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Two Substituted Pyrazolo[1′,2′:1,2]pyrazolo[4,3-*d*]tetrazolo[1,5-*b*]pyridazines

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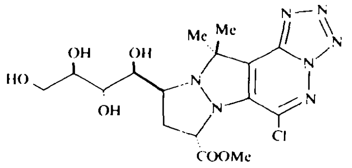
Abstract

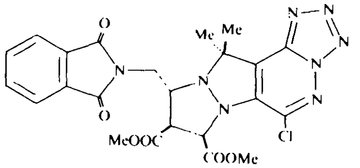
The compound methyl (1′*S*,8*S*,10*S*)-6-chloro-9,10-dihydro-12,12-dimethyl-10-(D-erythritol-1-yl)-8*H*,12*H*-pyrazolo[1′,2′:1,2]pyrazolo[4,3-*d*]tetrazolo-[1,5-*b*]pyridazine-8-carboxylate, $C_{16}H_{22}ClN_7O_6$ (I), is an example of a new C-nucleoside. Both (I) and dimethyl (6-chloro-9,10-dihydro-12,12-dimethyl-10-phthalimidomethyl-8*H*,12*H*-pyrazolo[1′,2′:1,2]pyrazolo[4,3-*d*]tetrazolo[1,5-*b*]pyridazine-8,9-dicarboxylate, $C_{23}H_{21}ClN_8O_6$, (II), contain heterocyclic systems consisting of four condensed fused rings. In each compound, the tetrazole ring is planar to within experimental error; the pyridazine ring and the pyrazole ring, which is fused to the pyridazine ring, deviate slightly from planarity, as does the phthalimido group of (II).

Comment

(I) was obtained by 1,3-dipolar cycloaddition of 2-diazopropane to 6-chorotetrazolo[1,5-*b*]pyridazine. This is highly regiospecific and proceeds as a cycloaddition across the partially localized C(7)=C(8) double bond of the pyridazine ring. Rearrangement of two H atoms produced NH—NH dihydro intermediates, which were then used for the regioselective synthesis of a C-nucleoside, employing D-ribose as a carbonyl reagent. The product was then converted with methyl acrylate into (I) (Žličar, Stanovnik & Tišler, 1992). The synthesis of (II) was analogous, with two exceptions: phthalimidoacetaldehyde was used as the carbonyl reagent and, instead of methyl acrylate, dimethyl maleate was employed. Views of the molecules with atomic numbering and of the molecular packing are presented in Figs. 1, 2, 3 and 4.



(I)



(II)

Although azolopyridazines with bridgehead N atoms are generally considered to be fully aromatic ten-π-electron systems, some reactions have indicated that these compounds have two localized double bonds (Golič, Leban, Stanovnik & Tišler, 1978). The double-bond character of these two bonds is also indicated by the bond lengths N(5)—C(1) [1.301 (3) in (I) and 1.303 (2) Å in (II)] and C(2)—C(7) [1.358 (2) Å in (II)]; the C(2)—C(7) bond in (I) [1.372 (3) Å] is slightly larger. The tetrazole unit is planar to within 0.004 (3) Å in (I) and 0.006 (4) Å in (II). The pyridazine unit deviates from planarity. The largest deviation is 0.020 (3) Å for C(8) in (I) and −0.013 (2) Å for C(2) in (II). The dihedral angles between tetrazole and pyridazine planes are 2.13 (8) in (I) and 1.2 (1)° in (II). The pyrazole ring that is fused to the pyridazine ring also deviates from planarity. The largest deviation in (I) is −0.050 (2) Å for C(7) and in (II) −0.075 (2) Å for C(6). The fact that Hückel's rule cannot be fulfilled indicates that this ring does not have aromatic character. The dihedral angles between the pyrazole and pyridazine ring planes are 4.87 (8) in (I) and 2.97 (7)° in (II). The dihedral angles between the best planes for both pyrazole rings are 34.29 (8) in (I) and 33.35 (6)° in (II). The remaining bond lengths and angles are within the normal ranges for such heterocyclic systems (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987; Golič *et al.*, 1978; Leban, Golič, Stanovnik & Tišler, 1987). The phenyl C atoms of the phthalimido group of (II) are coplanar to within 0.003 (3) Å. The whole phthalimido group deviates from planarity. The largest deviation is 0.031 (2) Å for O(5). The bond lengths and angles of groups bonded to the rings are within the normal ranges (Allen *et al.*, 1987). Methoxycarbonyl groups are bonded to the ring system on the side opposite to the phthalimidomethyl or erythritol group. This cor-

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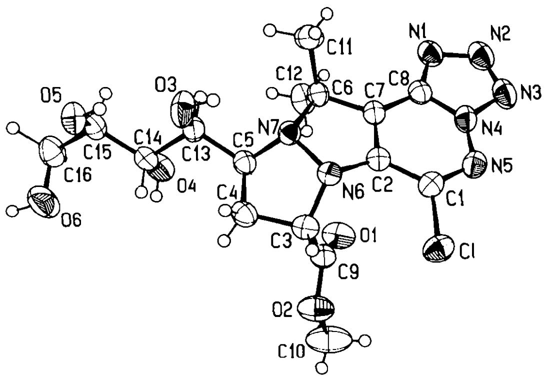

Fig. 1. *ORTEP* (Johnson, 1965) view of molecule (I), showing the labelling of the non-H atoms. Thermal ellipsoids are shown at 50% probability levels; H atoms are drawn as small circles of arbitrary size.

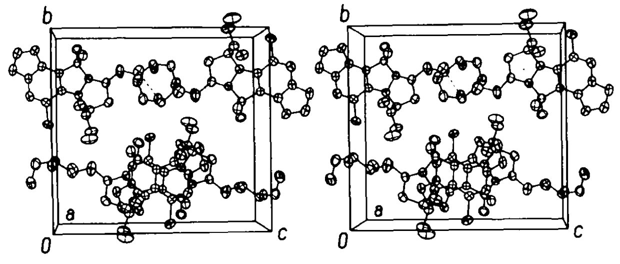

Fig. 2. Stereoview of the molecular packing in (I).

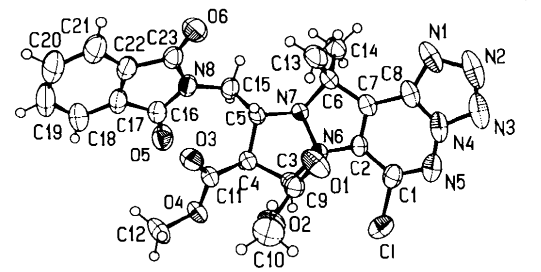

Fig. 3. View of molecule (II), showing the labelling of the non-H atoms. Thermal ellipsoids are shown at 50% probability levels, H atoms are drawn as small circles of arbitrary size.

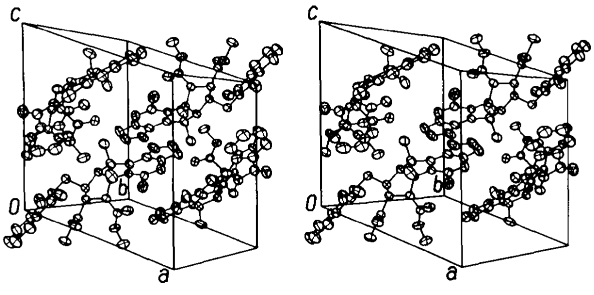

Fig. 4. Stereoview of the molecular packing in (II).

responds to minor steric hindrance among these groups. An intermolecular hydrogen bond exists in (I) between O(4) and O(5), of length 2.796 (3) Å. In (II) there are no intermolecular contacts of significance; the shortest contact is 3.229 (2) Å between C(3) and O(4).

Experimental

Compound (I)

Crystal data

$C_{16}H_{22}ClN_7O_6$
$M_r = 443.5$
Orthorhombic
$P2_12_12_1$
$a = 9.3226\ (6)$ Å
$b = 14.301\ (1)$ Å
$c = 15.042\ (1)$ Å
$V = 2005.4\ (4)$ Å^3
$Z = 4$
$D_x = 1.470$ Mg m^{-3}
$D_m = 1.46\ (2)$ Mg m^{-3}
D_m measured by flotation

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 75 reflections
$\theta = 8-15°$
$\mu = 0.2356$ mm^{-1}
$T = 293\ (1)$ K
Prism
0.52 × 0.40 × 0.33 mm
Orange

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans [width $(0.7 + 0.3\tan\theta)°$]
Absorption correction: none
10338 measured reflections
2731 independent reflections
2100 observed reflections [$I > 2.5\sigma(I)$]

$R_{\rm int} = 0.015$
$\theta_{\rm max} = 27.9°$
$h = 0 \rightarrow 12$
$k = -18 \rightarrow 18$
$l = -19 \rightarrow 19$
3 standard reflections
frequency: 333 min
intensity variation: −1.39%

Refinement

Refinement on F
$R = 0.032$
$wR = 0.040$
$S = 0.584$
2287 reflections
271 parameters

H-atom parameters not refined
Empirical weighting scheme
$(\Delta/\sigma)_{\rm max} = 0.185$
$\Delta\rho_{\rm max} = 0.26$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.11$ e Å^{-3}

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (I)

$$U_{\rm eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Cl	0.13756 (7)	0.03714 (4)	0.53711 (4)	0.0517 (3)
O(1)	0.3870 (2)	0.1337 (1)	0.3794 (2)	0.056 (1)
O(2)	0.3127 (2)	−0.0036 (1)	0.3228 (2)	0.059 (1)
O(3)	−0.0477 (2)	0.3202 (2)	0.1782 (1)	0.059 (1)
O(4)	0.3094 (2)	0.3102 (2)	0.0890 (1)	0.057 (1)
O(5)	−0.0577 (2)	0.3370 (1)	0.0013 (1)	0.049 (1)
O(6)	0.1651 (3)	0.2478 (2)	−0.1004 (1)	0.076 (1)
N(1)	0.2553 (2)	0.4245 (1)	0.5956 (1)	0.046 (1)
N(2)	0.2811 (3)	0.4085 (2)	0.6826 (1)	0.054 (1)
N(3)	0.2617 (3)	0.3220 (2)	0.7052 (1)	0.053 (1)
N(4)	0.2215 (2)	0.2783 (1)	0.6292 (1)	0.042 (1)
N(5)	0.1984 (2)	0.1855 (1)	0.6255 (1)	0.045 (1)
N(6)	0.0945 (2)	0.1925 (1)	0.3880 (1)	0.036 (1)
N(7)	0.0950 (2)	0.2801 (1)	0.3347 (1)	0.035 (1)

C(1)	0.1623 (2)	0.1556 (1)	0.5470 (1)	0.039 (1)
C(2)	0.1458 (2)	0.2148 (1)	0.4706 (1)	0.036 (1)
C(3)	0.1405 (2)	0.1134 (1)	0.3327 (1)	0.039 (1)
C(4)	0.1253 (2)	0.1530 (2)	0.2383 (1)	0.045 (1)
C(5)	0.1647 (2)	0.2562 (2)	0.2496 (1)	0.039 (1)
C(6)	0.1582 (2)	0.3578 (1)	0.3910 (1)	0.035 (1)
C(7)	0.1738 (2)	0.3086 (1)	0.4787 (1)	0.035 (1)
C(8)	0.2169 (2)	0.3422 (2)	0.5625 (1)	0.037 (1)
C(9)	0.2954 (2)	0.0839 (1)	0.3490 (1)	0.041 (1)
C(10)	0.4540 (4)	−0.0429 (2)	0.3318 (4)	0.086 (2)
C(11)	0.0505 (3)	0.4384 (2)	0.3943 (2)	0.051 (1)
C(12)	0.3046 (3)	0.3944 (2)	0.3613 (2)	0.050 (1)
C(13)	0.1046 (2)	0.3213 (2)	0.1775 (1)	0.040 (1)
C(14)	0.1587 (2)	0.2946 (1)	0.0849 (1)	0.040 (1)
C(15)	0.0921 (3)	0.3560 (1)	0.0122 (1)	0.042 (1)
C(16)	0.1623 (4)	0.3415 (2)	−0.0773 (2)	0.059 (1)

Table 2. *Selected geometric parameters* (Å, °) *for* (I)

Cl—C(1)	1.716 (2)	N(6)—C(3)	1.468 (3)
O(1)—C(9)	1.202 (3)	N(7)—C(5)	1.476 (3)
O(2)—C(9)	1.322 (3)	N(7)—C(6)	1.516 (3)
O(2)—C(10)	1.438 (4)	C(1)—C(2)	1.436 (3)
O(3)—C(13)	1.420 (3)	C(2)—C(7)	1.372 (3)
O(4)—C(14)	1.424 (3)	C(3)—C(4)	1.536 (3)
O(5)—C(15)	1.432 (3)	C(3)—C(9)	1.524 (3)
O(6)—C(16)	1.385 (4)	C(4)—C(5)	1.530 (3)
N(1)—N(2)	1.349 (3)	C(5)—C(13)	1.535 (3)
N(1)—C(8)	1.327 (3)	C(6)—C(7)	1.502 (3)
N(2)—N(3)	1.295 (4)	C(6)—C(11)	1.530 (3)
N(3)—N(4)	1.355 (3)	C(6)—C(12)	1.529 (3)
N(4)—N(5)	1.346 (3)	C(7)—C(8)	1.407 (3)
N(4)—C(8)	1.359 (3)	C(13)—C(14)	1.530 (3)
N(5)—C(1)	1.301 (3)	C(14)—C(15)	1.533 (3)
N(6)—N(7)	1.486 (2)	C(15)—C(16)	1.512 (3)
N(6)—C(2)	1.369 (3)		
N(5)—C(1)—Cl	116.0 (2)	C(12)—C(6)—N(7)	115.8 (2)
O(2)—C(9)—O(1)	126.0 (2)	C(6)—C(7)—C(2)	111.1 (2)
C(10)—O(2)—C(9)	116.9 (2)	C(9)—C(3)—C(4)	109.7 (2)
C(5)—C(13)—O(3)	110.7 (2)	C(13)—C(5)—C(4)	114.7 (2)
C(13)—C(14)—O(4)	104.3 (2)	C(11)—C(6)—C(7)	112.8 (2)
C(14)—C(15)—O(5)	111.6 (2)	C(8)—C(7)—C(6)	130.8 (2)
C(15)—C(16)—O(6)	111.4 (2)	C(15)—C(14)—C(13)	111.9 (2)
C(2)—C(1)—Cl	119.9 (2)	N(4)—C(8)—N(1)	108.1 (2)
C(3)—C(9)—O(1)	124.8 (2)	N(4)—N(3)—N(2)	104.9 (2)
C(3)—C(9)—O(2)	109.2 (2)	C(8)—N(4)—N(3)	108.8 (2)
C(14)—C(13)—O(3)	109.5 (2)	C(1)—N(5)—N(4)	113.8 (2)
C(15)—C(14)—O(4)	109.9 (2)	C(2)—C(1)—N(5)	124.1 (2)
C(16)—C(15)—O(5)	107.1 (2)	C(3)—N(6)—N(7)	110.1 (2)
C(8)—N(1)—N(2)	105.2 (2)	C(6)—N(7)—N(6)	108.5 (1)
N(3)—N(2)—N(1)	113.0 (2)	C(1)—C(2)—N(6)	128.9 (2)
C(7)—C(8)—N(1)	135.8 (2)	C(4)—C(3)—N(6)	102.3 (2)
N(5)—N(4)—N(3)	122.3 (2)	C(6)—N(7)—C(5)	118.9 (5)
C(8)—N(4)—N(5)	128.9 (2)	C(13)—C(5)—N(7)	108.2 (2)
C(7)—C(8)—N(4)	116.1 (2)	C(11)—C(6)—N(7)	108.4 (2)
C(2)—N(6)—N(7)	107.0 (1)	C(7)—C(2)—C(1)	118.9 (2)
C(5)—N(7)—N(6)	105.9 (1)	C(8)—C(7)—C(2)	118.0 (2)
C(3)—N(6)—C(2)	126.2 (2)	C(5)—C(4)—C(3)	103.3 (2)
C(7)—C(2)—N(6)	112.0 (2)	C(14)—C(13)—C(5)	111.8 (2)
C(9)—C(3)—N(6)	113.5 (2)	C(12)—C(6)—C(7)	109.3 (2)
C(4)—C(5)—N(7)	102.4 (2)	C(12)—C(6)—C(11)	109.7 (2)
C(7)—C(6)—N(7)	100.7 (1)	C(16)—C(15)—C(14)	112.4 (2)

Compound (II)

Crystal data

$C_{23}H_{21}ClN_8O_6$
$M_r = 540.5$
Monoclinic
$P2_1/c$
$a = 11.4371$ (8) Å
$b = 17.879$ (1) Å
$c = 12.7762$ (9) Å
$\beta = 109.406$ (6)°
$V = 2464.1$ (6) Å^3
$Z = 4$
$D_x = 1.458$ Mg m^{-3}
$D_m = 1.44$ (2) Mg m^{-3}
D_m measured by flotation

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 100 reflections
$\theta = 9-16°$
$\mu = 0.2067$ mm^{-1}
$T = 293$ (1) K
Irregular
0.72 × 0.72 × 0.56 mm
Orange

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans [width (0.8 + 0.3tanθ)°]
Absorption correction: none
12 330 measured reflections
5908 independent reflections
3723 observed reflections [$I > 2.5\sigma(I)$]

$R_{\rm int} = 0.02$
$\theta_{\rm max} = 27.9°$
$h = 0 \rightarrow 15$
$k = -23 \rightarrow 23$
$l = -16 \rightarrow 16$
3 standard reflections
frequency: 333 min
intensity variation: −5.04%

Refinement

Refinement on F
$R = 0.038$
$wR = 0.050$
$S = 0.998$
4492 reflections
426 parameters
All H-atom parameters refined

Empirical weighting scheme
$(\Delta/\sigma)_{\rm max} = 0.088$
$\Delta\rho_{\rm max} = 0.31$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.20$ e Å^{-3}
Extinction correction: Larson (1967)
Extinction coefficient: 1.508×10^{-3}

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (II)

$$U_{\rm eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Cl	0.3911 (1)	0.60021 (3)	0.21316 (5)	0.0678 (3)
O(1)	0.4129 (1)	0.4031 (1)	0.0944 (1)	0.068 (1)
O(2)	0.2813 (1)	0.4581 (1)	−0.0559 (1)	0.059 (1)
O(3)	0.0965 (1)	0.3226 (1)	−0.0889 (1)	0.055 (1)
O(4)	−0.0055 (1)	0.4313 (1)	−0.1132 (1)	0.046 (1)
O(5)	−0.1657 (1)	0.3185 (1)	−0.0154 (1)	0.070 (1)
O(6)	0.1353 (2)	0.1416 (1)	0.1126 (1)	0.065 (1)
N(1)	0.6318 (2)	0.3635 (1)	0.5066 (1)	0.068 (1)
N(2)	0.7371 (2)	0.4057 (2)	0.5467 (2)	0.082 (1)
N(3)	0.7279 (2)	0.4714 (2)	0.5030 (2)	0.078 (1)
N(4)	0.6116 (1)	0.4739 (1)	0.4282 (1)	0.060 (1)
N(5)	0.5682 (2)	0.5342 (1)	0.3647 (2)	0.061 (1)
N(6)	0.2637 (1)	0.4469 (1)	0.2225 (1)	0.037 (1)
N(7)	0.2287 (1)	0.3721 (1)	0.2535 (1)	0.038 (1)
N(8)	−0.0041 (1)	0.2394 (1)	0.0734 (1)	0.048 (1)
C(1)	0.4551 (2)	0.5258 (1)	0.2974 (1)	0.050 (1)
C(2)	0.3844 (1)	0.4589 (1)	0.2895 (1)	0.040 (1)
C(3)	0.2204 (1)	0.4551 (1)	0.1016 (1)	0.037 (1)
C(4)	0.1107 (1)	0.3998 (1)	0.0694 (1)	0.036 (1)
C(5)	0.1603 (1)	0.3342 (1)	0.1491 (1)	0.036 (1)
C(6)	0.3436 (2)	0.3351 (1)	0.[illegible]339 (1)	0.045 (1)
C(7)	0.4316 (1)	0.4001 (1)	0.3577 (1)	0.044 (1)
C(8)	0.5539 (2)	0.4074 (1)	0.4316 (1)	0.052 (1)
C(9)	0.3180 (1)	0.4349 (1)	0.0487 (1)	0.042 (1)
C(10)	0.3591 (2)	0.4372 (2)	−0.1206 (2)	0.076 (1)
C(11)	0.0681 (1)	0.3789 (1)	−0.0523 (1)	0.038 (1)
C(12)	−0.0556 (2)	0.4157 (1)	−0.2311 (1)	0.061 (1)
C(13)	0.3973 (2)	0.2699 (1)	0.2864 (2)	0.066 (1)
C(14)	0.3132 (2)	0.3125 (1)	0.4377 (2)	0.067 (1)
C(15)	0.0594 (2)	0.2855 (1)	0.1693 (1)	0.047 (1)
C(16)	−0.1102 (2)	0.2608 (1)	−0.0126 (2)	0.053 (1)
C(17)	−0.1334 (2)	0.1996 (1)	−0.0963 (2)	0.056 (1)
C(18)	−0.2269 (2)	0.1921 (2)	−0.1979 (2)	0.071 (1)
C(19)	−0.2223 (3)	0.1281 (2)	−0.2594 (2)	0.087 (2)
C(20)	−0.1308 (3)	0.0761 (2)	−0.2221 (2)	0.085 (2)

C(21)	−0.0369 (3)	0.0834 (1)	−0.1200 (2)	0.073 (1)
C(22)	−0.0417 (2)	0.1469 (1)	−0.0595 (2)	0.054 (1)
C(23)	0.0439 (2)	0.1714 (1)	0.0514 (1)	0.051 (1)

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

Cl—C(1)	1.715 (2)	N(6)—N(7)	1.487 (2)
O(1)—C(9)	1.192 (2)	N(6)—C(2)	1.378 (2)
O(2)—C(9)	1.326 (2)	N(6)—C(3)	1.464 (2)
O(2)—C(10)	1.450 (3)	N(7)—C(5)	1.470 (2)
O(3)—C(11)	1.199 (2)	N(7)—C(6)	1.525 (2)
O(4)—C(11)	1.326 (2)	N(8)—C(15)	1.456 (2)
C(16)—C(17)	1.491 (3)	C(21)—C(22)	1.385 (3)
C(17)—C(18)	1.387 (3)	C(22)—C(23)	1.495 (2)
C(17)—C(22)	1.371 (3)	N(8)—C(23)	1.401 (2)
C(18)—C(19)	1.399 (5)	C(1)—C(2)	1.429 (2)
C(19)—C(20)	1.362 (5)	C(2)—C(7)	1.358 (2)
C(20)—C(21)	1.394 (3)	C(3)—C(4)	1.542 (2)
O(4)—C(12)	1.450 (2)	C(3)—C(9)	1.528 (3)
O(5)—C(16)	1.206 (3)	C(4)—C(5)	1.533 (2)
O(6)—C(23)	1.201 (2)	C(4)—C(11)	1.515 (2)
N(1)—N(2)	1.368 (3)	C(5)—C(15)	1.535 (3)
N(1)—C(8)	1.327 (3)	C(6)—C(7)	1.501 (2)
N(2)—N(3)	1.289 (4)	C(6)—C(13)	1.533 (3)
N(3)—N(4)	1.356 (2)	C(6)—C(14)	1.532 (3)
N(4)—N(5)	1.341 (3)	C(7)—C(8)	1.409 (2)
N(4)—C(8)	1.368 (3)	N(8)—C(16)	1.392 (2)
N(5)—C(1)	1.303 (2)		
N(5)—C(1)—Cl	116.6 (2)	C(2)—C(1)—N(5)	123.9 (2)
C(2)—C(1)—Cl	119.5 (1)	C(2)—N(6)—N(7)	106.0 (1)
O(2)—C(9)—O(1)	125.0 (2)	C(3)—N(6)—N(7)	110.2 (1)
C(3)—C(9)—O(1)	125.1 (1)	C(5)—N(7)—N(6)	106.4 (1)
C(10)—O(2)—C(9)	116.5 (2)	C(6)—N(7)—N(6)	108.8 (1)
C(3)—C(9)—O(2)	109.8 (1)	C(3)—N(6)—C(2)	124.0 (1)
O(4)—C(11)—O(3)	124.6 (1)	C(1)—C(2)—N(6)	126.9 (1)
C(4)—C(11)—O(3)	124.8 (1)	C(7)—C(2)—N(6)	112.4 (1)
C(12)—O(4)—C(11)	115.3 (1)	C(4)—C(3)—N(6)	100.2 (1)
C(4)—C(11)—O(4)	110.6 (1)	C(9)—C(3)—N(6)	113.7 (1)
C(14)—C(6)—N(7)	107.7 (2)	C(9)—C(3)—C(4)	112.3 (1)
C(16)—N(8)—C(15)	124.6 (2)	C(5)—C(4)—C(3)	103.0 (1)
C(23)—N(8)—C(15)	122.8 (2)	C(11)—C(4)—C(3)	112.8 (1)
C(5)—C(15)—N(8)	111.8 (1)	C(11)—C(4)—C(5)	114.5 (1)
C(23)—N(8)—C(16)	112.2 (1)	C(15)—C(5)—C(4)	114.4 (1)
C(17)—C(16)—N(8)	105.4 (2)	C(13)—C(6)—C(7)	109.8 (2)
C(22)—C(23)—N(8)	105.5 (2)	C(14)—C(6)—C(7)	111.0 (1)
C(7)—C(2)—C(1)	120.5 (2)	C(8)—C(7)—C(6)	131.0 (2)
C(6)—C(7)—C(2)	111.9 (1)	C(14)—C(6)—C(13)	112.3 (2)
C(8)—C(7)—C(2)	116.9 (2)	C(18)—C(17)—C(16)	129.9 (2)
N(8)—C(16)—O(5)	124.8 (2)	C(22)—C(17)—C(16)	108.9 (2)
C(17)—C(16)—O(5)	129.8 (2)	C(22)—C(17)—C(18)	121.2 (2)
N(8)—C(23)—O(6)	124.6 (2)	C(19)—C(18)—C(17)	116.4 (3)
C(22)—C(23)—O(6)	129.9 (2)	C(21)—C(22)—C(17)	122.7 (2)
C(8)—N(1)—N(2)	103.9 (2)	C(23)—C(22)—C(17)	108.0 (2)
N(3)—N(2)—N(1)	114.0 (2)	C(20)—C(19)—C(18)	122.0 (3)
N(4)—C(8)—N(1)	108.8 (2)	C(21)—C(20)—C(19)	121.8 (3)
C(7)—C(8)—N(1)	135.0 (2)	C(22)—C(21)—C(20)	116.0 (2)
N(4)—N(3)—N(2)	104.7 (2)	C(23)—C(22)—C(21)	129.3 (2)
N(5)—N(4)—N(3)	122.1 (2)	C(6)—N(7)—C(5)	119.4 (1)
C(8)—N(4)—N(3)	108.7 (2)	C(4)—C(5)—N(7)	102.6 (1)
C(8)—N(4)—N(5)	129.2 (2)	C(15)—C(5)—N(7)	108.2 (1)
C(1)—N(5)—N(4)	113.1 (2)	C(7)—C(6)—N(7)	99.8 (1)
C(7)—C(8)—N(4)	116.2 (2)	C(13)—C(6)—N(7)	115.6 (1)

For (I), Friedel pairs were merged and the absolute configuration was assigned so as to agree with the known chirality at C(13), arising from its precursor D-ribose. Compound (II) is a racemate. The structures were solved by heavy-atom methods. H atoms were found from difference maps and included in the calculations for (II), but were not refined for (I). Refinement was by large-block-matrix least-squares methods. All calculations were performed on DEC10 and VAX8550 computers at the University Computer Center, Ljubljana. Atomic scattering factors were taken from Cromer & Mann (1968) for non-H atoms and from Stewart, Davidson & Simpson (1965) for H; anomalous-dispersion terms were taken from Cromer & Liberman (1970). Programs used for structure solution and refinement, and data reduction and interpretation: *XRAY76* (Stewart *et al.*, 1976). Molecular graphics: *ORTEP* (Johnson, 1965). Programs used for least-squares-planes calculations: *Xtal*3.0 (Hall & Stewart, 1990).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71524 (27 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: MU1060]

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