

Study of Short Hydrogen Bonds. IV.* Structures of Dimorphs of 2-Methylpiperidinium Hydrogen Bis(*p*-chlorobenzoate)

BY SHINTARO MISAKI, SETSUO KASHINO† AND MASAO HAISA

Department of Chemistry, Faculty of Science, Okayama University, Tsushima, Okayama 700, Japan

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Abstract. 2-Methylpiperidinium hydrogen bis(*p*-chlorobenzoate), $C_6H_{14}N^+ \cdot C_{14}H_9Cl_2O_4^-$, $M_r = 412.29$. Form 1, monoclinic, $C2/c$, $a = 21.746$ (3), $b = 8.404$ (3), $c = 23.777$ (3) Å, $\beta = 110.84$ (1)°, $V = 4061$ (2) Å³, $Z = 8$, $D_x = 1.349$ Mg m⁻³, $\mu = 3.13$ mm⁻¹, $F(000) = 1728$, final $R = 0.055$ for 2363 reflections with $|F_o|$ larger than $3\sigma(F_o)$; Form 2, monoclinic, $C2/c$, $a = 19.084$ (4), $b = 9.689$ (3), $c = 11.465$ (4) Å, $\beta = 90.56$ (2)°, $V = 2120$ (1) Å³, $Z = 4$, $D_x = 1.292$ Mg m⁻³, $\mu = 3.00$ mm⁻¹, $F(000) = 864$, final $R = 0.081$ for 975 reflections with $|F_o|$ larger than $3\sigma(F_o)$. $Cu K\alpha$, $\lambda = 1.54178$ Å, $T = 295$ K. In the crystal of Form 1 the 2-methylpiperidinium cation and hydrogen bis(*p*-chlorobenzoate) anion occupy general positions. The anion is composed of neutral and ionized benzoate residues which are held together through an asymmetric O—H \cdots O hydrogen bond of O \cdots O 2.469 (3) Å. In Form 2 the cation is disordered around a twofold axis, and the benzoate residues in the anion are linked by a short crystallographically symmetric O \cdots H \cdots O hydrogen bond of O \cdots O 2.437 (9) Å.

Introduction. As part of a study on short hydrogen bonds (Misaki, Kashino & Haisa, 1986, 1989*a,b*), the relationship between the symmetry of the hydrogen bond and the crystal structure is examined in the dimorphic structures of 2-methylpiperidinium hydrogen bis(*p*-chlorobenzoate).

Experimental. Experimental details are listed in Table 1. Crystals of Forms 1 and 2 were grown in the same batch by slow evaporation from a xylene solution. The intensities were collected on a Rigaku AFC-5 four-circle diffractometer equipped with a rotating anode with ω - 2θ -scan method [scan speed 4° min⁻¹ in ω , scan range (1.2 + 0.15 tan θ)° in ω , Ni-filtered $Cu K\alpha$ ($\lambda = 1.54178$ Å) at 40 kV, 200 mA]. Background was measured for 4 s on either side of peak. Three standard reflections were recorded after every 97 reflections. Lorentz and polarization corrections were applied, but no absorp-

tion correction. Non-zero reflections within $2\theta_{max}$ were used for the refinements.

The structure of Form 1 was solved by *MULTAN78*, and refined by block-diagonal least-squares method. The value minimized was $\sum w(|F_o| - |F_c|)^2$, where $w = 1/[\sigma(F_o)^2 + 0.0367|F_o| + 0.0016|F_o|^2]$. All the H atoms were located on a difference Fourier map. The non-H atoms were refined anisotropically and the H atoms isotropically. Correction for the secondary-extinction effect was applied for the strongest five reflections [$I_{corr} = I_o(1 + 8.11 \times 10^{-5}I_o)$].

The structure of Form 2 was solved by *MULTAN78*. The non-H atoms of the cation were found by successive Fourier and difference syntheses. The cation was disordered around a twofold axis. The structure was refined by full-matrix least-squares method. All the non-H atoms were refined anisotropically. The value minimized was $\sum w(|F_o| - |F_c|)^2$ with $w = 1/\sigma(F_o)^2$. The conformation, bond lengths and bond angles involving the non-H atoms, of the cation were restrained to the same values as those in Form 1. The positional parameters of the H atoms attached to the cation ring were calculated by assuming a usual geometry and were fixed; their thermal parameters were assumed to be identical with B_{sq} of the non-H atoms to which they were attached. The H atoms of the methyl group were not included in the refinement. The positional parameters of the H atoms attached to the phenylene ring were calculated by assuming a usual geometry and were fixed; only their thermal parameters were refined isotropically. The H atom participating in the O \cdots H \cdots O hydrogen bond was located at $\bar{1}$ on a difference Fourier map, and the position was fixed at $\bar{1}$ and the B_{iso} was refined.

The atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Programs used: *MULTAN78* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *RSSFR-5* (Sakurai, 1967), *HBL5* and *DAPH* (Ashida, 1973), modified version of *CRLS* (Takusagawa, 1982), *MOLCON* (Fujii, 1979) and *ORTEP* (Johnson, 1971). Computations were carried out at Okayama University Computer Center.

* Part III: Misaki, Kashino & Haisa (1989*b*).

† To whom correspondence should be addressed.

Table 1. *Experimental details*

Morphology	Form 1	Form 2
	Plate developed (101)	Prismatic <i>c</i>
Size of specimen (mm)	0.28 × 0.38 × 0.18	0.15 × 0.13 × 0.35
Range of 2θ (20 reflections) for lattice parameters (°)	19 to 36	10 to 37
Systematic absences	<i>h</i> + <i>l</i> odd for <i>hkl</i> <i>l</i> odd for <i>h0l</i> <i>k</i> odd for <i>0k0</i>	<i>h</i> + <i>l</i> odd for <i>hkl</i> <i>l</i> odd for <i>h0l</i> <i>k</i> odd for <i>0k0</i>
2θ _{max} (°)	125	125
<i>h</i> range	0 to 24	-21 to 21
<i>k</i> range	0 to 9	0 to 11
<i>l</i> range	-27 to 27	0 to 13
Fluctuation of standard reflections (%)	1.4	1.6
No. of unique reflections	3240	1687
No. of non-zero reflections	2949	1419
No. of reflections with <i>F</i> _o > 3σ(<i>F</i> _o)	2363	975
<i>R</i> / <i>wR</i> for non-zero reflections	0.072/0.071	0.110/0.082
<i>R</i> for reflections with <i>F</i> _o > 3σ(<i>F</i> _o)	0.055	0.081
<i>S</i>	1.23	1.46
(Δ/ <i>σ</i>) _{max} for non-H/H atoms	0.17/0.53	0.29/0.84
Δρ _{max} /Δρ _{min} (e Å ⁻³)	0.34/-0.27	0.30/-0.29

Table 2. *Final atomic coordinates and equivalent isotropic thermal parameters (Å²) with e.s.d.'s in parentheses*

$$B_{eq} = \frac{1}{3} \sum_i \beta_{ii} / a_i^2$$

	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq}
Form 1				
C(1)	0.1353 (1)	0.0485 (4)	0.0593 (1)	3.5 (1)
C(2)	0.1879 (2)	0.0418 (5)	0.0402 (1)	5.3 (2)
C(3)	0.1831 (2)	0.1065 (5)	-0.0151 (2)	5.9 (2)
C(4)	0.1261 (2)	0.1729 (4)	-0.0505 (1)	4.7 (2)
C(5)	0.0722 (2)	0.1796 (5)	-0.0330 (1)	5.6 (2)
C(6)	0.0777 (1)	0.1165 (4)	0.0227 (1)	4.7 (2)
C(7)	0.1438 (1)	-0.0127 (4)	0.1210 (1)	3.6 (1)
Cl(8)	0.12082 (6)	0.2549 (1)	-0.11894 (4)	7.39 (6)
O(9)	0.1954 (1)	-0.0661 (3)	0.15440 (9)	4.9 (1)
O(10)	0.09091 (9)	0.0021 (3)	0.13463 (8)	4.4 (1)
C(11)	0.1236 (1)	0.1725 (3)	0.3267 (1)	3.5 (1)
C(12)	0.0643 (1)	0.1358 (4)	0.3332 (1)	4.1 (1)
C(13)	0.0509 (1)	0.1911 (4)	0.3826 (1)	4.7 (2)
C(14)	0.0967 (2)	0.2811 (4)	0.4248 (1)	4.7 (2)
C(15)	0.1564 (2)	0.3149 (5)	0.4203 (2)	5.6 (2)
C(16)	0.1695 (2)	0.2610 (4)	0.3701 (1)	4.8 (2)
C(17)	0.1375 (1)	0.1159 (4)	0.2722 (1)	3.5 (1)
Cl(18)	0.07954 (5)	0.3532 (1)	0.48641 (4)	7.11 (6)
O(19)	0.18385 (9)	0.1792 (3)	0.26050 (9)	4.2 (1)
O(20)	0.1010 (1)	0.0065 (3)	0.24139 (8)	4.6 (1)
N(21)	0.3007 (1)	0.0050 (3)	0.2697 (1)	3.6 (1)
C(22)	0.3287 (2)	0.0100 (4)	0.3373 (1)	4.1 (1)
C(23)	0.4003 (2)	-0.0351 (4)	0.3583 (1)	4.6 (2)
C(24)	0.4392 (2)	0.0710 (4)	0.3315 (2)	4.9 (2)
C(25)	0.4091 (2)	0.0715 (4)	0.2635 (1)	5.3 (2)
C(26)	0.3375 (2)	0.1131 (4)	0.2421 (1)	4.6 (2)
C(27)	0.2879 (2)	-0.0984 (5)	0.3614 (2)	5.5 (2)
Form 2				
C(1)	0.1251 (3)	-0.1942 (5)	0.3671 (5)	5.8 (2)
C(2)	0.1754 (3)	-0.2889 (7)	0.4001 (5)	6.9 (3)
C(3)	0.2161 (3)	-0.3559 (7)	0.3170 (7)	8.2 (4)
C(4)	0.2034 (3)	-0.3277 (8)	0.2000 (6)	7.9 (3)
C(5)	0.1539 (3)	-0.2315 (8)	0.1645 (5)	7.9 (4)
C(6)	0.1151 (3)	-0.1669 (6)	0.2487 (5)	6.8 (3)
C(7)	0.0819 (3)	-0.1288 (6)	0.4587 (5)	6.9 (3)
Cl(8)	0.2506 (1)	-0.4191 (3)	0.0948 (2)	11.7 (2)
O(9)	0.0908 (3)	-0.1550 (6)	0.5624 (4)	9.8 (3)
O(10)	0.0353 (2)	-0.0443 (5)	0.4203 (4)	8.0 (2)
N(11)*	0.003 (2)	0.2150 (9)	0.260 (4)	6.7 (7)
C(12)*	-0.0340 (9)	0.331 (2)	0.199 (1)	9.5 (9)
C(13)*	-0.042 (1)	0.451 (2)	0.282 (2)	13 (1)
C(14)*	0.0286 (9)	0.498 (2)	0.330 (2)	12 (1)
C(15)*	0.067 (1)	0.380 (2)	0.387 (2)	16 (2)
C(16)*	0.0740 (7)	0.259 (2)	0.307 (1)	9.6 (9)
C(17)*	-0.103 (1)	0.278 (2)	0.151 (1)	11 (1)

* Occupancy factor was assumed to be 0.5.

Discussion. The final atomic parameters for Forms 1 and 2 are listed in Table 2.* The thermal ellipsoids of the molecules are shown in Fig. 1 with atomic numbering. Bond lengths and angles are listed in Table 3. Stereoviews of the crystal structures are shown in Fig. 2.

In Form 1, O(10) and O(20) in the anion are linked by an asymmetric O—H...O hydrogen bond [O(10)...O(20) 2.469 (3), O(10)—H(10) 1.12 (6), H(10)...O(20) 1.37 (6) Å, O(10)—H(10)...O(20) 164 (5)°]. O(19) accepts hydrogen bonds from N(21) [O(10)...N(21) 2.873 (3), O(19)...H(21*B*) 2.01 (3) Å, O(19)...H(21*B*)—N(21) 147 (3)°] and N(21) ($\frac{1}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$) [O(19)...N(21) 2.880 (3), O(19)...H(21*A*) 1.91 (4) Å, O(19)...H(21*A*)—N(21) 172 (4)°] to form a ribbon along a twofold screw axis. The ribbons related by a center of symmetry at ($\frac{1}{4}, \frac{1}{4}, 0$) form a sheet parallel to (400) by van der Waals interactions. The sheets related by a twofold axis are stacked along *a* to form the *C2/c* structure. The modes of formation of the ribbon and the sheet are the same as those in

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, and bond lengths and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51955 (32 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

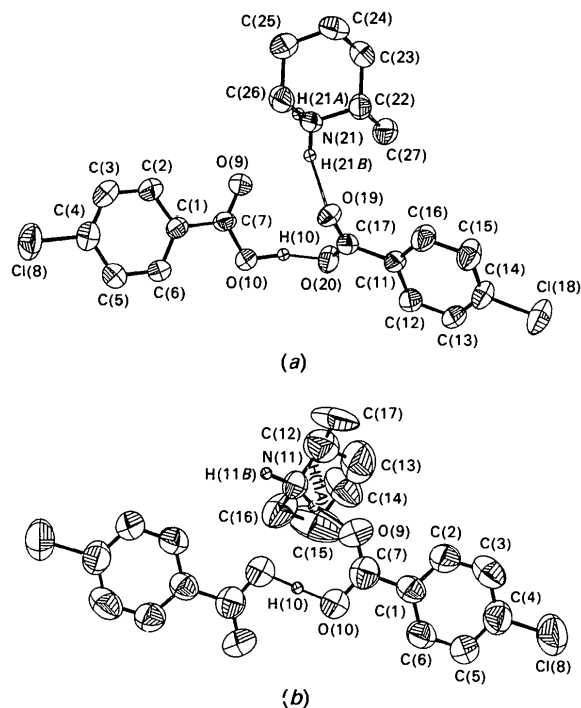


Fig. 1. The thermal ellipsoids (50% probability) with atomic numbering. The H atoms attached to the O and N atoms are represented as spheres equivalent to $B = 1.0 \text{ \AA}^2$. (a) Form 1. (b) Form 2. The disordered cation is omitted.

Table 3. Bond lengths (Å) and angles (°) with *e.s.d.*'s in parentheses

Form 1			
C(1)—C(2)	1.374 (5)	C(15)—C(16)	1.397 (5)
C(2)—C(3)	1.392 (6)	C(16)—C(11)	1.372 (5)
C(3)—C(4)	1.347 (5)	C(14)—C(18)	1.744 (4)
C(4)—C(5)	1.377 (6)	C(11)—C(17)	1.508 (4)
C(5)—C(6)	1.392 (6)	C(17)—O(19)	1.255 (4)
C(6)—C(1)	1.370 (5)	C(17)—O(20)	1.264 (4)
C(4)—Cl(8)	1.733 (4)	N(21)—C(22)	1.503 (4)
C(1)—C(7)	1.503 (4)	C(22)—C(23)	1.505 (5)
C(7)—O(9)	1.207 (4)	C(23)—C(24)	1.517 (5)
C(7)—O(10)	1.307 (4)	C(24)—C(25)	1.513 (5)
C(11)—C(12)	1.387 (4)	C(25)—C(26)	1.497 (5)
C(12)—C(13)	1.387 (5)	C(26)—N(21)	1.507 (4)
C(13)—C(14)	1.364 (5)	C(22)—C(27)	1.519 (5)
C(14)—C(15)	1.370 (5)		
C(6)—C(1)—C(2)	119.2 (3)	C(14)—C(15)—C(16)	119.1 (4)
C(1)—C(2)—C(3)	120.3 (3)	C(15)—C(16)—C(11)	120.2 (3)
C(2)—C(3)—C(4)	119.7 (4)	C(13)—C(14)—C(18)	119.5 (3)
C(3)—C(4)—C(5)	121.4 (4)	C(15)—C(14)—C(18)	119.0 (3)
C(4)—C(5)—C(6)	118.5 (4)	C(12)—C(11)—C(17)	120.3 (3)
C(5)—C(6)—C(1)	120.9 (3)	C(16)—C(11)—C(17)	120.2 (3)
C(3)—C(4)—Cl(8)	119.4 (3)	C(11)—C(17)—O(19)	118.6 (3)
C(5)—C(4)—Cl(8)	119.2 (3)	C(11)—C(17)—O(20)	116.8 (3)
C(2)—C(1)—C(7)	118.8 (3)	O(19)—C(17)—O(20)	124.6 (3)
C(6)—C(1)—C(7)	122.0 (3)	C(26)—N(21)—C(22)	111.9 (2)
C(1)—C(7)—O(9)	122.2 (3)	N(21)—C(22)—C(23)	109.0 (3)
C(1)—C(7)—O(10)	113.3 (3)	C(22)—C(23)—C(24)	112.2 (3)
O(9)—C(7)—O(10)	124.5 (3)	C(23)—C(24)—C(25)	110.9 (3)
C(16)—C(11)—C(12)	119.6 (3)	C(24)—C(25)—C(26)	111.5 (3)
C(11)—C(12)—C(13)	120.2 (3)	C(25)—C(26)—N(21)	111.1 (3)
C(12)—C(13)—C(14)	119.4 (4)	N(21)—C(22)—C(27)	108.5 (3)
C(13)—C(14)—C(15)	121.5 (3)	C(23)—C(22)—C(27)	113.5 (3)
Form 2 (bond lengths and angles for the cation are omitted because their values were restrained)			
C(1)—C(2)	1.378 (9)	C(6)—C(1)	1.394 (8)
C(2)—C(3)	1.40 (1)	C(4)—Cl(8)	1.753 (8)
C(3)—C(4)	1.39 (1)	C(1)—C(7)	1.484 (8)
C(4)—C(5)	1.39 (1)	C(7)—O(9)	1.226 (9)
C(5)—C(6)	1.37 (1)	C(7)—O(10)	1.283 (8)
C(6)—C(1)—C(2)	118.8 (5)	C(5)—C(4)—Cl(8)	119.4 (6)
C(1)—C(2)—C(3)	120.9 (6)	C(2)—C(1)—C(7)	118.7 (5)
C(2)—C(3)—C(4)	118.4 (7)	C(6)—C(1)—C(7)	122.4 (5)
C(3)—C(4)—C(5)	121.9 (7)	C(1)—C(7)—O(9)	121.7 (6)
C(4)—C(5)—C(6)	118.1 (7)	C(1)—C(7)—O(10)	114.7 (5)
C(5)—C(6)—C(1)	121.9 (6)	O(9)—C(7)—O(10)	123.6 (6)
C(3)—C(4)—Cl(8)	118.7 (6)		

4-methylpiperidinium hydrogen bis(*p*-methylbenzoate) (Misaki, Kashino & Haisa, 1986). However, the mode of the stacking of the sheets is different because of the difference in packing of the methyl groups of the cations. The piperidinium ring takes a chair conformation. N(21) and C(24) deviate by -0.667 (4) and 0.648 (5) Å, respectively, from the plane through C(22), C(23), C(25) and C(26). The methyl group is equatorially bonded to the ring: the torsion angles are $C(26)-N(21)-C(22)-C(27) = 178.6$ (3) and $C(24)-C(23)-C(22)-C(27) = 177.7$ (3)°.

The structure of Form 2 is disordered around a twofold axis. The center of the hydrogen bis(*p*-chlorobenzoate) anion lies on a $\bar{1}$ at (0,0,0). Keeping the $\bar{1}$ symmetry of the anion, the disordered structure would be reduced to one of the maximal subgroup $P\bar{1}$ by eliminating the twofold axis. The O...H...O hydrogen bond in the anion is crystallographically symmetric. The anions are linked through the N—H...O hydrogen bonds to form a chain along *c*

[N(11)...O(9) ($-x, -y, 1-z$) 2.79 (4), H(11A)...O(9) 1.74 Å, N(11)—H(11A)...O(9) 165°; N(11)...O(9) ($x, -y, -\frac{1}{2}+z$) 2.89 (4), H(11B)...O(9) 2.21 Å, N(11)—H(11B)...O(9) 119°]. A similar chain has been found in piperidinium hydrogen bis(*p*-bromobenzoate) ($P\bar{1}$, $Z = 2$) (Misaki, Kashino & Haisa, 1989a), in which the H atoms attached equatorially to the 2 and 6 positions of the piperidinium cation and the O atoms of the two nearest anions make contact with normal van der Waals distances and the dihedral angle between the anions is 14.7 (2)°. However, in Form 2 the corresponding dihedral angle is 85.8 (3)° to avoid unreasonable contacts between the 2-methyl group of the cation and O(10) of the nearest anion. The chains related by a center of symmetry at $(0, \frac{1}{2}, \frac{1}{2})$ form a sheet by disordering. The sheets related by a twofold screw axis are stacked along *a* to complete the whole structure. The mode of formation of the sheet is also similar to that in piperidinium hydrogen bis(*p*-bromobenzoate), but the mode of the stacking of the sheets is different because of the difference in the dihedral angles between the anions.

In Forms 1 and 2 the anions are arranged side by side along *a* and stacked along *b*, and the long axes of the anions are parallel to *c* in Form 1 and $[102]$ in Form 2. Thus, the cell dimensions of *a* and *b* of

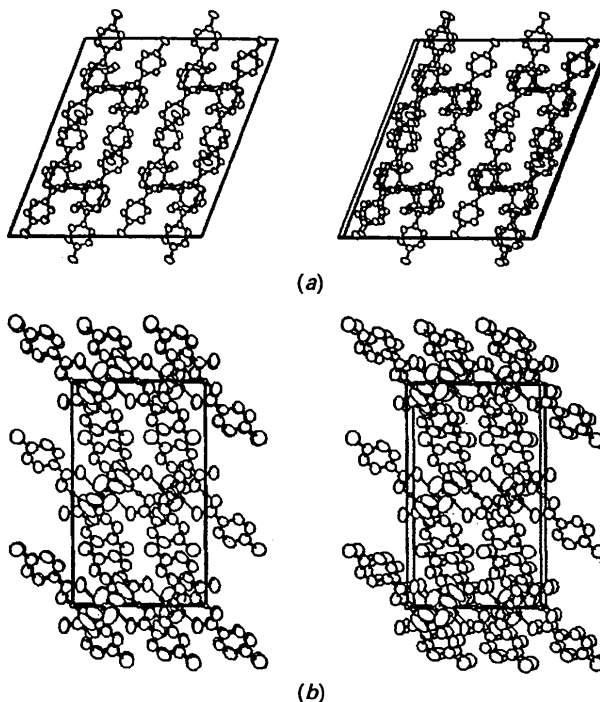


Fig. 2. Stereoscopic views of the crystal structures. The H atoms attached to the C atoms are omitted. (a) Form 1. The *a* axis points from left to right, the *b* axis downwards and the *c* axis onto the plane of the paper. (b) Form 2. The *a* axis points upwards, the *b* axis left to right and the *c* axis onto the plane of the paper. The disordered cation is included.

Form 1 are close to a and b respectively, of Form 2, and the direction of the c axis of Form 1 corresponds to that of $[\bar{1}02]$ of Form 2.

The O...O distance of the O...H...O hydrogen bond in Form 2 is significantly shorter than that in Form 1. The hydrogen bis(*p*-chlorobenzoate) anion in Form 2 has symmetric environments, while the same anion in Form 1 has asymmetric environments. Such a shortening of the O...O distance in symmetric environments has been seen for the same hydrogen bis(*p*-methylbenzoate) anion in environments of different symmetry (Misaki, Kashino & Haisa, 1989*b*). This fact is an indication that symmetric environments around the anion are suitable for decreasing the O...O distance. Observations of the asymmetric O—H...O hydrogen bonds show that the O—H bond lengthens as the O...O distance decreases (Misaki, Kashino & Haisa, 1986). Thus, it can be estimated that the O—H length in Form 2 is longer than the 1.12 (6) Å in Form 1. This means that the position of the H atom is within 0.1 Å of the center of the hydrogen bond. This is the reason why the peak of the H atom in a difference Fourier map appeared at the center of the hydrogen bond. The spacing between the planes of the O—C—O groups participating in the hydrogen bond is 0.121 (9) Å and the KKM effect was not observed (Misaki, Kashino & Haisa, 1989*a*).

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Structures of (*E*)-9-Styrylacridine and (*Z*)-9-(2,5-Dimethylstyryl)acridine

BY PAOLO SGARABOTTO* AND FRANCO UGOZZOLI

Istituto di Strutturistica Chimica, Università degli Studi di Parma,

Centro di Studio per la Strutturistica Diffraattometrica del CNR, Viale delle Scienze, I-43100 Parma, Italy

AND SALVATORE SORRISO

Dipartimento di Chimica, Università di Perugia, I-06100 Perugia, Italy

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Abstract. (*E*)-9-Styrylacridine, $C_{21}H_{15}N$, $M_r = 281.4$, triclinic, $P\bar{1}$, $a = 12.363$ (4), $b = 8.386$ (3), $c = 8.482$ (3) Å, $\alpha = 77.0$ (1), $\beta = 121.0$ (1), $\gamma = 96.9$ (1)°, $V = 734.5$ (9) Å³, $Z = 2$, $D_x = 1.27$ g cm⁻³, $Cu K\alpha$, $\lambda = 1.5418$ Å, $\mu = 5.3$ cm⁻¹, $F(000) = 296$, $T = 293$ K, final conventional $R = 0.038$ for 1346 symmetry-independent observed reflections. (*Z*)-9-(2,5-Dimethylstyryl)acridine, $C_{23}H_{19}N$, $M_r = 309.4$, triclinic,

$P\bar{1}$, $a = 11.905$ (4), $b = 8.955$ (3), $c = 8.429$ (3) Å, $\alpha = 99.5$ (1), $\beta = 73.3$ (1), $\gamma = 92.8$ (1)°, $V = 848.9$ (7) Å³, $Z = 2$, $D_x = 1.21$ g cm⁻³, $Cu K\alpha$, $\lambda = 1.5418$ Å, $\mu = 5.0$ cm⁻¹, $F(000) = 328$, $T = 293$ K, final conventional $R = 0.052$ for 2423 symmetry-independent observed reflections. The conformational geometry of the acridine moiety is similar in the two compounds and is characterized by the presence of an approximate mirror plane along the N(1)–C(8) line and of a good degree of planarity for the three-condensed-rings system.

* To whom correspondence should be addressed.