta \leq 57°$). The structure was deciphered by the direct method with the MULTAN program. It was specified by the method of least squares in the block-diagonal approximation initially isotropically to R = 0.122, and then anisotropically to R = 0.073. The hydrogen atoms were shown at this stage by the building up of the difference series; they were included in the specification with fixed and temperature ($V_{eq}^{iso} = 4$ Å^2) parameters. The final value of the divergence factor at the 1241 reflection with $F^2 \geqslant 2\sigma$ comprised R = 0.056 ($R_\omega = 0.059$). All calculations were performed on the Eclipse S/200 computer with the INEXTL programs [16]. The coordinates of all atoms and the isotropic equivalent temperature parameters of the non-hydrogen atoms are presented in Table 2; the bond lengths and angles are presented in Fig. 1.

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SYNTHESIS OF 5-HYDROXY-4-NITROSOBENZOTRIAZOLES AND 6-HYDROXY-7-NITROSOINDAZOLES AND THEIR SPLITTING INTO β-TRIAZOLYL- AND β-PYRAZOLYLACRYLIC ACIDS

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5-Hydroxy-4-nitrosobenzotriazoles and 6-hydroxy-7-nitrosoindazoles were synthesized. By the action of benzenesulfonyl chloride in an alkaline medium, only 5-hydroxy-4-nitroso-2-phenyl-benzotriazole and 1-methyl-6-hydroxy-7-nitrosoindazole split into 5-carboxyvinyl-2-phenyl-4-cyano-1,2,3-triazole- and β-(1-methyl-5-cyano-4-pyrazolyl)acrylic acid, respectively, while the fragmentation under electron impact proceeds by another scheme.

We have already shown that o-nitrosohydroxyarenes, which exist preferentially in the tautomeric form of o-quinone monooximes [1, 2], open the quinoid ring to form o-cyanocinnamic acids through the action of benzenesulfonyl chloride in an alkaline medium and on heating [3, 4]. The splitting of monooximes of isatins [5] proceeds in a similar way, and it was shown that the molecular ions of the latter also undergo a similar rearrangement in the mass spectrometer [6]. Therefore, in the present work, we studied the behavior of 1- and 2-methyl-6-hydroxy-7-nitrosoindazoles (I, II), 5-hydroxy-4-nitrosobenzotriazole (XIII) and 5-hydroxy-4-nitroso-2-phenyl-benzotriazole (XVII) both through the action of benzenesulfonyl chloride [7], and under electron impact.

Compounds I and II were synthesized by Scheme 1 from 6-nitroindazole (III), obtained by the method in [8].

In the mass spectrum of compound VIII an intense peak of molecular ion and the peak of the $[M-H]^+$ ion are observed, characteristic of 1-methylindazole [9]. In contrast, the molecular ion of hydroxyisoindazole IX is unstable and its primary decomposition involves a loss of a molecule of hydrocyanic acid (ion* 121), which then vigorously eliminates a molecule of CO (ion 93) or a methyl group (ion 106). This indicates a markedly lower aromatic-

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*Here and below, the m/z values are given for the ion peaks.

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