

The NALA structure is rather different from that of the pure L enantiomer. The latter optimizes the packing by forming wrinkled polar sheets, whose concavities accommodate very well the twisted side chains. Therefore the L enantiomer forms a slightly denser crystal (1.125 compared with 1.077 Mg m⁻³), but only two hydrogen bonds are established.

The melting point of the racemic NALA is also a little lower than those of the D-NALA and L-NALA crystals [401.0 (4) K against 404.1 and 403.2 K recently redetermined]. This temperature, however, results from an enthalpy-entropy ratio, where these two thermodynamic parameters are much smaller for the raceme than those recently found for the pure L enantiomer [2.8 (1) and 7.0 (3) against 16.5 (4) kJ mol⁻¹ and 40.9 (9) J mol⁻¹ K⁻¹, respectively]. These differences of an order of magnitude are unexpected; no solid-solid transitions were found in the range 250–404 K. It is possible that this discrepancy depends on a higher organization of the racemic liquid.

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Structure of Three Di-pyrrole Compounds

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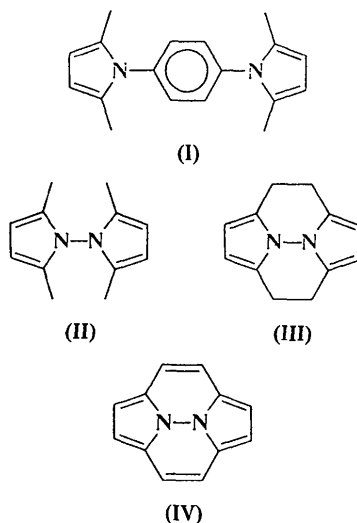
Abstract. All measurements with Mo K α radiation ($\lambda = 0.71073$ Å). (I) *p*-Phenylenebis(2,5-dimethylpyrrole), C₁₈H₂₀N₂, $M_r = 264.40$, orthorhombic, *Cc*mb, $a = 7.273$ (2), $b = 12.463$ (4), $c = 16.559$ (4) Å, $V = 1501.1$ Å³, $Z = 4$, $D_x = 1.17$ Mg m⁻³, $F(000) = 568$, $T = 295$ K, molecular symmetry 2/m. $R = 0.056$ ($wR = 0.053$) for 454 reflections having $I \geq 3\sigma(I)$ with the coordinates of all atoms refined, anisotropic thermal parameters for C and N atoms, and a fixed value of U_{iso} for H atoms. (II) 2,2',5,5'-Tetramethyl-1,1'-bipyrrrole, C₁₂H₁₆N₂, $M_r = 188.27$, orthorhombic, *Cc*2a, $a = 11.773$ (3), $b = 25.154$ (6), $c = 11.841$ (3) Å, $V = 3507$ (1) Å³, $Z = 12$, $D_x = 1.07$ Mg m⁻³, $F(000) = 1224$, $T = 292$ K, molecular symmetry 2 for three

independent molecules. $R = 0.078$ ($wR = 0.080$) for 605 reflections having $I \geq 3\sigma(I)$ with isotropic refinement for C, N and H atoms in calculated positions. (III) 13,14-Diazatetracyclo[8.2.1^{1,10}.-1^{4,7}.0^{13,14}]tetradeca-4,6,10,12-tetraene, C₁₂H₁₂N₂, $M_r = 182.6$, monoclinic, *P2*₁/*a*, $a = 7.667$ (2), $b = 8.191$ (2), $c = 8.231$ (2) Å, $\beta = 112.04$ (2)°, $V = 479.1$ (2) Å³, $Z = 2$, $D_x = 1.26$ Mg m⁻³, $F(000) = 196$, $T = 292$ K, molecular symmetry $\bar{1}$. $R = 0.087$ for 354 reflections having $I \geq 3\sigma(I)$ with C and N atoms refined anisotropically and H atoms in calculated positions. There is disorder in the —CH₂—CH₂— groups. In all three compounds, each 2,5-substituted pyrrole group is planar with unexceptional bond lengths and angles. In (I) the two pyrroles are strictly orthogonal to the benzene ring, in (II) they are

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orthogonal to each other, while in (III) they are coplanar. The crystal structures correlate well with the results of electron spin resonance measurements made on the corresponding radical cations in solution.

Introduction. The radical cations of heteroaromatic molecules, in particular four examples of molecules containing two pyrrole units, namely *p*-phenylenebis(2,5-dimethylpyrrole) (I), 2,2',5,5'-tetramethylbi(*N*-pyrrole) (II), 3,4,7,8-tetrahydro-8b,8c-diazapyracyclene (III), and 8b,8c-diazapyracyclene (IV) have been studied by Avila & Davies (1990). The crystal structure of (IV) has been published (Atwood, Hrnecir, Wong & Paudler, 1974).



We have determined the structures of (I), (II) and (III) to discover whether features of the molecular structures deduced from electron spin resonance (ESR) measurements in solution, are also found in the solid state.

Experimental. Details of the syntheses of the samples used in this work are published (Avila & Davies, 1990). All three compounds are colourless. For each compound a suitable crystal was mounted in random orientation on a Nicolet *R3m/V* diffractometer and carefully centred. Intensities of $5 \leq 2\theta \leq 50^\circ$ were collected by $\theta/2\theta$ scans at variable speed from 4 to $29^\circ \text{ min}^{-1}$ depending upon the intensity of a 2 s prescan; the range was 0.6° below $K\alpha_1$ to 0.6° above $K\alpha_2$ and backgrounds were measured at each side for a quarter of the scan time. Reflections were processed using profile analysis; Lorentz and polarization but no absorption corrections were applied. Three reference reflections were measured every 97 scans and none of the compounds showed deterioration in the beam. Table 1 gives details for the

Table 1. *Experimental details*

	(I)	(II)	(III)
Crystal size (mm)	$0.15 \times 0.25 \times 0.6$	$0.15 \times 0.20 \times 0.02$	$0.25 \times 0.30 \times 0.15$
μ (Mo $K\alpha$) (cm^{-1})	0.36	0.60	0.72
Orientation	$25, 13 < 2\theta < 22$	$42, 8 < 2\theta < 24$	$22, 10 < 2\theta < 23$
reflections, number, range ($^\circ$)			
Temperature (K)	295	292	292
Reference reflections	3T5,13T1,1T6	T32,T13,3T1	T31,22T,24T
Collection range	$h = 0$ to 10 $k = 0$ to 17 $l = 0$ to 22	$h = 0$ to 15 $k = 0$ to 30 $l = 0$ to 15	$h = 0$ to 10 $k = 0$ to 10 $l = -10$ to 10
Total collected	788	1713	903
Unique reflections	514	1553	834
R_{int}	0.03	—	0.07
Number of parameters	68	84	64
Largest shift/e.s.d.	0.038	0.03	0.001
Largest peak ($\text{e } \text{Å}^{-3}$)	0.16	0.29	0.21
g in weighting scheme	0.000102	0.000865	unit weights
$w = 1/(\sigma_F^2 + gF^2)$	—	0.18	0.18
All planes $R(n)$	—	0.18	0.18
S	2.24	2.04	0.83

individual compounds. Crystals of (II) sublime so the specimen was held in a glass capillary tube.

Structure determination and description. (I) The systematic absences, hkl with $h = k$ odd, $0kl$ with l odd (k odd), $hk0$ with k odd (h odd) correspond to two space groups, $Cc2a$ and $Ccmb$. The latter is a non-standard setting of $Ccma$, No. 64. The centrosymmetric space group was confirmed by the E statistics and by the satisfactory solution of the structure with the direct-methods program *SHELXTL-Plus* (Sheldrick, 1986). The equivalent positions are $\frac{1}{2}, \frac{1}{2}, 0 + (x, y, z; -x, y, \frac{1}{2} + z; x, \frac{1}{2} - y, z; -x, \frac{1}{2} - y, \frac{1}{2} + z; x, -y, \frac{1}{2} - z; -x, \frac{1}{2} + y, -z; x, \frac{1}{2} + y, \frac{1}{2} - z; -x, -y, -z)$; these give the origin on $\bar{1}$ and the position of $2/m$ symmetry at $\frac{1}{4}, \frac{1}{4}, 0$ etc. The centres of the molecules are on the latter sites. Refinement proceeded smoothly. H atoms were located in a difference map and their coordinates were refined but they were given a fixed isotropic temperature factor, $U = 0.08 \text{ Å}^2$, while the C and N atoms were allowed anisotropic thermal displacement parameters.

Fig. 1. shows a complete molecule with the designations of the atoms of the asymmetric unit whose coordinates are given in Table 2. The benzene ring lies in the plane of symmetry at $y = \frac{1}{4}$ as does N(1) and the centre of the C(5)—C(5a) bond. The atoms N(1), C(4), C(5), C(4a) and C(5a) form a plane necessarily normal to that of the benzene ring, with a mean deviation of 0.001 Å , while C(6) at $0.010(5) \text{ Å}$ is coplanar within experimental error. The molecules are packed in layers $b/2$ apart with the shortest contacts in that direction of more than 3 Å from the

methyl H atoms to the benzene ring in a molecule in the layer above. Within the layers the molecules are arranged in a herringbone fashion. The angle between N—N directions of adjacent rows is 80° and the shortest contact is 2.58 (5) Å from H(5) to C(4) in a molecule in the next row. Bond lengths and angles for C and N atoms are displayed in Fig. 2(a); those involving H atoms have been deposited* with the anisotropic displacement parameters and structure factor tables. The programs and the atomic scattering factors used were those in the *SHELXTL-Plus* package (version 2.2). We checked the program for generating H atoms in methyl groups and found these rotated by 12° about the C(4)—C(6) bond from the experimental values.

(II) The systematic absences are the same as those for (I) corresponding to the space groups *Ccmb* or *Cc2a*, the latter a non-standard setting of *Aba2*, No. 41. The structure was solved with difficulty. There were no identifiable Harker peaks in the Patterson synthesis which mainly showed pseudo fourfold symmetry down the *b* axis. The distribution of intensities clearly indicated a non-centrosymmetric structure and also that only 58% of the possible reflections were 'observed' in the critical range 1.1 to 1.2 Å. A recognizable solution was obtained after rejection of the reflections with the highest *E* values (*ca* 5.0). In the space group *Cc2a* the equivalent positions are $\frac{1}{2}, \frac{1}{2}, 0 = (x, y, z; \frac{1}{2} - x, y, \frac{1}{2} + z; \frac{1}{2} + x, y, \frac{1}{2} - z; -x, y, -z)$.

There are 12 molecules in the unit cell; the asymmetric unit consists of three independent half molecules each on the twofold axis at 0, *y*, 0 as shown in the stereoview (Fig. 3). Designations of the atoms in

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53814 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

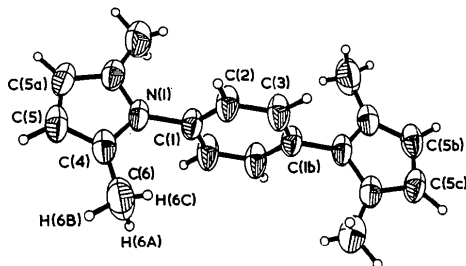


Fig. 1. Molecule of (I) showing the thermal ellipsoids at the 50% confidence level. The atoms of the asymmetric unit are designated thus: a single H atom has the same number as the C atom to which it is attached, while the three methyl H atoms are shown explicitly. Some of the symmetry-related atoms are labeled, the relations being (a) $x, \frac{1}{2} - y, z$; (b) $-\frac{1}{2} - x, \frac{1}{2} - y, 1 - z$; (c) $-\frac{1}{2} - x, y, 1 - z$.

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) in (I)

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
N(1)	436 (4)	2500	6108 (2)	52 (1)
C(1)	-1062 (5)	2500	5544 (2)	51 (1)
C(2)	-2843 (6)	2500	5811 (2)	64 (2)
C(3)	-4278 (6)	2500	5271 (2)	66 (2)
C(4)	1254 (3)	3400 (3)	6424 (2)	58 (1)
C(5)	2580 (4)	3060 (3)	6941 (2)	62 (1)
C(6)	680 (6)	4498 (4)	6194 (3)	93 (2)

* Equivalent isotropic *U* defined as one third of the trace of the orthogonalized *U*_{*ij*} tensor.

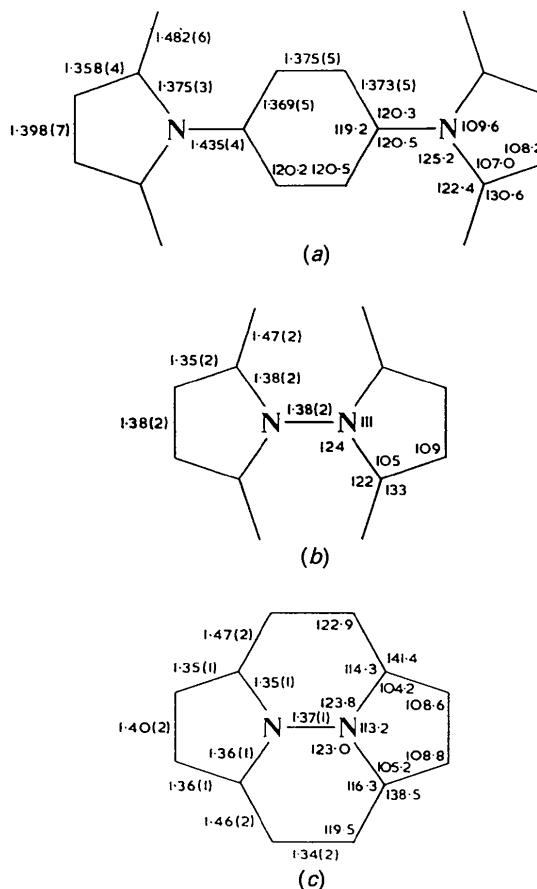


Fig. 2. Unique bond lengths (Å) and angles (°) for the C and N atoms are displayed for (I) and for (III), model A; those for (II) are the mean of three, four, or six independent values. The e.s.d.'s in the bond angles in (I) are 0.2° round N and 0.3–0.4° at C. In (II) they range from 0.8° for angles involving independent atoms to 1.9° for those involving symmetry-related atoms, and in (III) they range from 0.7° at N to 1.2° at C(5) and C(6).

complete molecules are in Fig. 4. To keep down the number of parameters the C and N atoms were refined isotropically and the H atoms included in calculated positions to give C—H = 0.96 Å and assigned a fixed isotropic *U* = 0.08 Å².

The coordinates are in Table 3 and the average values of the bond lengths and angles are displayed in Fig. 2(b). The individual bond lengths and angles, the coordinates of the H atoms, and the observed and calculated structure amplitudes have been deposited.*

Within experimental error in all three molecules the two constituent pyrrole groups are orthogonal. The angles between the normals to the five-membered rings are $89(1)^\circ$ for N(1) and N(1a), $88(1)^\circ$ for N(11) and N(11a) and $92(1)^\circ$ for N(21) and N(22). The average deviation of a methyl C atom from the plane of the corresponding pyrrole ring is $0.03(1) \text{ \AA}$, the largest $0.05(1) \text{ \AA}$ for C(26).

In the polar crystal the chains of molecules all run the same way as shown in Fig. 3. Along the chains

* See deposition footnote.

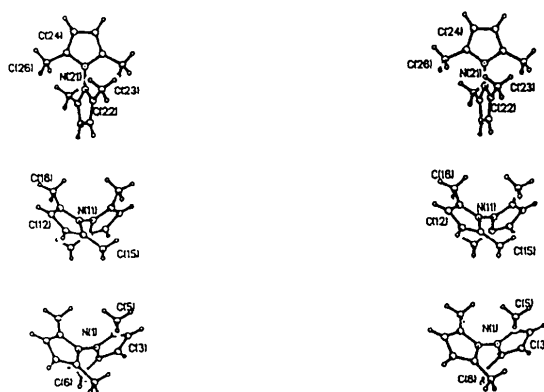


Fig. 3. A stereoview of the molecules of (II) lying at $0, y, 0$; the b axis is vertical, with the positive direction running down the page, and the view is down the a axis. The twofold axis passes through the centres of the N—N bonds of two molecules and along the N—N bond of the third.

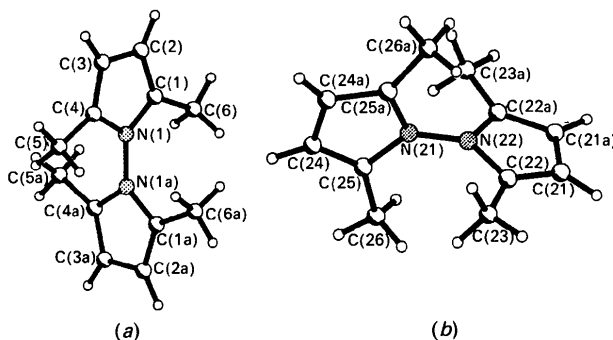


Fig. 4. (a) The designations of the atoms in one of the half molecules of the asymmetric unit (n), and the twofold axis related ones (na), the equivalent position (i) being $-x, y, -z$. The second molecule is similar with the designations ($1n$) for the asymmetric unit and ($1na$) in the other half. (b) The designations of the atoms in the molecule with the N—N bond along the twofold axis.

Table 3. Atomic coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) in (II)

	x	y	z	U_{iso}
N(1)	-342 (8)	8130	472 (7)	60 (3)
C(1)	-1295 (10)	8429 (6)	623 (11)	65 (4)
C(2)	-1708 (12)	8291 (7)	1659 (11)	78 (4)
C(3)	-1004 (10)	7893 (7)	2116 (11)	73 (4)
C(4)	-160 (10)	7800 (5)	1391 (10)	58 (3)
C(5)	823 (12)	7442 (8)	1447 (13)	103 (5)
C(6)	-1646 (12)	8822 (7)	-233 (12)	107 (6)
N(11)	461 (8)	4855 (4)	-365 (8)	63 (3)
C(11)	542 (10)	4566 (6)	-1326 (10)	62 (3)
C(12)	1565 (11)	4699 (7)	-1799 (11)	76 (4)
C(13)	2056 (11)	5084 (7)	-1109 (11)	76 (4)
C(14)	1389 (10)	5191 (6)	-222 (10)	59 (3)
C(15)	1511 (13)	5539 (8)	740 (13)	106 (5)
C(16)	-343 (11)	4180 (7)	-1643 (11)	98 (5)
N(21)	0	1220 (8)	0	66 (4)
N(22)	0	1763 (8)	0	68 (4)
C(21)	542 (11)	2581 (7)	206 (11)	81 (4)
C(22)	908 (11)	2078 (6)	338 (11)	70 (4)
C(23)	1980 (11)	1845 (7)	733 (11)	95 (5)
C(24)	196 (11)	405 (7)	-544 (11)	78 (4)
C(25)	304 (11)	914 (7)	-921 (11)	71 (4)
C(26)	711 (11)	1158 (7)	-1962 (10)	89 (5)

the shortest distance between molecules is 2.8 \AA for $\text{H}(21a)\cdots\text{H}(16b)$ while no $\text{C}\cdots\text{C}$ distance is less than 4.0 \AA . Each chain is surrounded by four others displaced by $b/2$, two at $\pm a/2$ which are in the same orientation and two at $\pm c/2$ which are twisted by the glide operation to reverse the direction along the c axis. The shortest corresponding $\text{C}\cdots\text{C}$ contacts are $3.57(2)$ and $3.74(2) \text{ \AA}$, and the shortest $\text{H}\cdots\text{H}$ contact is 3.0 \AA . The loose packing is reflected in the low density and ready volatility of the compound.

(III) The space group was determined unambiguously as $P2_1/a$ which, with $Z = 2$, requires a centre of symmetry in the molecule. Direct methods in *SHELXTL-Plus* (version 3.4; Sheldrick, 1987) revealed the C and N atoms. Refinement did not proceed at all smoothly because there is a conflict between the best fit to the electron density by crystallographic criteria and a chemically reasonable molecule. Four models were refined. In model *A* the C and N atoms were allowed anisotropic thermal displacement parameters, and the H atoms were in calculated positions to give $\text{C—H} = 0.96 \text{ \AA}$ and assigned a fixed isotropic displacement parameter $U = 0.08 \text{ \AA}^2$. With unit weights this gave $R = 0.087$ and the goodness of fit, $S = 0.83$. The corresponding molecule and the designations of the atoms are in Fig. 5. A refined weighting scheme, model *B*, led to higher R and S values, 0.092 and 3.05 , respectively. The coordinates for model *A* are in Table 4; the displacement parameters have been deposited.* The displacement parameters (Fig. 5) strongly suggest that the $-\text{CH}_2-\text{CH}_2-$ group is disordered, as do the short $\text{C}(5)-\text{C}(6a)$ bond length and large bond angles at C(5) and C(6) [Fig. 2(c)], and the torsion

* See deposition footnote.

Table 4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) in (III)

	x	y	z	U_{eq} *
N(1)	745 (8)	4785 (7)	739 (8)	52 (3)
C(1)	2316 (11)	4079 (10)	696 (14)	67 (4)
C(2)	3456 (12)	3890 (12)	2388 (15)	85 (5)
C(3)	2554 (12)	4511 (14)	3446 (13)	95 (5)
C(4)	839 (12)	5094 (11)	2397 (11)	71 (4)
C(5)	-857 (16)	5827 (19)	2481 (15)	157 (9)
C(6)	2319 (16)	3713 (17)	-1052 (16)	137 (8)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

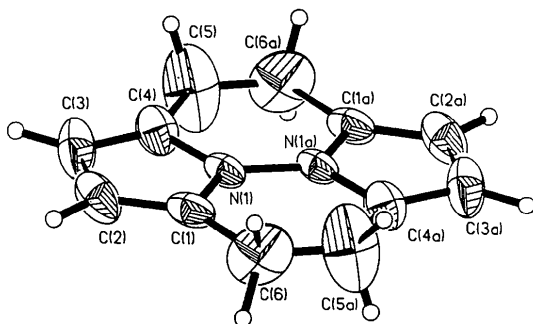


Fig. 5. One molecule of (III) with the thermal ellipsoids drawn at the 30% confidence level. The designations of the atoms and those related by a centre of symmetry are shown.

angle $C(4)-C(5)-C(6a)-C(1a)$ which is $5.5(2)$ instead of *ca* 60° . An electron density difference map with $C(5)$ and $C(6)$ omitted showed only one peak for each of these atoms. A model was calculated based on two isotropic half atoms $C(5)$ and $C(51)$, one on each side of the plane through $N(1)$, $C(1)$, $C(2)$, $C(3)$, $C(4)$ and at 1.5 \AA from $C(6a)$. Refinement with a weighting scheme, model *C*, and unit weights, model *D*, gave R values of 0.095 and 0.092 , respectively, and the corresponding S values of 2.68 and 0.94 . Although the isotropic thermal parameters for $C(5)$ and $C(51)$ refined satisfactorily to $0.082(7)$ and $0.073(6) \text{ \AA}^2$ in model *D*, the bond lengths to $C(6a)$ were $1.45(2)$ and $1.31(2) \text{ \AA}$ and the torsion angles 20 and $43(1)^\circ$, so the model was rejected. In all full-matrix least-squares refinements there were five correlation coefficients greater than 0.5 , so we must be content with an approximate structure. A table showing the bond lengths corresponding to the four models has been deposited* as have the observed and calculated structure factors for model *A*.

The ten atoms of the two five-membered rings are planar within 0.004 \AA . Deviations of $C(5)$ and $C(6)$ are $0.042(16)$ and $0.012(14) \text{ \AA}$, and disorder makes them appear nearly in the plane. On any model the CH_2 H atoms are out of the plane, as shown in the packing diagram (Fig. 6). Packing is in herringbone

* See deposition footnote.

fashion with an angle between the normals to the glide-related molecules of $52(1)^\circ$. The shortest contact is 2.58 \AA between $H(6A)$ and $N(1b)$ in the molecule at $\frac{1}{2} - x, -\frac{1}{2} + y, -z$.

Discussion. There is no significant difference in the dimensions of the pyrrole entities in the three structures, and the bond lengths within the five-membered rings are in good agreement with the mean values from over fifty structures in the *Cambridge Structural Database* (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987).

The $C_{sp^2}-C_{sp^3}$ bonds in (I) and (II) are all in the range $1.46-1.48 \text{ \AA}$, rather shorter than the average for such bonds, 1.502 \AA , (Allen *et al.*, 1987). Model *A* for (III) (Fig. 2), gives the same length whereas longer values resulted from model *D*. For (IV), Atwood *et al.* (1981) found all the peripheral bonds to be 1.40 \AA within 0.03 \AA , and all the atoms, including hydrogen, coplanar. Packing in (IV) is closer than in (III) giving a density of 1.41 Mg m^{-3} .

The $C(1)-N(1)$ bond in (I) is longer than that quoted by Allen *et al.* (1987) for $C_{ar}-N_{sp^2}$, $1.371(16) \text{ \AA}$, which is probably the average for coplanar aromatic and N_{sp^2} entities. In the *N*-(2,4-dinitrophenyl)-4-(1-pyrrolyl)pyridinium ion (Ferguson & McAlees, 1990) there are two $C_{ar}-N_{sp^2}$ bonds, one of $1.378(3)$ and the other $1.445(3) \text{ \AA}$, corresponding to coplanar and non-coplanar (dihedral angle 59.5°) entities. In (I) the dihedral angle is 90° suggesting that there is no delocalization of electrons between the pyrrole and benzene rings and that $1.435(5) \text{ \AA}$ is the length of a single bond.

The features of the molecular structure found in the crystals correlate well with the deductions from ESR measurements in solution (Avila & Davies,

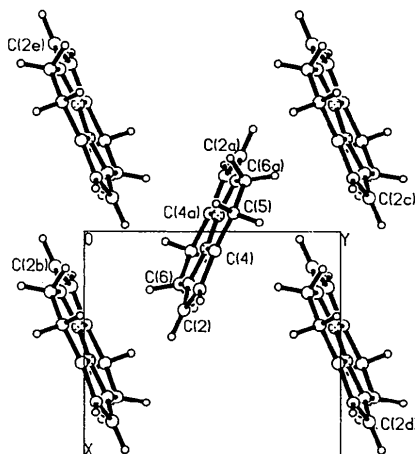


Fig. 6. Projection of the structure of (III) down the c axis. Some of the symmetry related atoms are labelled: the relations are (b) $\frac{1}{2} - x, -\frac{1}{2} + y, -z$; (c) $-\frac{1}{2} + x, \frac{3}{2} - y, z$; (d) $\frac{1}{2} + x, \frac{3}{2} - y, z$; (e) $-\frac{1}{2} - x, -\frac{1}{2} + y, -z$.

1990). No radical cation could be found for (III), this being attributed to the lability of an H atom out of the molecular plane whereas (IV) gave a radical cation with the electron delocalized over the whole molecule. For (II) also the electron of the radical cation was shared between the two halves of the molecule while in (I) it was isolated on one pyrrole entity.

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Structures Cristallines et Electroniques de Deux Dérivés de l'Oxaphénalène: les 2-Acétylet et 2-Méthoxycarbonyl-6-méthoxynaphto[1,8-*bc*]pyranes

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Abstract. 2-Methoxy-8-oxatricyclo[7.3.1.0^{5,13}]trideca-1(13),2,4,6,9,11-hexen-7-yl methyl ketone, C₁₅H₁₂O₃ (I), $M_r = 240.3$, orthorhombic, $P2_12_1$, $a = 6.893$ (1), $b = 11.108$ (1), $c = 15.320$ (3) Å, $V = 1173$ Å³, $Z = 4$, $D_x = 1.361$ Mg m⁻³, $\lambda(\text{Cu } K\alpha) = 1.54178$ Å, $\mu = 0.684$ mm⁻¹, $F(000) = 504$, $T = 298$ K, $R = 0.041$ for 1158 observed reflections. 2-Methoxy-8-oxatricyclo[7.3.1.0^{5,13}]trideca-1(13),2,4,6,9,11-hexene-7-carboxylic acid methyl ester, C₁₅H₁₂O₄, (II), $M_r = 256.3$, monoclinic, $P2_1/n$, $a = 13.561$ (4), $b = 5.034$ (1), $c = 18.277$ (4) Å, $\beta = 104.42$ (3)°, $V = 1208$ Å³, $Z = 4$, $D_x = 1.409$ Mg m⁻³, $\lambda(\text{Cu } K\alpha) = 1.54178$ Å, $\mu = 0.86$ mm⁻¹, $F(000) = 536$, $T = 298$ K, $R = 0.034$ for the 1301 observed reflections. The oxaphenylene nuclei of (I) and (II) are quasi-planar and the double bond between C(2) and C(3) showed a greater ethylenic character than that observed in the 2-nitronaphthofuran series.

Introduction. Parmi les substances les plus génotoxiques actuellement connues figurent certains dérivés des arénofurannes et particulièrement des 2-nitronaphto[2,1-*b*]furannes (Royer & Buisson, 1986;

Ajana, Bideau, Cotrait, Buisson, Demerseman, Einhorn & Royer, 1988).

Il a été montré que des 2-nitro oxaphénalènes, méthoxylés ou non, possèdent également un très haut pouvoir génotoxique (Royer, Buisson, Vlemineckx & Moens, 1986). Ces oxaphénalènes substitués en 2 dérivent d'un squelette qui possède certaines analogies avec celui des aréno-furannes déjà évoqués. Au cours des études spectroscopiques dont ils ont fait l'objet (Platzer, Buisson & Demerseman, 1991), il est apparu en RMN du proton, des déplacements chimiques assez surprenants de certains signaux caractéristiques de ces molécules, qui impliquent des distributions perturbées. C'est afin de pouvoir établir des relations structure-activité comparatives entre les deux séries naphthofurannique et oxaphénalique que nous avons entrepris une étude structurale radiocristallographique et électronique de deux représentants de cette dernière série: le 2-acétylet-6-méthoxynaphto[1,8-*bc*]pyrane (I) et le 2-méthoxycarbonyl-6-méthoxynaphto[1,8-*bc*]pyrane (II).

Les dérivés nitrés en position 2, avec un groupement nitro à la place des groupements 2-acétylet (I) et