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A SCF MO Treatment of Some Tropone Derivatives*

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Recent work in these laboratories has led to the development of a semiempirical SCF MO treatment which seems to give extremely good results for ground states of conjugated molecules of all kinds composed of carbon, hydrogen, nitrogen and oxygen. We have now applied this treatment to a problem of current interest, namely the structures of tropolone and tropone derivatives. The calculations lead to the conclusion that neither of these ring systems is in itself aromatic, while tropone is now recognized to be polyenoid, tropolone still seems to be generally regarded as aromatic. This belief, however, arose from the behavior of tropolone derivatives in strong acid solution, where they exist as hydroxy tropylium derivatives, or in alkali where they form mesomeric anions. Calculated heats of formation, resonance energies, and bond lengths are reported.

INTRODUCTION

Some time ago one of us[1] concluded on the basis of available chemical evidence that stipitatic acid and colchicine must contain a novel aromatic system, tropolone (I), containing a seven-membered ring. Subsequent work not only confirmed this conclusion but also led to the synthesis of tropolone[2] itself, and of the related tropone[3] (II); both these compounds seemed to show stability characteristics of typical aromatic systems, and it was quickly realized that this might be due to the fact that both I and II can be regarded as derivatives of the tropylium ion, $C_7H_7^+$, which Hückel[4] in 1931 had predicted to be aromatic, a prediction which has been fully confirmed.[5] However although an enormous amount of experimental work has been carried out since then on the synthesis and properties of numerous tropone and tropolone derivatives, very few theoretical studies seem as yet to have been reported. The only published investigations of ground state properties have been based on the HMO method,[6,7] and a little work has also been reported on excited states.[8]

While the HMO method is known to be quite unreliable for compounds containing heteroatoms, more satisfactory procedures, based on the Pople SCF MO treatment, have been described in recent years. The best of them, in so far as ground states are concerned, is a semiempirical SCF MO treatment that has been developed in these laboratories[9–12]. In its current form, this

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enables the heats of formation of a very wide variety of conjugated molecules, both aromatic and non-aromatic, and containing nitrogen and/or oxygen as well as carbon and hydrogen, to be calculated within the limits of experimental errors in the available thermochemical data. We therefore thought it would be of interest to apply this technique to a variety of tropone and tropolone derivatives; the present paper describes the results of these calculations.

THEORETICAL APPROACH AND CHOICE OF PARAMETERS

Using the Hückel σ, π approximation, the heat of atomisation (ΔH_a) of a conjugated system can be written in the form:

$$-\Delta H_a = \Sigma E^r_{\sigma b} + E_{\pi b} + \Sigma E_{X-H} \tag{1}$$

where $E^r_{\sigma b}$ is the bond energy of a particular X—Y σ bond of length r, $E_{\pi b}$ is the total π binding energy, calculated by a suitable MO procedure, and E_{X-H} is the bond energy of X—H bond (X being C, N or O). In the present work, $E_{\pi b}$ was calculated by a SCF MO procedure based on the Pople treatment[13], in which the F-matrix is given by:

$$F_{ii} = W_i + {}^1/_2\, q_i\, (ii, ii) + \Sigma_{j(\neq i)}\ (q_j - c_j)\, (ii, jj) \tag{2}$$

$$F_{ij} = \beta^c_{ij} - {}^1/_2\, p_{ij}\, (ii, jj) \tag{3}$$

Here W_i is the valence state ionisation potential of the p AO of atom i and (ii, ii) the corresponding one-center repulsion integral; (ii, jj) is the usual repulsion integral between AOs of atoms i and j and β^c_{ij} the corresponding core resonance integral; and q_i and p_{ij} are respectively the π electron density of atom i and the bond order between atoms i and j.

The quantities W_i and (ii, ii) were found by the method of Pariser and Parr[14], using the valence state ionization potentials of Hinze and Jaffé[15]. Table I shows values for carbon, pyrrole- and pyridine-type nitrogen and ketone- and ether-type oxygen.

TABLE I

One-center Integrals

Atom or Ion	Valence State	W_i (eV)	(ii, ii) (eV)
C	$tr^1tr^1tr^1\pi$	— 11.16	11.13
N^+	$tr^1tr^1tr^1\pi$ (> N —)	— 28.59	16.63
O	$tr^2tr^2tr^1\pi$ (> C = O)	— 17.70	15.23
O^+	$tr^2tr^1tr^1\pi$ (> O)	— 33.90	18.60

The two-center repulsion integrals were found as before[9–12] from the following expression (cf. Ohno[16]):

$$(ii, jj) = e^2\, [r_{ij}^2 + (R_i + R_j)^2]^{-1/2} \tag{4}$$

where:

$$2R_i = e^2 / (ii, ii);\ 2R_j = e^2 / (jj, jj) \tag{5}$$

The core resonance integral β^c_{ij} was evaluted from the thermocycle procedure of Dewar and Schmeising[17,18], as indicated in Eq. (6):

$$\begin{array}{ccccccc} & R' & C' & R & E_{\pi b} & R & -C'' \quad R'' \\ X{-}Y & \longrightarrow & X{-}Y & \longrightarrow & X{=}Y & \longrightarrow & X{=}Y \\ \downarrow & & & & & & \uparrow \\ \multicolumn{7}{c}{(D'{-}D'')} \end{array} \qquad (6)$$

Here R′ and R″ are the equilibrium bond lengths, and D′ and D″ the bond energy, of *pure* XY single and double bonds respectively, while C′ and C″ are compression energies evaluated from Morse potential functions. The π binding energy ($E_{\pi b}$) is equal to minus the π bond energy of the X=Y bond stretched to length R and in our case is given by the following expression:

$$E_{\pi b} = q_x/W_x + {}^1/_4 q_x\,(xx, xx)/ + q_y/W_y + {}^1/_4 q_y\,(yy, yy)/ + 2p_{xy}\beta^c_{xy} + \\ + (q_x - c_x)(q_y - c_y)(xx, yy) - {}^1/_2 p^2_{xy}\,(xx, yy) - W_x - W_y \qquad (7)$$

From Eqs. (6) and (7):

$$\beta^c_{xy} = \frac{1}{2p_{xy}} / (1 - q_x)W_x + (1 - q_y)W_y - {}^1/_4 q^2_x\,(xx, xx) - {}^1/_4 q^2_x\,(yy, yy) - \\ - (q_x - c_x)(q_y - c_y)(xx, yy) + {}^1/_2 p^2_{xy}\,(xx, yy) + D' - D'' - C' + C''/ \qquad (8)$$

In our procedure (variable β-procedure[10]) β^c_{ij} and (ii, jj) are recalculated for each bond at each stage in the iterative treatment of the molecule we are considering. In order to estimate β^c_{ij} we need to know six quantities: R′, R″, D′, D″, a′ and a″; a′ and a″ being the Morse constants for a CC *sigma* bond and for a CC double bond, respectively. These quantities can be estimated quite easily in the case of hydrocarbons[9–11], but difficulties arise[12] in the case of bonds involving nitrogen or oxygen. Apart from the dearth of experimental data, double bonds involving pyrrole-type nitrogen or ether-type oxygen involve charged species (*e. g.* $R_2N^+ = CR_2$, $RO^+ = CR_2$); not only it is impossible to estimate the heat of atomisation of such ions in the gas phase, with sufficient accuracy, but it is also questionable if parameters determined in this way can legitimately be used to describe neutral molecules such as pyrrole or furan. The parameters for bonds of this type were therefore determined from semiempirical relations between bond length and other bond properties; *viz.*:

(a) A linear relation was assumed (*cf.* 9—12) between bond order and bond length:

$$r_{ij} = F - Gp_{ij} \qquad (9)$$

(b) A tratrix relation[18] was assumed between bond energy and bond length:

$$Br = A\ln[A + (A^2 - D^2)^{1/2}] - A\ln D - (A^2 - D^2)^{1/2} \qquad (10)$$

(c) An inverse power series relation[18] was assumed between force constant (k) and bond length:

$$k = Cr^{-2} + Dr^{-4} + Er^{-6} \qquad (11)$$

Values for the parameters A—E were found by fitting suitable experimental data and used to estimate the quantities D, R, and a; the results are listed in Table II.

TABLE II

Thermocycle Data

Bond	D″ (eV)	D′ (eV)	R″ (Å)	R′ (Å)	a″ (Å^{-1})	a′ (Å^{-1})	F (Å)	G (Å)
CC	5.5600	3.9409	1.338	1.512	2.3177	2.0022	1.512	0.174
CN	5.1766	3.3463	1.270	1.448	2.5161	1.9209	1.448	0.178
CO	7.1011	3.9987	1.230	1.395	2.1787	1.7870	1.395	0.165

As before[12], we found it necessary to allow for the effects of polarity of the σ bonds linking dissimilar atoms (*i. e.* C and N, or C and O). We assumed that resulting charges (q_i) on the atoms forming a heteroatomic bond to be proportional to the difference in electronegativity between the atoms concerned, and the corresponding changes in the valence state ionization potentials were then calculated from the parabolic relation:

$$W_i = a + bq_i + cq_i^2 \tag{12}$$

Here a, b, and c are parameters found by fitting the valence state ionization potentials of a neutral atom and two ions derived from it. Table III shows values of W_i and (ii, ii) for various atoms and bonds, after correction for σ polarization.

TABLE III

One-center Integrals After σ Polarization Corrections

Type of Bond	Atom	Core Charge	W_i (eV)	(ii, ii) (eV)
C—N̈	C	1.035	— 11.5516	11.3236
	N	1.926	— 27.4161	16.2842
C=O	C	1.100	— 12.2872	11.6786
	O	0.900	— 16.0190	14.4871
C—Ö	C	1.093	— 12.2075	11.6406
	O	1.814	— 30.5989	17.6709

The σ bond energies (E_σ^r) are found automatically in the calculation of β_{ij}^c by the thermocycle, being given by:

$$E_\sigma^r = D' - C' \tag{13}$$

where C′ is found from the Morse function:

$$C' = D' \{1 - \exp [a' (R' - R)^2]\} \tag{14}$$

The X—H bond energies were also estimated during the parametrization procedure; they are listed in Table IV.

TABLE IV

X—H Bond Energies

Bond	Bond Energy (eV)
C—H	4.4375
N—H	4.0418
O—H	4.7700

RESONANCE ENERGY

We have defined[9–11] the resonance energy (E_R) of conjugated hydrocarbons as the difference in heat of atomisation between it and corresponding classical polyene, the latter value being found by summing appropriate bond energies. This definition is superior to others that have been proposed, for two reasons.

First, the quantity in which chemists are primarily interested concerning a conjugated molecule is not its stability relative to some idealized structure with *pure* single and double bonds, but rather its stability relative to an open chain analog. Since the latter is a classical polyene, the quantity in question is precisely the one we have defined as resonance energy.

Secondly, our definition is independent of theory; for the polyene bond energies could (and should) be estimated from thermochemical data. In our work[11] we have estimated their bond energies from calculated heats of atomisation of classical polyenes only because the necessary thermochemical data are still lacking; while it is to be hoped that such data will become available in the near future, the available evidence support that the values based on theory are not far from the truth[19].

This definition of resonance energy can be carried over to compounds containing heteroatoms only if a similar additivity can be established for bond energies in corresponding classical compounds. Here the situation regarding thermochemical data is even more disastrous than in the case of hydrocarbons, but recent theoretical studies[20,21] in this laboratory seem to suggest that the necessary additivity does indeed hold with sufficient accuracy. The heat of atomisation of classical conjugated compounds containing nitrogen or oxygen and calculated by our SCF MO method are well represented by sums of appropriate bond energies. The values used in the present work are listed in Table V.

TABLE V

Bond Energies

Bond	Bond Energy (eV)
C—C	4.3499
C=C	5.5378
C—Ö	4.1594
C=O	7.1575
C—N̈	3.5903
C=N	5.1654

RESULTS AND DISCUSSION

The compounds studied here are shown in Fig. 1 and their calculated total σ and π binding energies, heats of atomisation, and resonance energies are listed in Table VI. Since most of the compounds are either still unknown, or have only recently been prepared, hardly any thermochemical data are available. Indeed, the only experimental heat of atomisation so far reported is for tropolone[22]; it differs from our calculated value by only 0.056 eV or 1.3 kcal/mole.

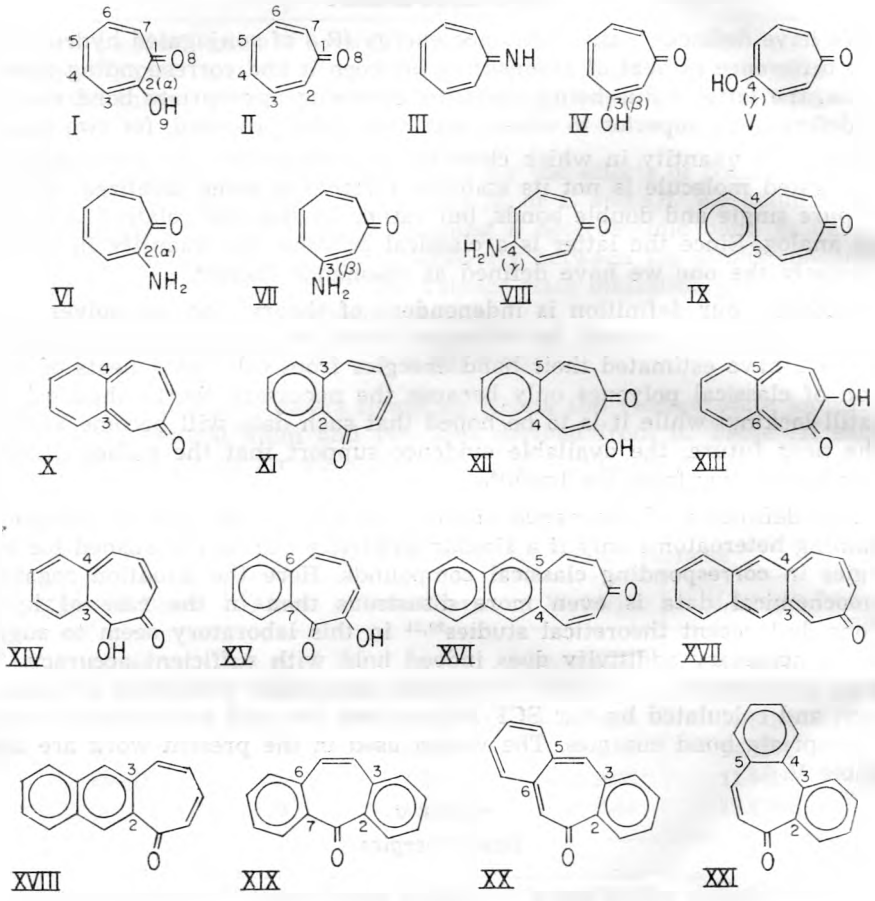

Fig. 1. Atomic skeletal structure for investigated molecules.

The resonance energies in the last column of Table VI are interesting and surprising, implying that tropone, tropolone, and the corresponding nitrogen derivatives, are non-aromatic. The only compounds with large resonance energies are those containing benzene or naphthalene rings and their resonance energies are almost identical with those estimated[11] for the benzenoid compounds. This conclusion is of course diametrically opposed to the current

TABLE VI

Calculated Total Energies, Heats of Atomisation and Resonance Energies

Compound	-(Total Energy) (eV)		-(Heat of Atomisation) (eV)	Resonance Energy (kcal/mole)
	$-E_{\pi b}$	$-E_{\sigma b}$		
α-Tropolone (I)	11.8420	33.3665	72.266[a]	— 0.5
Tropone (II)	11.7355	23.4678	67.828[b]	0.8
Azatropone (III)	10.5739	28.7376	69.968	2.8
β-Tropolone (IV)	11.9189	33.4748	72.351	1.5
γ-Tropolone (V)	11.9162	33.4765	72.350	1.5
α-Aminotropone (VI)	11.9481	32.8390	75.058	0.6
β-Aminotropone (VII)	11.9679	32.8258	75.065	0.8
γ-Aminotropone VIII)	11.9497	32.8288	75.050	0.4
4,5-Benzotropone (IX)	17.9436	48.1617	101.605[b]	18.7
3,4-Benzotropone (X)	17.3294	48.1142	100.944	3.4
2,3-Benzotropone (XI)	18.0038	48.1884	101.692	20.6
4,5-Bentropolone (XII)	18.0471	52.1574	106.037	17.3
5,6-Benzotropolone (XIII)	17.4343	52.1139	105.381	2.2
3,4-Benzotropolone (XIV)	17.4320	52.1152	105.380	2.1
6,7-Benzotropolone (XV)	18.1071	52.1826	106.122	19.3
4,5-Naphthotropone (XVI)	23.8694	66.7903	135.035[b]	28.6
3,4-Naphhotropone (XVII)	22.9013	66.7694	134.046	5.8
2,3-Naphthotropone (XVIII)	23.9953	66.8217	135.192	32.2
2,3,6,7-Dibenzotropone (XIX)	24.2700	66.9211	135.566	40.8
2,3,5,6-Dibenzotropone (XX)	23.6011	66.8101	134.786	22.8
2,3,4.5-Dibenzotropone (XXI)	24.2201	66.9055	135.501	39.3

[a] Experimental heat of atomisation for tropolone is 72.21 eV (Ref. 22)

[b] Experimental heats of atomization for tropone, 4,5-benzotropone and 4,5-naphthotropone are 67.43 eV, 101.44 eV, and 135.03 eV, respectively. (Private communication from Professor E. Heilbronner).

assumption that tropolone, and perhaps also tropone, are aromatic,[23] an assumption that is strongly supported by HMO calculations[7,23]; the available chemical and spectroscopic evidence does, however, seem to suggest that it is wrong[24]. Thus tropone very readily undergoes Diels-Alder reactions[25], under neutral or basic conditions, and a recent structure analysis[26] of 4,5-benzotropone shows that the bonds in the seven membered ring alternate strongly and indeed approximate closely to the values expected for single and double bonds in classical polyene (1.46 Å and 1.35 Å).

The idea that tropolone is aromatic arose from its ability to undergo facile aromatic substitutions (*e. g.* diazo coupling), and its stability to strong acids. These reactions are, however, carried out under basic or acidic conditions where the compound exists as a symmetrical anion $C_7H_5O_2^-$, or cation $C_7H_7O_2^+$. Both these must be highly resonance-stabilized; thus the latter must approximate in structure to a dihydroxy derivative of the aromatic tropylium ion. Similar reasons apply of course to the stability of tropone in strong acid, where it exists as hydroxytropylium; under these conditions the ring is very inert. One might add that the fact that tropone is quite strong base must

imply that the conjugated acid has a very much larger resonance energy than tropone itself; the parent base must therefore be much less aromatic than tropylium.

The theoretical procedure[9-12] used here leads automatically to estimates of bond lengths; these, and corresponding π electron densities, are presented in diagramatic form in Fig. 2. Unfortunately no adequate structure determination have as yet been reported, except for the 4,5-benzotropone (IX)[26] and even here the possible errors in the experimental bond lengths, are rather large. In view of this, the agreement between them and our calculated values must be regarded as satisfactory. In the case of tropone and tropolone, electron diffraction studies[27-31] have lead to the conclusion that the rings in them are

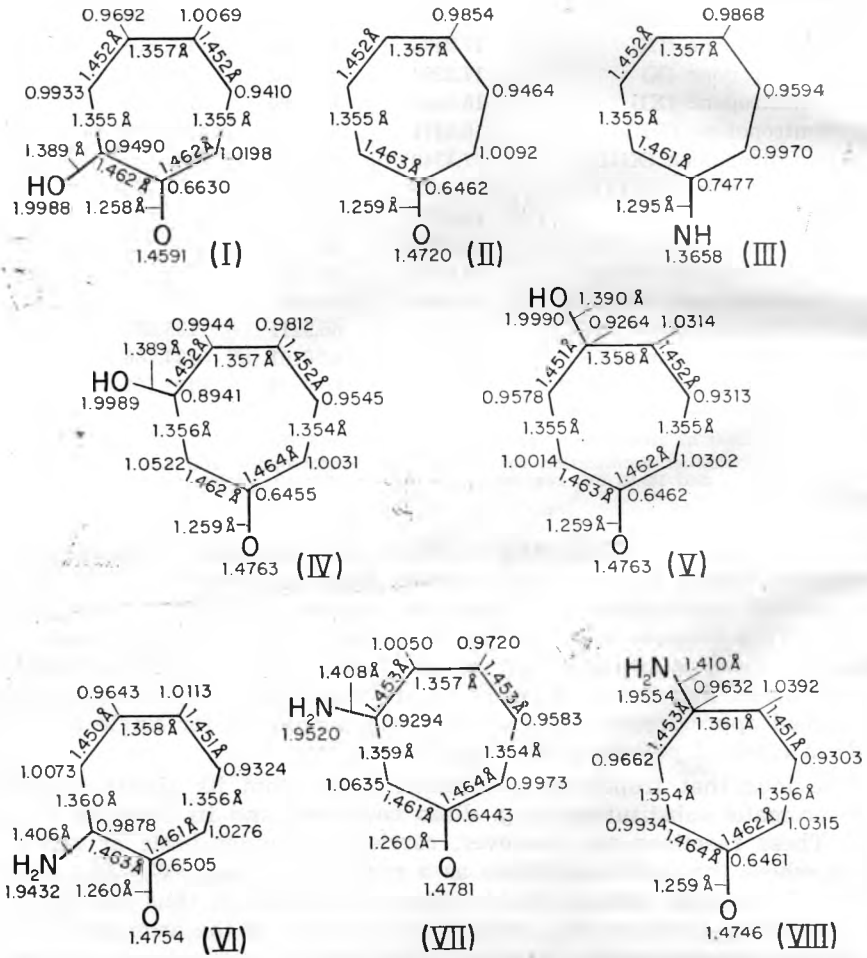

Fig. 2. Molecular orbital diagrams (bond lengths and charge densities) for molecules I—XXI. Preliminary determination of the structure of 4,5-benzotropone (in brackets) by X-ray investigation from Ref. 26.

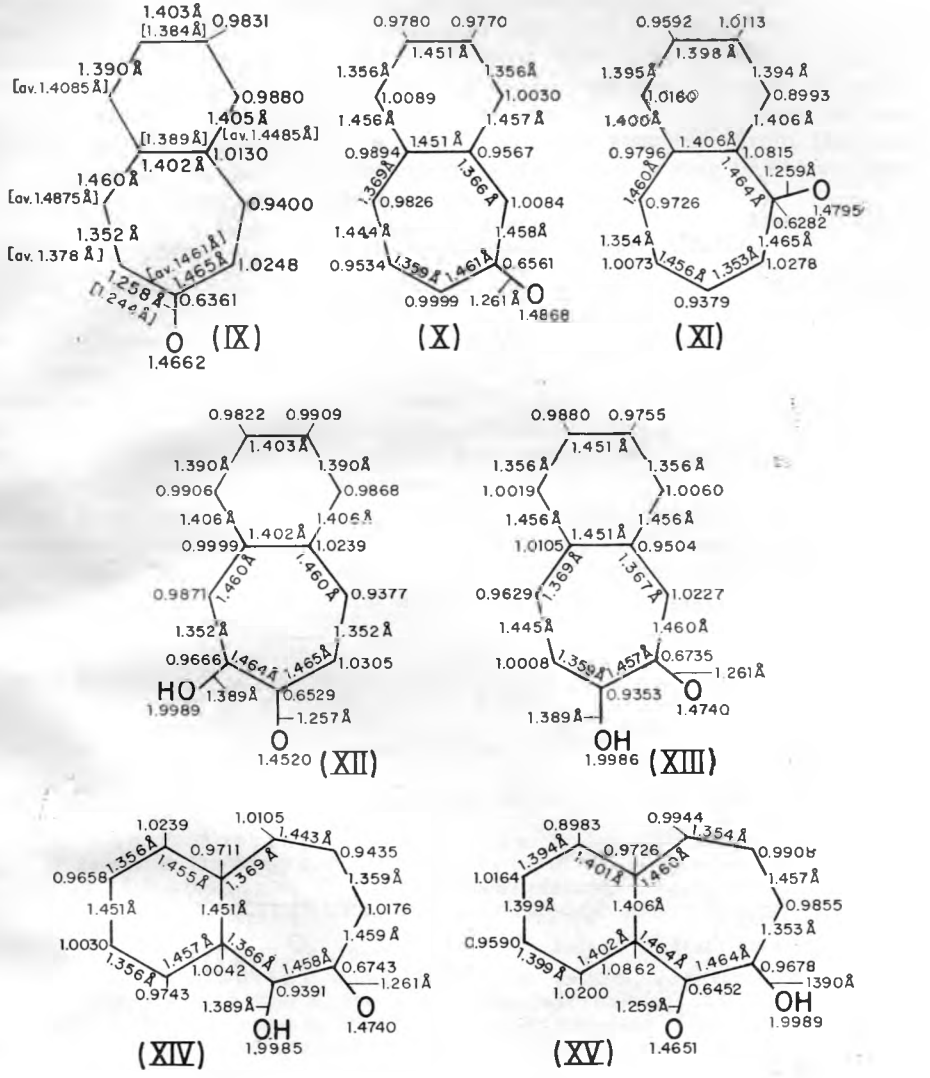

Fig. 2b

planar with average CC bond distances of 1.40 Å; it could not however be established whether or not the bond lengths alternate. The reported C=O (1.26 Å) and C—O (1.36 Å) bond lengths agree very well with our calculated values.

If tropone and tropolone are indeed non-aromatic one would expect gross difference in behaviour between polycyclic compounds formed from them by annelation in various positions[32]. Thus (IX) and (XI) should be aromatic, the benzene rings being unaffected by attachment at the polyenoid C_5 moiety,

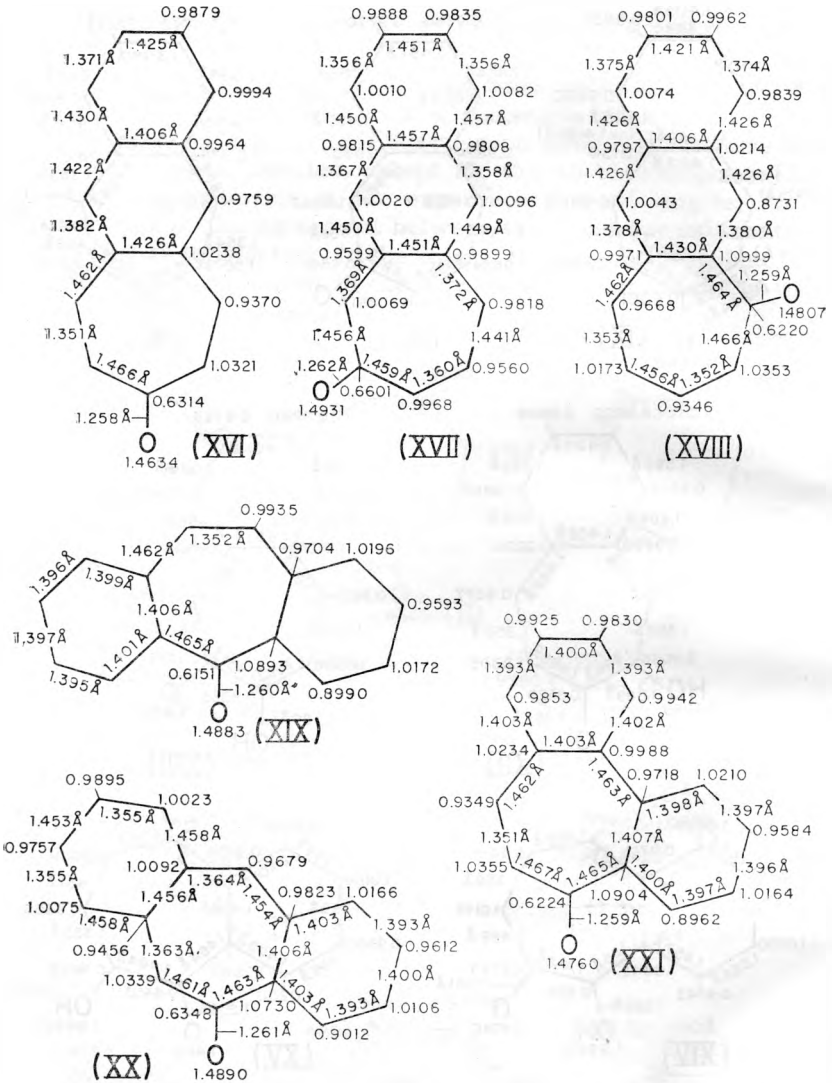

Fig. 2c

where as (X) should have a non-aromatic quinonoid structure. Likewise the position of the hydroxyl proton in annelated tropolones should be unambiguous, one isomer in each case being aromatic and the other non-aromatic (*cf.* (XII) with (XIII) or (XIV) with (XV). These intuitive conclusions are fully confirmed both by the calculations reported here (Table VI and Fig. 2), which imply that the non-aromatic annelated compounds should have low resonance energies and strongly alternating bonds, and also by the available experimental evidence[32]. Thus none of the non-aromatic tropones has as yet been

synthesized, although a number of the aromatic isomers are known and are stable. Note also that the π electron distribution in tropolone, and aromatic annelated derivatives, corresponds closely to that expected for a classical structure with localized single and double bonds; thus the π charges on carbon are close to unity and on oxygen close to two. On the other hand the non-aromatic benzotropone (X) shows relatively large departure from this classical picture, due to the desperate efforts of the benzene ring to recover some at least of its aromaticity.

SUMMARY AND CONCLUSIONS

The most important conclusion from the work reported here is the definitive prediction that neither tropone nor tropolone is aromatic, in direct contradiction to the results of HMO calculations. Since the procedure used here has proved uniformly satisfactory for all systems which properties are known experimentally, its predictive power seems strong; tropone and tropolone therefore seem likely to prove additional nails in the coffin of HMO theory, representing yet two more cases when HMO erroneously predicts non-aromatic compounds to be aromatic.

We hope that the present communication may stimulate further experimental work to settle this point, in particular a synthesis of (X); though if we are right, (X) should not only be difficult to synthesize but probably impossible to isolate in view of facile polymerisation.

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IZVOD

Račun SCF MO za neke derivate tropona

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Račun SCF MO je primijenjen na izračunavanje svojstava osnovnoga stanja (toplina atomiziranja, totalna energija molekule, energija rezonancije, dužina veze, π-elektronska raspodjela) tropona, tropolona i njihovih derivata. Najvažniji zaključak rada jest to da tropon i tropolon nisu aromatske molekule, suprotno ranijim predviđanjima baziranim na HMO računima. Značajan je i zaključak rada da postoji osnovna razlika između molekula dobivenih pripajanjem benzena troponu (ili tropolonu) u položaju 2,3- ili 4,5- (to su onda aromatske molekule), ili pripajanjem benzena u položaju 3,4- (to je onda ne-aromatska, kinoidna molekula).

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