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266. ESR.-Studies of Nonalternant Radicals Structurally Related to Phenalenyl

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(11. IX. 75)

Summary. The radical anion and the radical cation of azuleno[1,2,3-*cd*]phenalene (III) have been investigated by ESR. spectroscopy, along with the radical anion of 2-phenylazulene (IV). Also studied has been the neutral radical obtained by one-electron reduction of cyclohepta[*cd*]phenalenium-cation ($VI^{\oplus}$). Assignment of the proton coupling constants for the radical ions $III^{\cdot\ominus}$, $III^{\cdot\oplus}$ and $IV^{\cdot\ominus}$, and the radical $VI^{\cdot}$ is supported by comparison with the ESR. spectra of specifically deuteriated derivatives $III\text{-}d_5^{\cdot\ominus}$, $III\text{-}d_5^{\cdot\oplus}$, $IV\text{-}d_2^{\cdot\ominus}$ and $VI\text{-}d_1^{\cdot}/VI\text{-}d_1'^{\cdot}$. The experimental results are in full accord with qualitative topological arguments and predictions of HMO models. Whereas the radical anion $III^{\cdot\ominus}$ exhibits π-spin distribution similar to that of $IV^{\cdot\ominus}$, the corresponding radical cation $III^{\cdot\oplus}$ and the neutral radical $VI^{\cdot}$ are related in this respect to phenalenyl ($V^{\cdot}$). It is noteworthy that oxidation of III by conc. H_2SO_4 yields a paramagnetic species ($IIIa^{\cdot\oplus}$) which has a similar – but not an identical – structure as the radical cation $III^{\cdot\oplus}$ produced from III with $AlCl_3$ in CH_3NO_2.

We have reported previously [1] on the radical anion of azuleno[5,6,7-*cd*]phenalene (I) which resembles that of 6-phenylazulene (II) with respect to its ease of formation and π-spin distribution. A corresponding relationship is expected to hold for the radical anions of 2-phenylazulene (IV) and azuleno[1,2,3-*cd*]phenalene (III), a nonalternant hydrocarbon synthesized recently [2]. The radical anion of III should thus be adequately described by the formula $III^{\cdot\ominus}$ which represents $IV^{\cdot\ominus}$ linked to two isolated double bonds.

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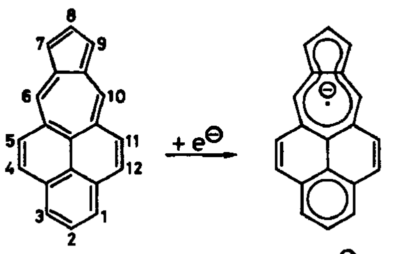
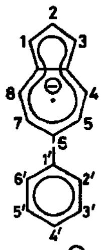
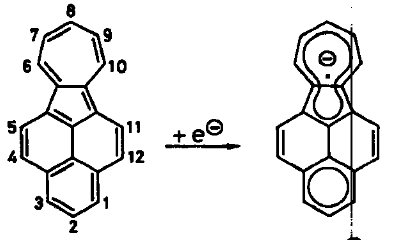


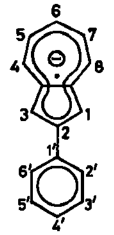
I → I·⊖



II·⊖

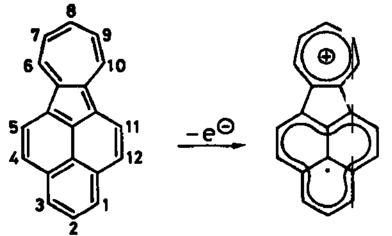


III → III·⊖

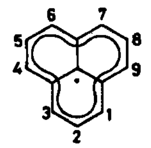


IV·⊖

On the other hand one might anticipate that the radical cations of I and III would be related to the extremely stable phenalenyl radical (V·). However, experimental evidence points to a rather low stability of I·⊕, since attempts to generate this radical cation by standard techniques have not been successful[3]). This result can be explained qualitatively by considering the topology of the π-system of I; it is not possible to formulate I·⊕ as V· linked to a cationic fragment of low energy. An analogous argument applied to the isomeric π-system of III suggests, however, that the radical cation of this hydrocarbon would be much more favoured. Such viewpoint is expressed by the formula III·⊕ in which the phenalenyl radical (V·) is coupled to the stable tropylium cation.



III → III·⊕



V·

Similar considerations indicate that a neutral radical should be readily produced from the cyclohepta[*cd*]phenalenium cation (VI⊕), another novel nonalternant

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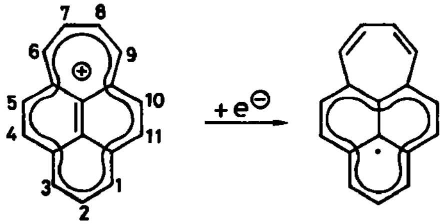
[3]) Dissolution of azuleno[5,6,7-*cd*]phenalene (I) in conc. sulfuric acid leads exclusively to the addition of a proton in the 7- (or 9-) position. Also the formation of the radical cation I·⊕ cannot be detected when I reacts with $SbCl_5$ in methylene chloride. On the other hand, an ESR. spectrum of low intensity is observed upon treatment of I with $AlCl_3$ in nitromethane. However, the hyperfine structure of this spectrum (three coupling constants of 3.5, 2.4 and 0.8 Gauss, each due to four equivalent or nearly equivalent protons [3]) seems incompatible with the π-spin distribution expected for the radical cation I·⊕.

π-system synthesized by the same research group [4]. This radical would be well characterized by the formula VI· representing V· coupled to the *cis*-1,3-butadiene π-system.



VI$^{\oplus}$ VI·

In this paper we present the ESR. spectra of the radical ions III$^{\cdot\ominus}$, IV$^{\cdot\ominus}$, and III$^{\cdot\oplus}$, in addition to that of the neutral radical VI·. Also reported are the investigations of some specifically deuteriated derivatives such as the radical ions III-$d_5^{\cdot\ominus}$ and III-$d_5^{\cdot\oplus}$ of 6,7,8,9,10-pentadeuterioazuleno[1,2,3-*cd*]phenalene, the radical anion IV-$d_2^{\cdot\ominus}$ of 1,3-dideuterio-2-phenylazulene, and the neutral radicals VI-d_1· and VI-d_1'· derived from a 5:6 mixture of 6- and 7-deuteriocyclohepta[*cd*]phenalenium cations.

Experimental Part. – The syntheses of azuleno[1,2,3-*cd*]phenalene (III) and its 6,7,8,9,10-pentadeuterio-derivative (III-d_5) have been described in a recent paper [2]. 2-Phenylazulene (IV) was a gift of Prof. *Takase* of Tohoku University, Sendai, who prepared it according to a procedure reported previously [5]. 1,3-Dideuterio-2-phenylazulene (IV-d_2) was obtained by an isotope exchange between IV and 85 percent D_3PO_4 (*Merck*, Darmstadt). The synthesis of cyclohepta[*cd*]phenalenium cation (VI$^{\oplus}$) has also been described recently [4]. When in one of its steps (involving the reduction of cyclohepta[*cd*]phenalen-6-one) $LiAlH_4$ was replaced by $LiAlD_4$, a 5:6 mixture of the two isomeric 6- and 7-deuterio-cyclohepta[*cd*]phenalenium cations (VI-$d_1^{\oplus}$ and VI-$d_1'^{\oplus}$, respectively) resulted as a final product.

Reduction of III, IV, VI$^{\oplus}$ and their deuterio-derivatives to the corresponding radical anions (III$^{\cdot\ominus}$, III-$d_5^{\cdot\ominus}$, IV$^{\cdot\ominus}$ and IV-$d_2^{\cdot\ominus}$) or neutral radicals (VI·, VI-d_1· and VI-d_1'·) was performed chemically (reaction with an alkali metal in an ethereal solvent) and/or electrolytically (in N,N-dimethylformamide, with a tetraalkylammonium perchlorate as the supporting salt). The radical anions III$^{\cdot\ominus}$ and III-$d_5^{\cdot\ominus}$ exhibited rather low stability. On the other hand, relatively stable paramagnetic species were produced from III and III-d_5 by several oxidative procedures: (1) conc. H_2SO_4 or D_2SO_4, (2) $SbCl_5 + O_2$ in $SbCl_3$; (3) O_2 in CF_3COOH, and (4) $AlCl_3$ in CH_3NO_2. However, only the species obtained by the last method could be unambiguously identified by ESR. spectroscopy as the radical cations III$^{\cdot\oplus}$ and III-$d_5^{\cdot\oplus}$ (see following section).

Results and Discussion. – *Radical anions.* Reaction of azuleno[1,2,3-*cd*]phenalene (III) with lithium, sodium or potassium in 1,2-dimethoxyethane (DME) or tetrahydrofuran (THF) yielded only small concentrations of the radical anion III$^{\cdot\ominus}$ in solution, whereas electrolytic reduction of III in N,N-dimethylformamide (DMF) resulted merely in a secondary species. This handicap is thought to be caused by a combined effect of (*1*) the uptake of a second electron with the formation of the diamagnetic dianion III$^{2\ominus}$, and (*2*) the low solubility and rapid decomposition of both III$^{\cdot\ominus}$ and III$^{2\ominus}$. Fig. 1 shows an ESR. spectrum of III$^{\cdot\ominus}$ obtained upon reaction of III with Na in DME. Its quality is only modest, since the small concentration of the radical anion required a high amplification of the signal and a large modulation

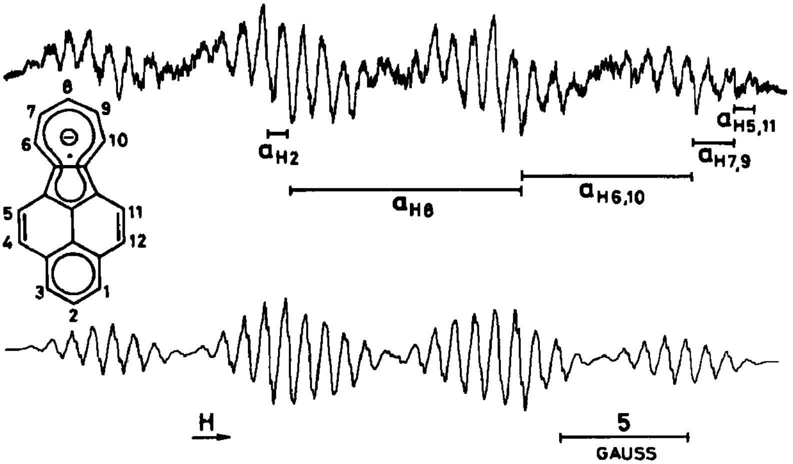


Fig. 1. *ESR. spectra of the radical anion III* ·$^{\ominus}$. Top: Experimental spectrum. Solvent: DME; counter-ion: Na$^{\oplus}$; temp.: +20°. Bottom: Computer-simulated spectrum. Coupling constants given in Table 1; line-width: 0.13 Gauss; line-shape: Lorentzian

amplitude. Nevertheless, the hyperfine structure could be reliably analyzed, as confirmed by the computer-simulated curve also reproduced in Fig. 1. The assignment of the proton coupling constants (a_{H_μ}) listed in Table 1 is based on comparison with the spectrum of the 6,7,8,9,10-pentadeuterio-derivative III-d_5·$^{\ominus}$. This spectrum, which consists of a broad signal extending over 11–12 Gauss[4]), proves that the

Table 1. *Proton coupling constants* a_{H_μ} (in Gauss = 10^{-4} Tesla) *for the radical anions III* ·$^{\ominus}$, *IV* ·$^{\ominus}$ *and VII* ·$^{\ominus}$

	III·$^{\ominus}$		IV·$^{\ominus}$	VII·$^{\ominus}$
μ a)	$a_{H\mu}$ b)	μ c)	$a_{H\mu}$ d)	$a_{H\mu}$ e)
1,3	0.2 f)g)	3',5'	0.38	
2	0.8	4'	1.50	
4,12	0.1 f)g)			
5,11	0.8 f)			
6,10	6.7 h)	4,8	6.09	6.22
7,9	1.6 h)	5,7	1.15 f)	1.27
8	9.0 h)	6	8.48	8.87
		1,3	0.18 h)	0.28
		2',6'	1.37 f)	
		2	–	3.98

a) Numbering of the positions in azuleno[1,2,3-*cd*]phenalene (*cf.* formula III). b) Experimental error: ±0.1 for $a_{H7,9}$ and a_{H8}, and ±0.05 Gauss for the remaining a_{H_μ} values. c) Numbering of the positions in azulene and 2-phenylazulene (*cf.* formula IV). d) Experimental error: ±0.02 and ±0.01 Gauss for a_{H_μ} values larger and smaller than 1 Gauss, respectively. e) Values taken from [6b]. f) Assignment uncertain. g) Only partially resolved splitting. h) Replaced by a_{D_μ} = (0.1535) a_{H_μ} in the ESR. spectra of the deuterio-derivatives.

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[4]) 1 Gauss = 10^{-4} Tesla.

three largest a_{H_μ} values must be assigned to the deuteriated positions. The pertinent coupling constants strongly resemble the analogous data for the radical anions IV$\cdot^{\ominus}$ and VII$\cdot^{\ominus}$ of 2-phenylazulene and azulene [6], respectively. These data are also contained in Table 1, while Fig. 2 and 3 present the experimental and computer-simulated spectra of IV$\cdot^{\ominus}$ and its 1,3-dideuterio-derivative IV-$d_2\cdot^{\ominus}$.

Radical cations. As mentioned in the Exper. Part, azuleno[1,2,3-*cd*]phenalene (III) could be converted into relatively stable paramagnetic species by a variety of oxidizing agents. A single ESR. signal of 30±5 Gauss width appeared upon mere admission of oxygen to a solution of III in trifluoroacetic acid at room temperature. Furthermore, seven broad hyperfine components spaced by 4±1 Gauss and of approximately binomial intensity distribution were observed at + 100° when III was dissolved in an unpurified antimony trichloride which usually contains traces of $SbCl_5$ and O_2 [7]. More conventional methods, however, had to be applied in order to obtain well-resolved multiline ESR. spectra such as those shown in Fig. 4 and 5. Even a cursory consideration of these spectra, which resulted from oxidation of III at room temperature by aluminum trichloride in nitromethane (Fig. 4) and by conc. sulfuric acid (Fig. 5), reveals substantial differences in their splitting patterns. The presumption that the two spectra arise from different species is supported by the analysis of their hyperfine structures which yields the proton coupling constants (a_{H_μ}) listed in Table 2 and used for computer-simulation of the corresponding

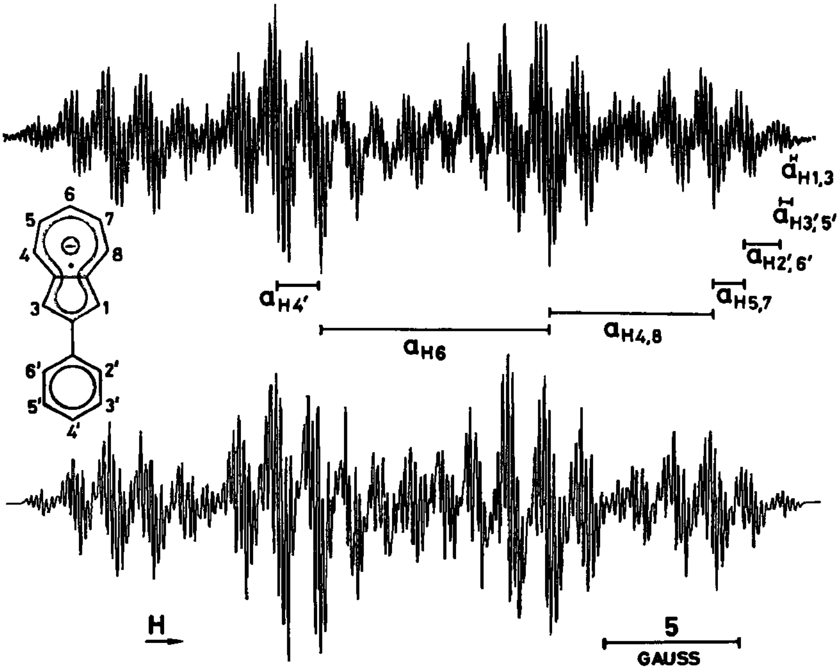

Fig. 2. *ESR. spectra of the radical anion IV*$\cdot^{\ominus}$. Top: Experimental spectrum. Solvent: DME; counter-ion: $K^{\oplus}$; temp.: −60°. Bottom: Computer-simulated spectrum. Coupling constants given in Table 1; line-width: 0.09 Gauss; line-shape: Lorentzian

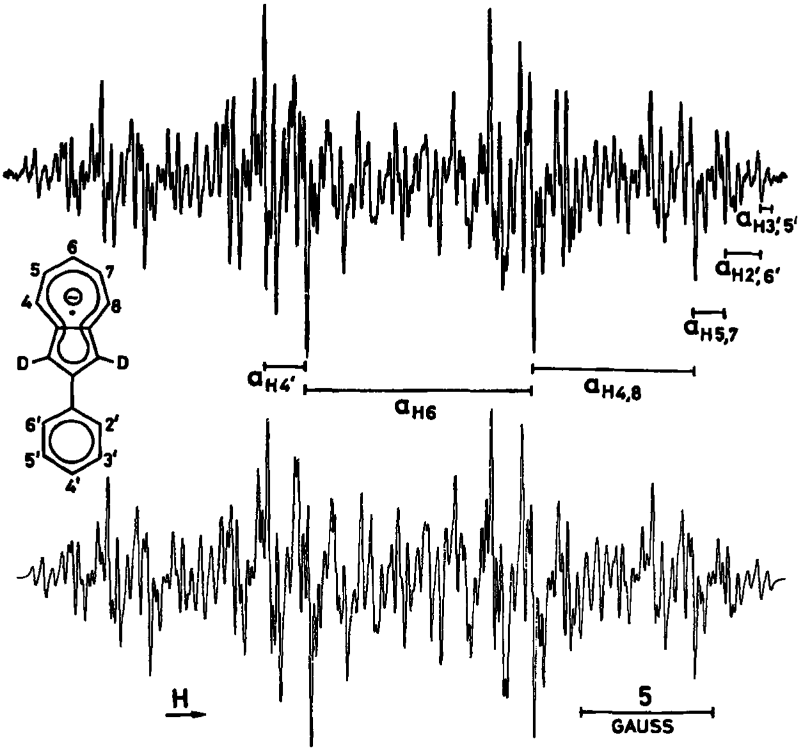

Fig. 3. *ESR. spectra of the radical anion* $IV\text{-}d_2\,\cdot^{\ominus}$. Top: Experimental spectrum. Solvent: DME; counter-ion: $K^{\oplus}$; temp.: $-60°$. Bottom: Computer-simulated spectrum. The same coupling constants as used for $IV\,\cdot^{\ominus}$, except $a_{H1,3}$ which has been omitted; line-width: 0.13 Gauss; line-shape: Lorentzian

derivative curves (Fig. 4 and 5). As will be confirmed by MO calculations (see *HMO models*), the π-spin distribution expected for the radical cation of III is borne out much more satisfactorily by the a_{H_μ} values obtained from the spectrum of Fig. 4 ($AlCl_3/CH_3NO_2$) than from that of Fig. 5 (conc. H_2SO_4). The former (Fig. 4) has therefore been attributed to the radical cation $III\cdot^{\oplus}$, leaving the interpretation of the latter (Fig. 5) open to discussion. Since the structure of the species giving rise to the spectrum in question (Fig. 5) could not yet be completely elucidated (see below), a provisional notation $IIIa\cdot^{\oplus}$ has been introduced for that species in the present paper.

The assignment of the proton coupling constants in Table *2* is consistent with the ESR. spectra of the 6,7,8,9,10-pentadeuterio-derivatives $III\text{-}d_5\cdot^{\oplus}$ in $AlCl_3/CH_3NO_2$ and $IIIa\text{-}d_5\cdot^{\oplus}$ in conc. H_2SO_4[5]. The most prominent feature of these spectra is the splitting into five major components spaced by *ca.* 4.7 Gauss and of almost binomial intensity distribution; it requires the that two largest a_{H_μ} values observed for $III\cdot^{\oplus}$ and $IIIa\cdot^{\oplus}$ should be assigned to two pairs of equivalent protons in positions which are undeuteriated in $III\text{-}d_5\cdot^{\oplus}$ and $IIIa\text{-}d_5\cdot^{\oplus}$. By analogy with the ESR. data for

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[5] In this context, one has to emphasize that the ESR. spectrum of $IIIa\,\cdot^{\oplus}$ in Fig. 5 is obtained with either conc. H_2SO_4 or D_2SO_4 and that the same holds for the spectrum of $IIIa\text{-}d_5\cdot^{\oplus}$.

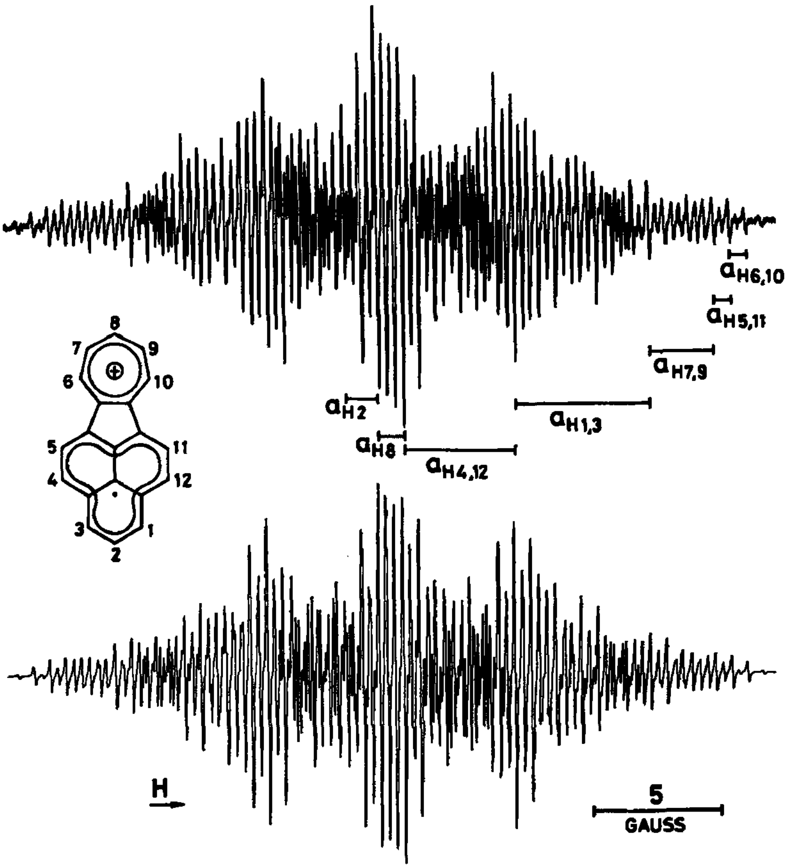

Fig. 4. *ESR. spectra of the radical cation III* ·⊕. Top: Experimental spectrum. Solvent: CH_3NO_2; temp.: +20°. Bottom: Computer-simulated spectrum. Coupling constants given in Table 2; line-width: 0.07 Gauss; line-shape: Lorentzian

phenalenyl radical (V·) [8], also given in Table 2, these positions can be identified as 1,3 and 4,12[6]).

Neutral radicals. No ESR. signals could be detected upon reaction of the cyclohepta[*cd*]phenalenium-cation (VI⊕) with alkali metals in ethereal solvents. More successful was an electrolytic reduction of VI⊕ in N,N-dimethylformamide (DMF) with tetraethylammonium perchlorate as the supporting salt. Fig. 6 shows the ESR. spectrum of the neutral radical VI· generated from VI⊕ during a continuous electro-

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[6]) It is noteworthy that, in addition to the hyperfine splittings from the five sets of two equivalent protons, only one splitting (0.9 Gauss) due to a single proton is found in the spectrum of Fig. 5. Since in the spectrum of IIIa-d_5 ·⊕ this splitting has been replaced by one arising from a deuteron, the pertinent coupling constant of 0.9 Gauss must be assigned to the proton in the position 8, and the splitting due to the second single proton in the position 2 is either missing or unresolved (*i.e.*, smaller than the line-width of *ca.* 0.1 Gauss). The absence of such a splitting, which is expected to have an absolute value of 1 to 1.5 Gauss, presents a convincing argument against attributing the spectrum of Fig. 5 to *the* radical cation of III. It strongly suggests that some change in the molecular structure occurs at the position 2 upon oxidation of III by conc. sulfuric acid.

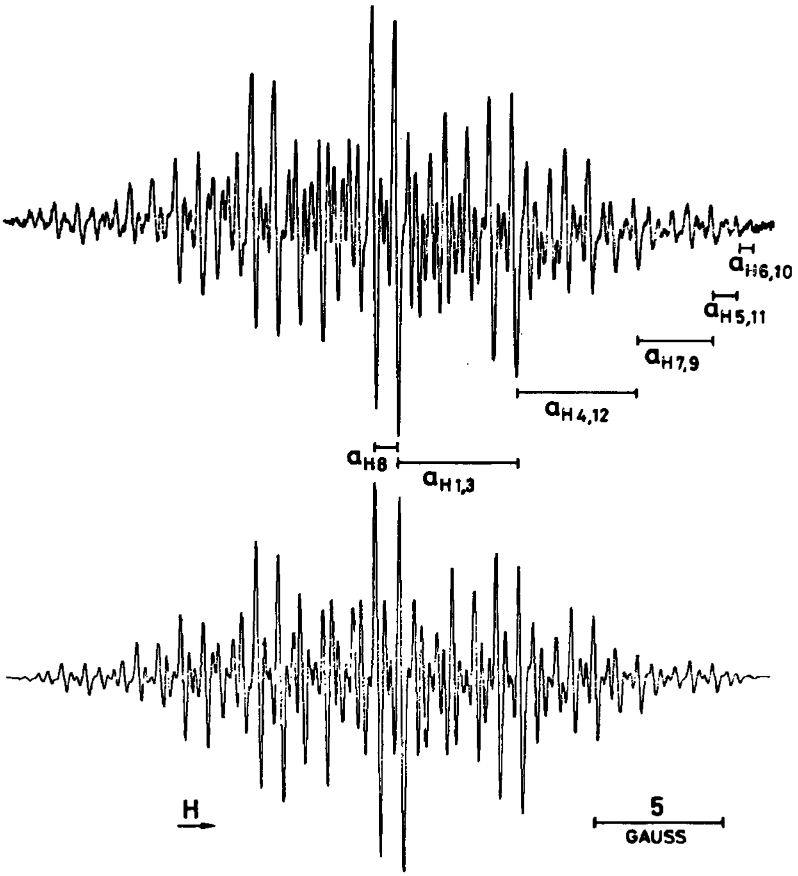

Fig. 5. *ESR. spectra of the radical cation IIIa* $\cdot^{\oplus}$. Top: Experimental spectrum. Solvent: conc. H_2SO_4; temp.: +20°. Bottom: Computer-simulated spectrum. Coupling constants given in Table 2; line-width: 0.12 Gauss; line-shape: Lorentzian

Table 2. *Proton coupling constants* a_{H_μ} (in Gauss = 10^{-4} Tesla) *for the radical cations III* $\cdot^{\oplus}$ *and IIIa* $\cdot^{\oplus}$ *and for the neutral radicals V* $\cdot$ *and VI* $\cdot$

	III·⊕	IIIa·⊕		V·		VI·
μ a)	$a_{H\mu}$ b)	$a_{H\mu}$ b)	μ c)	$a_{H\mu}$ d)	μ e)	$a_{H\mu}$ b)
1,3	5.23	4.66	1,3	6,29	1,3	5.01
2	1.26	<0.1	2	1,81	2	1.36
4,12	4.29	4.66	4,9	6,29	4,11	4.80
5,11	0.62	0.90	5,8	1,81	5,10	1.55
6,10	0.62 f)	0.55 f)			6,9	0.28 f)
7,9	2.56 f)	2.94 f)			7,8	2.95 f)
8	0.94 f)	0.90 f)				
			6,7	6.29		

a) Numbering of the positions in azuleno[1,2,3-*cd*]phenalene (*cf.* formula III). b) Experimental error: ±0.02 and ±0.01 Gauss for a_{H_μ} values larger and smaller than 1 Gauss, respectively. c) Numbering of the positions in phenalenyl (*cf.* formula V ·). d) Values taken from [8b]. e) Numbering of the positions in cyclohepta[*cd*]phenalenium cation (*cf.* formula VI⊕). f) Replaced by $a_{D_\mu} = (0.1535)\, a_{H_\mu}$ in the ESR. spectra of the deuterio-derivatives.

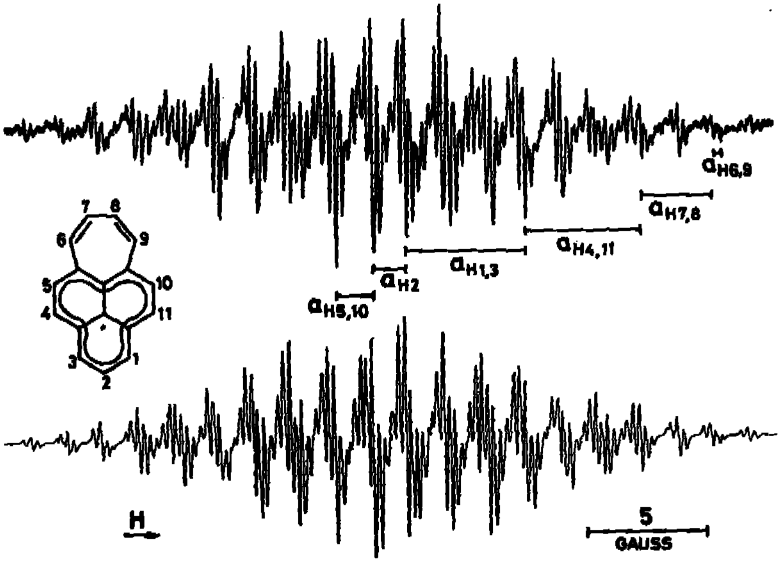

Fig. 6. *ESR. spectra of the radical VI·*. Top: Experimental spectrum. Solvent: DMF; temp.: −40°. Bottom: Computer-simulated spectrum. Coupling constants given in Table 2; line-width: 0.10 Gauss; line-shape: Lorentzian

lysis at −40°. It also displays a derivative curve which has been computer-simulated with the use of the proton coupling constants (a_{H_μ}) listed in Table 2. The assignment of the a_{H_μ} values is mainly based on analogy with the ESR. data for phenalenyl radical (V·); a partial check has been provided by the ESR. study of a DMF solution of the 6- and 7-deuterio-derivatives, VI-d_1· and VI-d_1'·, respectively. Their spectrum was obtained upon an electrolytic reduction of a 5:6 mixture of the corresponding cations VI-$d_1^{\oplus}$ and VI-$d_1'^{\oplus}$ (see Exper. Part).

HMO models. Fig. 7 presents the diagrams and energy levels of the singly occupied HMO's in the radical ions of azulene (VII), its phenyl-derivatives II and IV, and the two isomeric azulenophenalenes I[7]) and III. The radical cations of VII and III and all the radical anions have been characterized by ESR. spectroscopy, either previously [1] [6] [9] or in this work.

As might be anticipated, the singly occupied HMO's in II$^{\cdot\ominus}$, IV$^{\cdot\ominus}$, II$^{\cdot\oplus}$ and IV$^{\cdot\oplus}$ strongly resemble the corresponding azulene orbitals in VII$^{\cdot\ominus}$ and VII$^{\cdot\oplus}$. Interestingly, this statement also holds for the radical anions I$^{\cdot\ominus}$ and III$^{\cdot\ominus}$ of the two isomeric azulenophenalenes with respect to both the energy ($\alpha - 0.40\beta$) and the shape of the HMO's. On the other hand, although the singly occupied HMO's in the radical cations I$^{\cdot\oplus}$ and III$^{\cdot\oplus}$ correlate with those in II$^{\cdot\oplus}$ and IV$^{\cdot\oplus}$, respectively, the models predict a distinct shift of the unpaired electron population from the azulene fragments of the molecules into the fused phenalenyl π-systems. As evident from the diagrams of Fig. 7, this shift should be more pronounced for III$^{\cdot\oplus}$ than for I$^{\cdot\oplus}$; it is reflected by the sequence of the HMO energies: VII$^{\cdot\oplus}$ $\approx$ II$^{\cdot\oplus}$ $\approx$ IV$^{\cdot\oplus}$ ($\alpha + 0.48\beta$) <

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[7]) Consult [1] for the energy sequence of the lowest antibonding HMO's in I and its occupancy in the radical anion I$^{\cdot\ominus}$.

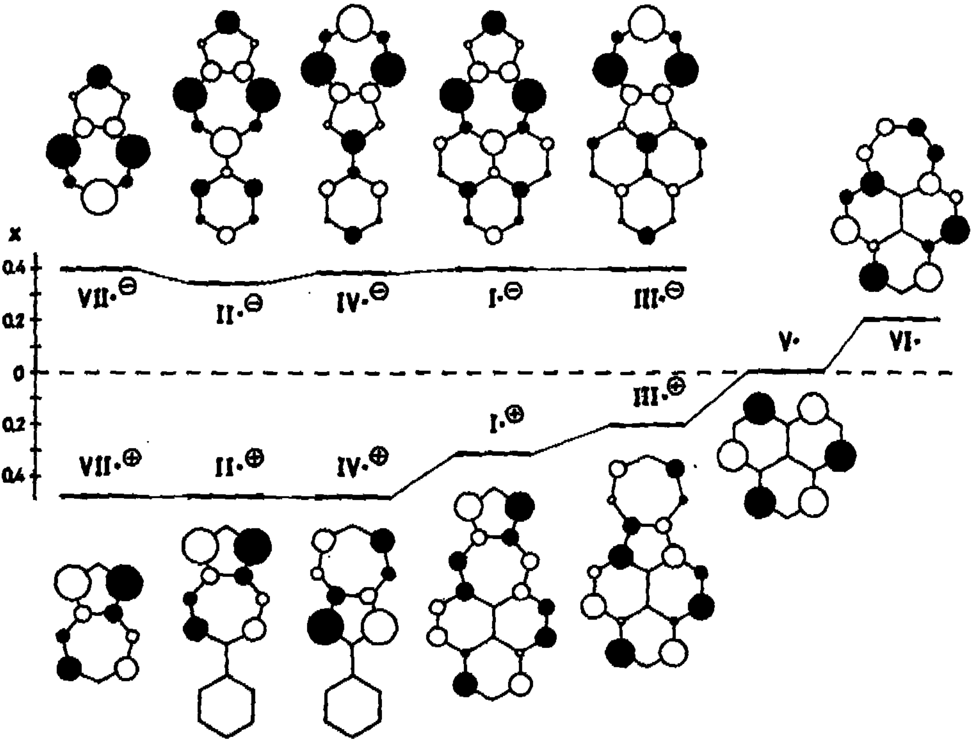

Fig. 7. *Orbital diagrams and energy levels of the singly occupied HMO's in the radical ions* $VII^{\cdot\ominus}$, $VII^{\cdot\oplus}$, $II^{\cdot\ominus}$, $II^{\cdot\oplus}$, $IV^{\cdot\ominus}$, $IV^{\cdot\oplus}$, $I^{\cdot\ominus}$7), $I^{\cdot\oplus}$, $III^{\cdot\ominus}$ *and* $III^{\cdot\oplus}$, *and in the neutral radicals* $V\cdot$ *and* $VI\cdot$. The areas of the circles in the diagrams are proportional to the squares of the LCAO coefficients; blank and filled areas symbolize different signs of these coefficients. The energies E are in units of $x = (1/\beta)\ (E\text{-}\alpha)$

$I^{\cdot\oplus}$ $(\alpha + 0.32\beta)$ $<$ $III^{\cdot\oplus}$ $(\alpha + 0.21\beta)$ $<$ $V\cdot$ (α). The singly occupied HMO in $III^{\cdot\oplus}$ can thus be considered as having more «phenalenyl character» than the corresponding orbital in $I^{\cdot\oplus}$. The diagram and energy level of the pertinent HMO in $V\cdot$ are also displayed by Fig. 7, along with those in the cyclohepta[*cd*]phenalenyl radical ($VI\cdot$). Clearly, the unpaired electron distribution over the phenalenyl π-systems is predicted to be very similar in $III^{\cdot\oplus}$, $V\cdot$ and $VI\cdot$.

Table 3 lists the π-spin populations (ϱ_μ) calculated by the *McLachlan* [10] procedure for the proton bearing centers (μ) in those radical ions ($III^{\cdot\ominus}$, $III^{\cdot\oplus}$ and $IV^{\cdot\ominus}$) and the neutral radical ($VI\cdot$) which have been investigated in this work. The good correlation of the HMO theoretical ϱ_μ values with the observed proton coupling constants (a_{H_μ}) corroborates the assignment made in Tables 1 and 2. Moreover, in the case of III, it clearly favours the radical cation produced by $AlCl_3/CH_3NO_2$ ($III^{\cdot\oplus}$) over that formed in conc. H_2SO_4 ($IIIa^{\cdot\oplus}$).

Concluding Remarks. – The results of ESR. studies reported in this paper are in excellent agreement both with qualitative arguments based on topology and with the predictions of HMO models. In particular, the physico-chemical properties of the radical cation $III^{\cdot\oplus}$ (ease of formation and relative stability) are fully in line with

Table 3. *π-Spin populations ρ_μ at the proton bearing centers μ in the radical ions $IV^{\cdot\ominus}$, $III^{\cdot\ominus}$ and $III^{\cdot\oplus}$, and the neutral radical $VI^{\cdot}$*

	$IV^{\cdot\ominus}$		$III^{\cdot\ominus}$	$III^{\cdot\oplus}$		$VI^{\cdot}$	$VI^{\cdot}$
μ a)	ρ_μ b)	μ c)	ρ_μ b)	ρ_μ b)	μ d)	ρ_μ b)e)	ρ_μ b)f)
3',5'	-0.013	1,3	-0.011	0.212	1,3	0.179	0.204
4'	0.039	2	0.019	-0.057	2	-0.056	-0.056
		4,12	-0.012	0.182	4,11	0.161	0.175
		5,11	0.013	-0.022	5,10	-0.015	-0.025
4,8	0.291	6,10	0.303	-0.017	6,9	0.036	0.022
5,7	-0.082	7,9	-0.079	0.063	7,8	0.089	0.078
6	0.347	8	0.374	-0.025			
1,3	-0.008						
2',6'	0.033						

a) Numbering in 2-phenylazulene (*cf.* formula IV). b) Calculated by the *McLachlan* procedure with the parameter $\lambda = 1.2$. c) Numbering in azuleno[1,2,3-*cd*]phenalene (*cf.* formula III). d) Numbering in cyclohepta[*cd*]phenalenium cation (*cf.* formula $VI^{\oplus}$). e) Using polarizabilities $\pi_{\mu\nu}$ of the cation $VI^{\oplus}$. f) Using polarizabilities $\pi_{\mu\nu}$ of the anion $VI^{\ominus}$.

expectation. This accord stresses once more the merits of the simple theories of planar π-systems, whether in terms of a topological approach or by means of HMO treatment.

We thank Prof. *K. Takase*, Tohoku University, for a sample of 2-phenylazulene (IV). Support by the *Schweizerischer Nationalfonds zur Förderung der wissenschaftlichen Forschung* (Project Nr. 2.163.74) is acknowledged, as well as financial assistance by *Ciba-Geigy SA*, *Sandoz SA* and *F. Hoffmann-La Roche SA*.

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