Table 1. *Final positional parameters* ($\times 10^4$) *and their e.s.d.'s and equivalent isotropic temperature factors* ($\mathring{A}^2$)

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
C(1)	1826 (5)	5135 (4)	3492 (3)	2·72
C(2)	830 (5)	5646 (4)	4151 (3)	3·02
C(3)	−481 (5)	5189 (5)	4334 (3)	3·83
C(4)	−1279 (7)	5550 (5)	5016 (4)	5·22
C(5)	−821 (7)	6344 (6)	5527 (4)	5·14
C(6)	458 (6)	6807 (4)	5344 (3)	4·20
C(7)	1272 (6)	6459 (4)	4664 (3)	3·30
C(8)	1042 (5)	4665 (4)	2721 (3)	2·69
C(9)	−170 (6)	5150 (4)	2407 (3)	3·51
C(10)	−812 (6)	4787 (5)	1668 (3)	4·26
C(11)	−286 (6)	3936 (4)	1242 (3)	4·00
C(12)	923 (6)	3466 (4)	1534 (3)	3·92
C(13)	1601 (6)	3831 (4)	2268 (3)	3·40
C(14)	2857 (5)	5926 (4)	3084 (3)	2·68
C(15)	4264 (6)	5669 (4)	2924 (4)	4·06
C(16)	5125 (7)	6380 (5)	2494 (4)	5·36
C(17)	4616 (7)	7307 (5)	2205 (4)	4·65
C(18)	3222 (7)	7554 (4)	2343 (4)	4·44
C(19)	2354 (6)	6875 (4)	2781 (3)	3·34
N(20)	2668 (4)	4310 (3)	3923 (3)	2·80
C(21)	1937 (6)	3329 (4)	4211 (3)	3·90
C(22)	2615 (6)	3145 (4)	5081 (3)	4·11
C(23)	2621 (6)	4221 (4)	5469 (3)	3·71
C(24)	3457 (5)	4656 (4)	4710 (3)	3·00
C(25)	4675 (7)	3899 (4)	4707 (4)	3·79
O(26)	4127 (4)	2960 (3)	4925 (2)	4·56
O(27)	5897 (4)	4025 (3)	4523 (3)	5·33
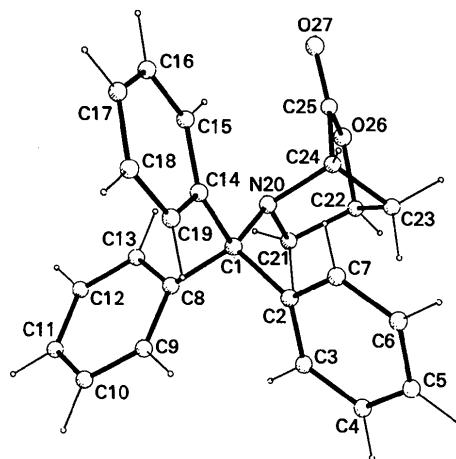
Fig. 1. The atom numbering of the molecule.

Table 2. *Bond distances* ($\mathring{A}$) *and angles* (°)

N(20)—C(21)	1·508 (6)	C(21)—N(20)—C(24)	103·5 (4)
C(21)—C(22)	1·522 (7)	N(20)—C(21)—C(22)	101·6 (4)
C(22)—C(23)	1·509 (7)	C(21)—C(22)—C(23)	102·5 (4)
C(23)—C(24)	1·532 (7)	C(22)—C(23)—C(24)	91·5 (4)
C(24)—N(20)	1·506 (6)	N(20)—C(24)—C(23)	105·3 (4)
C(24)—C(25)	1·512 (7)	C(23)—C(22)—O(26)	102·1 (4)
C(25)—O(26)	1·357 (6)	C(22)—O(26)—C(25)	105·7 (4)
O(26)—C(22)	1·477 (6)	O(26)—C(25)—C(24)	106·1 (5)
C(25)—O(27)	1·208 (6)	C(25)—C(24)—C(23)	99·4 (4)

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Structure of 5-Methyl-2'-deoxycytidine 5'-Monophosphate Dihydrate

BY H. N. LALITHA, S. RAMAKUMAR AND M. A. VISWAMITRA

Department of Physics and ICMR Centre for Genetics and Cell Biology, Indian Institute of Science, Bangalore 560012, India

Abstract. $C_{10}H_{16}N_3O_7P.2H_2O$, $M_r = 357·2$, triclinic, $P1$, $a = 4·8520$ (8), $b = 8·3703$ (8), $c = 10·0199$ (12) $\mathring{A}$, $\alpha = 104·578$ (9), $\beta = 102·332$ (13), $\gamma = 93·670$ (11)°, $V = 381·75$ $\mathring{A}^3$, $Z = 1$, $D_x = 1·55$, $D_m = 1·53$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 $\mathring{A}$, $\mu = 2·01$ mm^{-1}, $F(000) = 188$, $T = 290$ K, $R = 0·049$ for 1568 unique reflections.

The glycosidic torsion angle $\chi = -173.8\ (0.5)°$, the cytosine base is *anti*, the sugar pucker is C3'-*endo*–C2'-*exo* $(^3T_2)$, the phase angle of pseudo-rotation, $P = 2.2°$, and the maximum amplitude of pucker, $\tau_{max} = 34.0°$. The phosphate torsion angles, φ_{OO} (O5—C5'—C4'—O4') $= -70.0\ (0.6)°$ and φ_{OC} (O5—C5'—C4'—C3') $= 48.6\ (0.6)°$, show a *gauche-gauche* conformation. Base protonation at N(3) (by migration of the proton from phosphate O) results in widening of the angle C(2)—N(3)—C(4) to $124.0\ (0.5)°$. The associated changes in bond lengths and angles are in agreement with those for other protonated bases. The phosphate group carries a single negative charge, the molecule existing as a zwitterion.

Experimental. Small crystal, $0.17 \times 0.09 \times 0.06$ mm, grown from an aqueous solution of the compound by the slow diffusion of the precipitant, ethanol. The density was determined by flotation in C_6H_6 and $CHBr_3$. Enraf–Nonius CAD-4 diffractometer, Ni-filtered radiation, ω–2θ scan mode, maximum $\sin\theta/\lambda = 0.58$ Å^{-1}, lattice parameters from 24 reflections with $9 < 2\theta < 42°$ ($h = -6$ to 6, $k = -10$ to 10, $l = -12$ to 12), three reflections ($\bar{1}01$, $0\bar{2}1$, and $\bar{1}10$) as intensity standards measured every hour of exposure time, intensity variation $< 2\%$, no evidence of crystal decay, Lorentz and polarization corrections applied, no absorption corrections, Friedel pairs averaged, anomalous-dispersion corrections not applied. The correct enantiomorphic form corresponds to the structure of a β-nucleotide. 1568 unique reflections out of 3139 measured, 213 excluded during refinement $[|F_o| < 2\sigma(|F_o|)]$. P and three O atoms initially located from *RANTAN* (*SDP*, Enraf–Nonius, 1979). Repeated full-matrix least-squares refinement and difference Fourier calculations revealed the entire structure gradually. Parameters x, y, z and U_{ij} varied for all non-H atoms; x, y, z and U for all H atoms obtained from difference Fourier calculations. $w(|F_o| - |F_c|)^2$ minimized, $w = \sigma^{-2}(F)$, $R = 4.9\%$, $wR = 4.9\%$, $(\Delta/\sigma)_{max} = 0.03$ in the final cycle. Residual electron density in the final difference synthesis was between -0.37 and 0.32 e Å^{-3}.

Scattering factors from *International Tables for X-ray Crystallography* (1974). Table 1 gives the atomic parameters.* Fig. 1 shows the molecule and Fig. 2 the packing in the unit cell. Table 2 lists bond lengths, bond angles, torsion angles and hydrogen-bond parameters. All calculations were performed on VAX 11/785 and PDP 11/44 computers using

* 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 51908 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final fractional coordinates and temperature factors of the non-*H *atoms with e.s.d.'s in parentheses*

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

	x	y	z	$U_{eq}(\text{Å}^2)$
P	0.5460	0.5670	0.8390	0.023 (1)
O8	0.2474 (8)	0.5598 (5)	0.7630 (4)	0.034 (1)
O7	0.7443 (9)	0.6531 (6)	0.7645 (5)	0.038 (2)
O6	0.6500 (9)	0.4080 (5)	0.8572 (5)	0.033 (1)
O5	0.5807 (9)	0.6974 (5)	0.9906 (4)	0.031 (1)
C5'	−0.1477 (12)	0.7372 (7)	1.0915 (6)	0.030 (2)
C4'	0.8723 (11)	0.9094 (7)	1.1862 (6)	0.026 (2)
C3'	0.6172 (11)	0.9471 (6)	1.2504 (5)	0.025 (2)
C2'	0.6108 (12)	1.1314 (7)	1.2659 (6)	0.028 (2)
C1'	0.7155 (12)	1.1559 (7)	1.1397 (6)	0.027 (2)
O4'	0.8911 (8)	1.0303 (5)	1.1060 (4)	0.027 (1)
O3'	0.6465 (10)	0.9150 (5)	1.3860 (4)	0.034 (1)
N1	0.4806 (9)	1.1408 (5)	1.0110 (5)	0.023 (1)
C2	0.3062 (11)	1.2631 (6)	1.0204 (6)	0.026 (2)
N3	0.0923 (10)	1.2493 (6)	0.9012 (5)	0.025 (1)
C4	0.0669 (11)	1.3359 (6)	0.7756 (6)	0.025 (2)
C5	0.2582 (12)	1.0151 (6)	0.7648 (5)	0.025 (2)
C6	0.4568 (11)	1.0233 (6)	0.8849 (6)	0.025 (2)
N4	−0.1377 (11)	1.1451 (6)	0.6679 (5)	0.033 (2)
C7	0.2394 (15)	0.8881 (7)	0.6269 (6)	0.036 (2)
O2	0.2380 (9)	1.3782 (5)	1.1275 (5)	0.035 (1)
OW1	0.1190 (15)	0.4599 (8)	0.4681 (6)	0.058 (2)
OW2	0.6199 (15)	1.5876 (6)	1.3767 (6)	0.053 (2)

Table 2. *Bond distances* (Å), *bond angles* (°), *torsion angles* (°) *and hydrogen-bond parameters* (Å,°) *with e.s.d.'s in parentheses*

P—O8	1.483 (4)	C1'—O4'	1.420 (6)
P—O7	1.582 (4)	C1'—N1	1.504 (6)
P—O6	1.494 (4)	N1—C2	1.371 (6)
P—O5	1.600 (4)	C2—O2	1.229 (7)
O5—C5'	1.447 (7)	C2—N3	1.383 (7)
C5'—C4'	1.498 (7)	N3—C4	1.348 (6)
C4'—O4'	1.453 (6)	C4—N4	1.326 (7)
C4'—C3'	1.525 (7)	C4—C5	1.419 (7)
C3'—O3'	1.431 (6)	C5—C7	1.497 (7)
C3'—C2'	1.514 (7)	C5—C6	1.358 (7)
C2'—C1'	1.515 (8)	C6—N1	1.369 (6)

O8—P—O7	109.0 (2)	C2'—C1'—N1	113.2 (4)
O8—P—O6	117.8 (2)	O4'—C1'—N1	108.7 (4)
O8—P—O5	105.5 (2)	C1'—N1—C2	116.4 (4)
O7—P—O6	109.4 (2)	C1'—N1—C6	122.7 (4)
O7—P—O5	104.1 (2)	C6—N1—C2	120.4 (4)
O6—P—O5	110.1 (2)	N1—C2—O2	123.8 (5)
P—O5—C5'	120.0 (3)	N3—C2—O2	120.1 (5)
O5—C5'—C4'	108.8 (4)	N1—C2—N3	116.2 (4)
C5'—C4'—C3'	115.9 (4)	C2—N3—C4	124.0 (5)
O4'—C4'—C5'	109.7 (4)	N3—C4—N4	117.2 (5)
C4'—O4'—C1'	110.6 (4)	N4—C4—C5	123.7 (5)
O4'—C4'—C3'	104.9 (4)	N3—C4—C5	119.1 (5)
C4'—C3'—O3'	113.3 (4)	C4—C5—C6	116.3 (4)
C2'—C3'—O3'	109.9 (4)	C4—C5—C7	120.8 (5)
C4'—C3'—C2'	103.3 (4)	C7—C5—C6	122.9 (5)
C3'—C2'—C1'	102.9 (4)	C5—C6—N1	123.6 (5)
C2'—C1'—O4'	106.8 (4)		

χ	(O4'—C1'—N1—C2)	−173.8 (4)	φ_{OC} (C3'—C4'—C5'—O5)	48.6 (6)
ν_0	(C4'—O4'—C1'—C2')	9.5 (6)	φ_{OO} (O4'—C4'—C5'—O5)	−70.0 (6)
ν_1	(O4'—C1'—C2'—C3')	−27.1 (6)	C4'—C5'—O5—P	152.7 (4)
ν_2	(C1'—C2'—C3'—C4')	33.5 (5)	C5'—O5—P—O6	53.4 (5)
ν_3	(C2'—C3'—C4'—O4')	−28.4 (5)	C5'—O5—P—O7	−63.8 (4)
ν_4	(C3'—C4'—O4'—C1')	12.0 (6)	C5'—O5—P—O8	−178.5 (4)

X—H$\cdots Y$	$X\cdots Y$	X—H	H$\cdots Y$	X—H$\cdots Y$	Symmetry
N3—H3$\cdots$O6	2.61	1.06 (12)	1.70	140.8	−1 1 0
N4—H1N4$\cdots$O6	2.92	1.06 (12)	2.15	127.0	−1 1 0
O7—H7O$\cdots$O8	2.61	0.96 (11)	1.70	158.7	1 0 0
N4—H2N4$\cdots$O3'	2.92	1.00 (08)	2.04	145.6	−1 0−1
OW2—H1W2$\cdots$O2	2.70	1.12 (08)	1.61	164.7	0 0 0
O3'—HO3'$\cdots$OW2	2.71	1.08 (08)	1.65	166.9	0−1 0
OW2—H2W2$\cdots$OW1	2.78	0.81 (10)	2.05	158.0	1 1 1
OW1—H1W1$\cdots$OW2	3.00	0.76 (10)	2.57	118.0	0−1−1
OW1—H1W1$\cdots$O8	2.78	0.76 (10)	2.52	102.3	0 0 0

$C_{10}H_{16}N_3O_7P.2H_2O$

*SHELX*76 (Sheldrick, 1976) and *SDP* (Enraf–Nonius, 1979).

Related literature. The C(2)—O(2) bond distance is 1·229 (7) Å, which is longer than both the value of 1·207 Å typical of conjugated systems (*International Tables for X-ray Crystallography*, 1962) and the value of 1·209 (4) Å in 5-methylcytosine (Padmaja, Ramakumar & Viswamitra, 1987). Similar elongation of this bond has also been observed in other

Fig. 1. View of the molecule.

Fig. 2. Packing in the unit cell.

structures where O(2) is involved in strong hydrogen bonding, as in 3-methyldeoxycytidine methosulfate (1·223 Å) (Lalitha, Ramakumar & Viswamitra, 1988) and cytosine hydrochloride (1·226 Å) (Mandel, 1977); a further lengthening (to 1·242 Å) occurs in dCMP (Na salt) (Pandit, Seshadri & Viswamitra, 1983) where O(2) participates in two hydrogen bonds. The structure of the title compound is stabilized by a series of hydrogen bonds. There is no base stacking. Protonated and methylated cytosines have generally shown no preference for base stacking (Bugg, Thomas, Sundaralingam & Rao, 1971).

Metabolic activities of 5-methylated cytosine bases with a key role in a variety of biochemical regulation processes have been discussed by Doerfler (1983, 1984), Razin & Riggs (1980), and Ehrlich & Wang (1981). The structure of the title compound resembles deoxycytidine 5′-monophosphate (dCMP) free acid (Viswamitra, Reddy, Lin & Sundaralingam, 1971), but is significantly different from that of dCMP Na salt (Pandit, Seshadri & Viswamitra, 1983); other conformational changes resulting from protonation of the base are similar to those reported by Sundaralingam & Jensen (1965) and Bugg, Thomas, Sundaralingam & Rao (1971). The pseudo-rotation angle and amplitude of pucker, calculated according to Altona & Sundaralingam (1972) and Rao, Westhof & Sundaralingam (1981), compare well with those for other protonated cytosines (Trus & Marsh, 1972; Mandel, 1977).

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2-Ethyl-6-(p-nitrophenyl)dihydro-1,5,2-dioxazine

By M. Shoja, S. Saba and R. Kabbani

Department of Chemistry, Fordham University, Bronx, NY 10458, USA

Abstract. $C_{11}H_{14}N_2O_4$, $M_r = 238 \cdot 24$, triclinic, $P\bar{1}$, $a = 5 \cdot 383$ (1), $b = 10 \cdot 940$ (2), $c = 12 \cdot 074$ (2) Å, $\alpha = 103 \cdot 09$ (2), $\beta = 100 \cdot 16$ (2), $\gamma = 117 \cdot 59$ (2)°, $V = 580 \cdot 3$ (2) Å^3, $Z = 2$, $D_x = 1 \cdot 37$ g cm^{-3}, Cu $K\alpha$ radiation, $\lambda = 1 \cdot 5418$ Å, $\mu = 8 \cdot 9$ cm^{-1}, $F(000) = 252$, $T = 293$ K, final $R = 0 \cdot 047$ for 1385 observed reflections. The dioxazine ring is in a chair conformation. The dihedral angle between the phenyl ring and the dioxazine moiety is 142·3 (1)°. The torsion angle C(2')—C(1')—C(6)—O(5) is −4·8 (4)°. The ethyl group is in the equatorial position. The torsion angle for C(8)—C(7)—N(2)—O(1) is 78·6 (3)°.

Experimental. The title compound was prepared by thermal rearrangement of the corresponding oxazolidine *N*-oxide. Colorless crystals obtained from a solution of petroleum ether at room temperature; dimensions $0 \cdot 4 \times 0 \cdot 4 \times 0 \cdot 4$ mm. Data collected on a CAD-4 diffractometer, graphite monochromator. Cell parameters measured on the diffractometer using 25 reflections in the 2θ range 20–40°. Range of indices $0 \le h \le 6$, $-10 \le k \le 10$, $-13 \le l \le 13$ ($\theta \le 60°$). Three standards ($\bar{1}1\bar{1}$, $11\bar{2}$, $02\bar{4}$) measured after every 200 reflections showed a variation of 0·6%. No absorption corrections. Lorentz and polarization corrections. 1709 unique reflections measured. 1385 observed reflections with $I > 3 \cdot 0\sigma(I)$. Direct methods (*MULTAN*82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) used for structure determination. H atoms located by difference Fourier synthesis. Anisotropic full-matrix least-squares refinement (on *F*) for non-H atoms, isotropic for H atoms. All attempts to refine the coordinates of HC(4) atoms led to meaningless H—C(4) distances. These H atoms were held at a fixed distance, 0·96 Å, with temperature factors of 4·8 Å^2. $\sum w(|F_o| - |F_c|)^2$ minimized. $wR = 0 \cdot 047$, max. $\Delta/\sigma = 0 \cdot 8$. Max. peak height in the final difference Fourier map 0·54 e Å^{-3}, $S = 0 \cdot 51$. Atomic scattering factors from *International Tables for X-ray*

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-*H *atoms with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{eq}(\text{Å}^2)$
O(1)	0·0973 (4)	0·1315 (2)	0·3827 (2)	3·64 (5)
O(3)	−0·2476 (6)	−0·4743 (2)	−0·0813 (2)	7·05 (8)
O(4)	−0·5888 (6)	−0·4476 (3)	−0·1744 (2)	6.65 (8)
O(5)	−0·0313 (4)	0·2230 (2)	0·2411 (2)	4·37 (5)
N(1)	−0·3707 (6)	−0·4061 (3)	−0·0902 (2)	4·91 (8)
N(2)	0·2534 (5)	0·2770 (2)	0·4800 (2)	3·68 (6)
C(1')	−0·0101 (6)	0·0071 (3)	0·1794 (2)	3.40 (7)
C(2')	−0·2616 (6)	−0·0489 (3)	0·0846 (3)	4·17 (8)
C(3)	0·0711 (7)	0·3401 (3)	0·4530 (3)	4·54 (8)
C(3')	−0·3831 (7)	−0·1847 (3)	−0·0039 (3)	4·35 (8)
C(4)	0·0784 (7)	0·3609 (3)	0·3341 (3)	4·91 (9)
C(4')	−0·2464 (6)	−0·2627 (3)	0·0065 (2)	3·87 (8)
C(5')	0·0024 (7)	−0·2120 (3)	0·1009 (3)	4·49 (8)
C(6)	0·1273 (6)	0·1560 (3)	0·2747 (2)	3·60 (7)
C(6')	0·1217 (7)	−0·0754 (3)	0·1882 (3)	4·34 (8)
C(7)	0·2383 (7)	0·2400 (3)	0·5891 (3)	4·20 (8)
C(8)	0·4645 (8)	0·2008 (3)	0·6290 (3)	5·91 (9)

Table 2. *Bond distances (*Å*), bond angles (°) and selected torsion angles (°) with e.s.d.'s in parentheses*

O(1)—N(2)	1·477 (2)	C(1')—C(2')	1·373 (4)
O(1)—C(6)	1·408 (4)	C(1')—C(6)	1·503 (4)
O(3)—N(1)	1·216 (5)	C(1')—C(6')	1·391 (6)
O(4)—N(1)	1·223 (4)	C(2')—C(3')	1·381 (4)
O(5)—C(4)	1·434 (3)	C(3)—C(4)	1·507 (5)
O(5)—C(6)	1·421 (4)	C(3')—C(4')	1·370 (6)
N(1)—C(4')	1·482 (4)	C(4')—C(5')	1·374 (4)
N(2)—C(3)	1·469 (5)	C(5')—C(6')	1·385 (4)
N(2)—C(7)	1·468 (4)	C(7)—C(8)	1·511 (6)
N(2)—O(1)—C(6)	107·7 (2)	N(2)—C(3)—C(4)	107·6 (3)
C(4)—O(5)—C(6)	110·2 (2)	C(2')—C(3')—C(4')	117·9 (3)
O(3)—N(1)—O(4)	124·1 (2)	O(5)—C(4)—C(3)	110·6 (3)
O(3)—N(1)—C(4')	118·0 (2)	N(1)—C(4')—C(3')	118·1 (3)
O(4)—N(1)—C(4')	118·0 (3)	N(1)—C(4')—C(5')	119·1 (3)
O(1)—N(2)—C(3)	104·2 (2)	C(3')—C(4')—C(5')	122·8 (2)
O(1)—N(2)—C(7)	103·6 (2)	C(4')—C(5')—C(6')	118·3 (3)
C(3)—N(2)—C(7)	111·8 (3)	O(1)—C(6)—O(5)	110·3 (3)
C(2')—C(1')—C(6)	121·5 (3)	O(1)—C(6)—C(1')	106·7 (2)
C(2')—C(1')—C(6')	119·6 (2)	O(5)—C(6)—C(1')	108·4 (2)
C(6)—C(1')—C(6')	118·9 (2)	C(1')—C(6')—C(5')	120·2 (3)
C(1')—C(2')—C(3')	121·1 (4)	N(2)—C(7)—C(8)	111·7 (3)
O(1)—N(2)—C(3)—C(4)	−64·0 (3)	C(4)—O(5)—C(6)—O(1)	59·2 (3)
N(2)—C(3)—C(4)—O(5)	58·5 (4)	O(5)—C(6)—O(1)—N(2)	−67·3 (3)
C(3)—C(4)—O(5)—C(6)	−54·3 (4)	C(6)—O(1)—N(2)—C(3)	69·0 (3)