$V = 2799.80 (18) \text{ Å}^3$

Mo $K\alpha$ radiation $\mu = 0.19 \text{ mm}^{-1}$

 $0.3 \times 0.2 \times 0.2 \text{ mm}$

Z = 4

T = 293 K

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3-(6-Benzyloxy-2,2-dimethylperhydrofuro[2,3-*d*][1,3]dioxolan-5-yl)-5-(4chlorophenyl)-4-nitro-2-phenyl-2,3,4,5tetrahydroisoxazole

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.088; data-to-parameter ratio = 13.4.

In the title compound, $C_{29}H_{29}ClN_2O_7$, the isoxazole and dioxolane rings adopt envelope conformations, and the furan ring adopts a twisted conformation. The crystal structure is stabilized by intermolecular $C-H\cdots\pi$ interactions between a benzyloxy methylene H atom and the 4-chlorophenyl ring of an adjacent molecule, and by weak non-classical intermolecular $C-H\cdots$ O hydrogen bonds. In addition, the crystal structure exhibits a $Cl\cdots$ O halogen bond of 3.111 (3) Å, with a nearly linear $C-Cl\cdots$ O angle of 160.7 (1)°.

Related literature

For general background to 1,3-dipolar cycloaddition reactions, see: Gothelf & Jorgensen (1998); Bernotas *et al.* (1996); Breuer (1982); Colombi *et al.* (1978); Hossain *et al.* (1993). For ring puckering parameters, see: Cremer & Pople (1975); Nardelli (1983). For halogen bonds, see: Politzer *et al.* (2007).



Experimental

Crystal data

 $\begin{array}{l} C_{29}H_{29}{\rm CIN}_2{\rm O}_7 \\ M_r = 552.99 \\ {\rm Orthorhombic}, \ P2_12_12_1 \\ a = 12.7862 \ (5) \ {\rm \AA} \\ b = 13.0160 \ (5) \ {\rm \AA} \\ c = 16.8232 \ (6) \ {\rm \AA} \end{array}$

Data collection

Bruker Kappa APEXII CCD
diffractometer17056 measured reflections
4764 independent reflectionsAbsorption correction: multi-scan
(SADABS; Bruker 2004)
 $T_{min} = 0.926, T_{max} = 0.964$ 17056 measured reflections
4764 independent reflections
3446 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.088$	$\Delta \rho_{\rm max} = 0.15 \text{ e} \text{ Å}^{-3}$
S = 1.02	$\Delta \rho_{\rm min} = -0.14 \text{ e} \text{ Å}^{-3}$
4764 reflections	Absolute structure: Flack (1983),
355 parameters	1975 Friedel pairs
1 restraint	Flack parameter: -0.05 (8)

Table 1Hydrogen-bond geometry (Å, °).

	рн	Ш 4	D 4	
$D = \Pi \cdots A$	D = H	$\Pi \cdots A$	$D \cdots A$	$D = \Pi \cdots A$
$C13-H13\cdots O2^{i}$	0.98	2.54	3.298 (3)	134
$C17 - H17B \cdots O1^{ii}$	0.97	2.46	3.218 (3)	135
$C21 - H21 \cdots Cg1^{i}$	0.93	2.75	3.598 (1)	152

Symmetry codes: (i) $x - \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$. Cg1 is the centroid of the C1–C6 ring.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2103).

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3-(6-Benzyloxy-2,2-dimethylperhydrofuro[2,3-*d*][1,3]dioxolan-5-yl)-5-(4-chlorophenyl)-4-nitro-2-phenyl-2,3,4,5-tetrahydroisoxazole

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Comment

The 1,3-dipolar cycloaddition of nitrones with olefinic dipolarophiles proceeds through a concerted mechanism yielding highly substituted isoxazolidines (Gothelf & Jorgensen, 1998). The cornerstone for cycloaddition reactions, nitrones, are excellent spin traping (Bernotas *et al.*, 1996) and highly versatile synthetic intermediates (Breuer, 1982). Highly substituted spiro-isoxazolidines result from the 1,3-dipolar cycloaddition of exocylic olefins with nitrones and these spiro-isoxazolidines have also been transformed into complex heterocycles (Colombi *et al.*, 1978, Hossain *et al.*, 1993). Here we report the crystal structure of the title compound (Fig. 1).

The dihedral angle between the phenyl rings C1-C6 and C18-C23, C18-C23 and C24-C29, and, C1-C6 and C24-C29 are 8.4 (2), 83.9 (1) and 75.7 (1)°, respectively. The five membered tetrahydrofuran ring (C10-C13/O4) adopts a twisted conformation and the other five membered rings, isoxazole ring (C7-C9/O1/N1) and the dioxolan ring (C12-C14/O5/O6), adopt envelope conformations on C11 and C10, O1 and O5 with a pseudo-twofold axis passing through C12–C11, C9–C8 and C13–O6 bonds. The puckering parameters (Cremer & Pople, 1975) and the lowest displacement asymmetry parameters (Nardelli, 1983)as follows: for the tetrahydrofuran ring q₂ = 0.365 (1) Å, φ = 304.9 (1)°, Δ_S (C10) is 12.8 (1)° and Δ_2 (C13) is 1.8 (1)°, for the isoxazolidine ring q₂ = 0.377 (1) Å, φ = 359.7 (1)°, Δ_S (O1) is 1.0 (1)° and Δ_2 (C8) is 19.6 (1)° and for the dioxolone ring q₂ = 0.248 (1) Å, φ = 181.2 (1)°, Δ_S (O5) is 0.3 (1)° and Δ_2 (C13) is 13.3 (1)°.

The molecular packing is stabilized by weak non-classical intermolecular C–H···O hydrogen bonds (Table 1 and Fig. 2; symmetry code as in Fig. 2). Additionally, the crystal structure exhibits a Cl···O halogen bond (Politzer *et al.*, 2007) between the chlorine atom and the oxygen of a neighbouring NO₂ group, with a Cl1···O2^{iv} distance of 3.111 (3) Å (symmetry code as in Fig. 2). The molecular packing (Fig. 3) is further stabilized by an intermolecular C–H···π interactions between the methylene H atom of benzyloxy substituent and the 4-chlorophenyl ring of an adjacent molecule, with a C21–H21···Cg1ⁱⁱⁱ separation of 2.75 Å (Table 1, Cg1 is the centroid of C1-C6 benzene ring).

Experimental

A mixture of D-glucose derived nitrone (0.5 mmol) and β -nitrostyrene (0.5 mmol) was refluxed in dry toluene (10 ml) until completion of the reaction as evidenced by TLC analysis. The solvent was evaporated under reduced pressure. The crude was purified by column chromatography on silica gel (Merck, 100-200 mesh, ethylacetate-petroleum ether (10 : 90) to afford pure isoxazolidine. Single crystals of the title compound suitable for X-ray diffraction was recrystallized from ethanol.

Refinement

All H atoms were positioned geometrically, with C–H = 0.93-0.98 Å and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C, N)$, where x = 1.5 for methyl H and x = 1.2 for all H atoms.

Figures



Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

Fig. 2. The C–H···O interactions, and Cl1···O halogen bond (dashed lines) in the title compound. [Symmetry codes: (i) x - 1/2, -y + 1/2, -z + 1; (ii) -x + 1, y - 1/2, -z + 3/2; (iv) x - 1/2, -y + 3/2, -z + 1.]



Fig. 3. C–H··· π interactions (dashed lines) in the title compound. Cg denotes the ring centroid. [Symmetry codes: (iii) x + 1/2, -y + 1/2, -z + 1; (v) x - 1/2, -y + 1/2, -z + 1.]

3-(6-Benzyloxy-2,2-dimethylperhydrofuro[2,3-*d*][1,3]dioxolan-5-yl)- 5-(4-chlorophenyl)-4-nitro-2-phenyl-2,3,4,5-tetrahydroisoxazole

Crystal data	
C29H29ClN2O7	$F_{000} = 1160$
$M_r = 552.99$	$D_{\rm x} = 1.312 \ {\rm Mg \ m^{-3}}$
Orthorhombic, $P2_12_12_1$	Mo <i>K</i> α radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 3652 reflections
a = 12.7862 (5) Å	$\theta = 2.5 - 25^{\circ}$
b = 13.0160 (5) Å	$\mu = 0.19 \text{ mm}^{-1}$
c = 16.8232 (6) Å	T = 293 K
$V = 2799.80 (18) \text{ Å}^3$	Needle, colourless
Z = 4	$0.3 \times 0.2 \times 0.2$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	4764 independent reflections
Radiation source: fine-focus sealed tube	3446 reflections with $I > 2\sigma(I)$

Monochromator: graphite	$R_{\rm int} = 0.034$
T = 293 K	$\theta_{max} = 25.0^{\circ}$
ω and ϕ scans	$\theta_{\min} = 2.9^{\circ}$
Absorption correction: Multi-scan (SADABS; Bruker 2004)	$h = -15 \rightarrow 15$
$T_{\min} = 0.926, \ T_{\max} = 0.964$	$k = -13 \rightarrow 14$
17056 measured reflections	$l = -16 \rightarrow 20$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.2549P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.088$	$(\Delta/\sigma)_{max} < 0.001$
<i>S</i> = 1.02	$\Delta \rho_{max} = 0.15 \text{ e} \text{ Å}^{-3}$
4764 reflections	$\Delta \rho_{\rm min} = -0.13 \text{ e } \text{\AA}^{-3}$
355 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.0045 (6)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1975 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: -0.05 (8)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2 \text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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Fractional atomic coordinates a	nd isotropic or a	auivalant isotropic o	isnlacomont i	naramators l	(14	
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	x	У	Z	Uiso*/Ueq
C1	0.33984 (19)	0.6866 (2)	0.65294 (16)	0.0602 (7)
H1	0.3415	0.6459	0.6983	0.072*
C2	0.2814 (2)	0.7761 (2)	0.65257 (18)	0.0692 (7)
H2	0.2457	0.7964	0.6981	0.083*
C3	0.2765 (2)	0.8340 (2)	0.5857 (2)	0.0673 (7)
C4	0.3326 (2)	0.8082 (2)	0.5200 (2)	0.0760 (9)
H4	0.3301	0.8493	0.4749	0.091*
C5	0.3933 (2)	0.7205 (2)	0.52082 (18)	0.0691 (8)
Н5	0.4332	0.7039	0.4764	0.083*

C6	0.39575 (17)	0.65738 (18)	0.58632 (15)	0.0471 (6)
C7	0.45334 (17)	0.55719 (17)	0.58177 (14)	0.0455 (6)
H7	0.5181	0.5658	0.5513	0.055*
C8	0.38927 (17)	0.46762 (17)	0.54776 (13)	0.0427 (6)
H8	0.3143	0.4808	0.5544	0.051*
C9	0.42248 (17)	0.37460 (18)	0.59803 (14)	0.0434 (6)
Н9	0.4536	0.3214	0.5643	0.052*
C10	0.33056 (15)	0.33112 (18)	0.64465 (14)	0.0434 (6)
H10	0.3092	0.3802	0.6857	0.052*
C11	0.34793 (16)	0.22621 (18)	0.68184 (14)	0.0448 (6)
H11	0.3831	0.2310	0.7335	0.054*
C12	0.23650 (18)	0.18767 (19)	0.68975 (14)	0.0474 (6)
H12	0.2314	0.1126	0.6886	0.057*
C13	0.17952 (16)	0.23875 (19)	0.62140 (14)	0.0460 (6)
H13	0.1606	0.1884	0.5805	0.055*
C14	0.08681 (19)	0.2635 (2)	0.73843 (15)	0.0582 (7)
C15	0.0626 (3)	0.3618 (3)	0.7812 (2)	0.1063 (12)
H15A	0.1132	0.4131	0.7668	0.159*
H15B	0.0653	0.3503	0.8375	0.159*
H15C	-0.0060	0.3849	0.7666	0.159*
C16	0.0104 (2)	0.1788 (3)	0.7552 (2)	0.0866 (10)
H16A	-0.0575	0.1981	0.7359	0.130*
H16B	0.0069	0.1669	0.8114	0.130*
H16C	0.0328	0.1171	0.7289	0.130*
C17	0.4468 (2)	0.0741 (2)	0.66159 (16)	0.0585 (7)
H17A	0.3903	0.0319	0.6819	0.070*
H17B	0.4917	0.0925	0.7058	0.070*
C18	0.50869 (17)	0.01390 (19)	0.60141 (15)	0.0493 (6)
C19	0.5602 (2)	-0.0733 (2)	0.62669 (19)	0.0713 (8)
H19	0.5570	-0.0928	0.6798	0.086*
C20	0.6160 (2)	-0.1312 (3)	0.5736 (2)	0.0875 (10)
H20	0.6507	-0.1899	0.5910	0.105*
C21	0.6215 (2)	-0.1038 (3)	0.4954 (2)	0.0811 (9)
H21	0.6591	-0.1439	0.4597	0.097*
C22	0.5717(2)	-0.0176 (2)	0.46998 (17)	0.0713 (8)
H22	0.5757	0.0018	0.4169	0.086*
C23	0.5151 (2)	0.0412 (2)	0.52292 (16)	0.0608 (7)
H23	0.4809	0.1000	0.5052	0.073*
C24	0.60915 (17)	0.3964 (2)	0.63870 (14)	0.0489 (6)
C25	0.63995 (19)	0.2974 (2)	0.62056 (17)	0.0639 (8)
H25	0.5905	0.2457	0.6140	0.077*
C26	0.7453 (2)	0.2761 (3)	0.61224 (17)	0.0790 (9)
H26	0.7663	0.2100	0.5988	0.095*
C27	0.8194 (2)	0.3512 (3)	0.62345 (18)	0.0847 (11)
H27	0.8901	0.3359	0.6187	0.102*
C28	0.7876 (2)	0.4485 (3)	0.64162 (19)	0.0805 (10)
H28	0.8373	0.4999	0.6485	0.097*
C29	0.68311 (17)	0.4720 (2)	0.64995 (16)	0.0618 (7)
H29	0.6626	0.5384	0.6631	0.074*

N1	0.50029 (14)	0.41439 (15)	0.65469 (12)	0.0476 (5)
N2	0.4148 (2)	0.45251 (17)	0.46170 (13)	0.0574 (6)
O1	0.47679 (12)	0.52172 (12)	0.66073 (9)	0.0517 (4)
O2	0.4993 (2)	0.4215 (2)	0.44423 (13)	0.0993 (8)
O3	0.3483 (2)	0.4733 (2)	0.41370 (13)	0.1086 (8)
O4	0.24623 (11)	0.31531 (12)	0.59000 (9)	0.0503 (4)
O5	0.19043 (12)	0.23172 (14)	0.75864 (9)	0.0588 (5)
O6	0.08979 (12)	0.28308 (14)	0.65527 (10)	0.0613 (5)
O7	0.40491 (11)	0.16447 (12)	0.62710 (9)	0.0478 (4)
Cl1	0.19572 (8)	0.94167 (6)	0.58228 (7)	0.1059 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0647 (16)	0.0588 (18)	0.0572 (16)	0.0114 (14)	-0.0014 (14)	-0.0080 (14)
C2	0.0688 (17)	0.070 (2)	0.0692 (16)	0.0167 (16)	-0.0049 (15)	-0.0232 (13)
C3	0.0706 (18)	0.0432 (17)	0.0883 (19)	0.0018 (14)	-0.0139 (17)	-0.0167 (13)
C4	0.099 (2)	0.0429 (18)	0.086 (2)	-0.0020 (17)	-0.0028 (19)	0.0106 (16)
C5	0.088 (2)	0.0506 (18)	0.0687 (19)	-0.0036 (16)	0.0181 (16)	-0.0007 (15)
C6	0.0449 (13)	0.0404 (15)	0.0559 (15)	-0.0077 (11)	0.0023 (12)	-0.0126 (13)
C7	0.0447 (13)	0.0421 (15)	0.0497 (15)	-0.0055 (11)	0.0041 (11)	-0.0071 (12)
C8	0.0416 (12)	0.0425 (14)	0.0439 (14)	-0.0004 (11)	0.0024 (10)	-0.0035 (11)
C9	0.0385 (12)	0.0433 (15)	0.0485 (14)	0.0025 (10)	-0.0014 (11)	-0.0027 (12)
C10	0.0388 (12)	0.0432 (15)	0.0482 (14)	0.0006 (11)	-0.0034 (10)	-0.0004 (11)
C11	0.0452 (13)	0.0443 (15)	0.0450 (13)	0.0031 (11)	-0.0028 (11)	0.0019 (12)
C12	0.0530 (14)	0.0414 (15)	0.0479 (14)	0.0007 (12)	0.0052 (11)	0.0001 (12)
C13	0.0439 (12)	0.0471 (15)	0.0471 (13)	-0.0059 (12)	0.0000 (10)	-0.0003 (12)
C14	0.0540 (15)	0.0662 (19)	0.0544 (16)	0.0074 (14)	0.0049 (13)	-0.0018 (14)
C15	0.120 (3)	0.101 (3)	0.099 (3)	0.031 (2)	0.007 (2)	-0.033 (2)
C16	0.0640 (18)	0.104 (3)	0.091 (2)	-0.0119 (19)	0.0126 (16)	0.026 (2)
C17	0.0702 (17)	0.0496 (17)	0.0556 (16)	0.0215 (14)	-0.0020 (13)	0.0105 (13)
C18	0.0447 (13)	0.0441 (16)	0.0592 (17)	0.0053 (12)	0.0004 (11)	0.0064 (13)
C19	0.0730 (18)	0.065 (2)	0.076 (2)	0.0201 (17)	0.0068 (15)	0.0156 (16)
C20	0.078 (2)	0.069 (2)	0.115 (3)	0.0330 (17)	0.018 (2)	0.013 (2)
C21	0.0659 (19)	0.065 (2)	0.112 (3)	0.0099 (17)	0.0286 (18)	-0.014 (2)
C22	0.0799 (19)	0.069 (2)	0.0653 (19)	-0.0030 (18)	0.0187 (16)	-0.0046 (16)
C23	0.0703 (17)	0.0506 (17)	0.0615 (18)	0.0124 (14)	0.0001 (14)	0.0040 (14)
C24	0.0386 (13)	0.0631 (19)	0.0451 (15)	0.0009 (13)	-0.0026 (11)	0.0005 (12)
C25	0.0474 (14)	0.070 (2)	0.0742 (18)	0.0103 (14)	-0.0031 (13)	-0.0081 (15)
C26	0.0579 (17)	0.100 (3)	0.080 (2)	0.0289 (19)	0.0031 (15)	-0.0037 (19)
C27	0.0411 (16)	0.138 (3)	0.075 (2)	0.015 (2)	0.0063 (14)	0.023 (2)
C28	0.0423 (15)	0.117 (3)	0.082 (2)	-0.0142 (18)	-0.0024 (14)	0.024 (2)
C29	0.0479 (14)	0.0722 (19)	0.0652 (17)	-0.0065 (14)	-0.0031 (12)	0.0012 (15)
N1	0.0396 (11)	0.0478 (13)	0.0553 (12)	0.0014 (9)	-0.0010 (9)	-0.0058 (10)
N2	0.0776 (15)	0.0449 (13)	0.0497 (14)	-0.0107 (12)	-0.0008 (13)	-0.0059 (11)
01	0.0526 (9)	0.0512 (11)	0.0513 (11)	0.0034 (8)	-0.0048 (7)	-0.0116 (9)
02	0.1055 (18)	0.123 (2)	0.0690 (14)	0.0167 (16)	0.0285 (13)	-0.0203 (13)
O3	0.136 (2)	0.125 (2)	0.0645 (14)	0.0038 (17)	-0.0251 (14)	0.0137 (14)

$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	04	0 0404 (8)	0 0540 (11)	0.0565 (10)	-0.0071(8)	-0.0082(7)	0 0133 (8)
06 0.0485 (1) 0.072 (13) 0.0591 (11) 0.0070 (9) 0.0053 (8) 0.0097 (10) 07 0.0547 (9) 0.0422 (10) 0.0467 (9) 0.0116 (8) $-0.0055 (7)$ 0.0056 (8) C11 0.1104 (7) 0.0618 (5) 0.1454 (9) 0.0290 (5) $-0.0323 (6)$ $-0.0224 (6)$ Geometric parameters (Å, °) C1-C2 1.383 (4) C15-H115A 0.9600 C2-C3 1.355 (4) C16-H16A 0.9600 C3-C4 1.350 (4) C16-H16C 0.9600 C3-C4 1.380 (4) C17-O7 1.417 (3) C4-C5 1.380 (4) C17-H17A 0.9700 C5-C6 1.375 (4) C17-H17A 0.9700 C5-C6 1.375 (3) C19-C20 1.369 (4) C7-C1 1.500 (3) C18-C19 1.380 (3) C7-O1 1.438 (3) C19-C20 1.369 (4) C7-C8 1.557 (3) C20-C21 1.360 (4) C8-H2 1.497 (3) C22-C23 1.380 (4)	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	05	0.0541 (10)	0.0757 (13)	0.0465 (10)	0.0024 (9)	0.0008 (8)	0.0010 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	06	0.0485 (10)	0.0762 (13)	0.0591 (11)	0.0070 (9)	0.0053 (8)	0.0097 (10)
Cline Cline <t< td=""><td>C1 0.1104 (7) 0.0618 (5) 0.1434 (9) 0.0290 (5) -0.0323 (6) -0.0224 (6) Geometric parameters (Å, ?) C1-C6 1.383 (3) C15-H15A 0.9600 C1-H1 0.9300 C15-H15B 0.9600 C2-C3 1.355 (4) C16-H16B 0.9600 C3-C4 1.360 (4) C16-H16B 0.9600 C3-C4 1.360 (4) C17-C18 1.395 (3) C4-C5 1.380 (4) C17-C18 1.395 (3) C4-C5 1.380 (4) C17-H17A 0.9700 C5-C6 1.375 (4) C17-H17B 0.9700 C5-H5 0.9300 C18-C23 1.396 (4) C7-C8 1.535 (3) C19-H19 0.3800 C6-C7 1.500 (3) C18-C23 1.369 (4) C7-H7 0.9800 C20-C21 1.369 (4) C7-H7 0.9800 C21-H21 0.9300 C8-C9 1.537 (3) C21-C22 1.369 (4) C8-H8 0.9800 C21-H21 0</td><td>07</td><td>0.0547 (9)</td><td>0.0422(10)</td><td>0.0467 (9)</td><td>0.0116 (8)</td><td>-0.0005(7)</td><td>0.0056 (8)</td></t<>	C1 0.1104 (7) 0.0618 (5) 0.1434 (9) 0.0290 (5) -0.0323 (6) -0.0224 (6) Geometric parameters (Å, ?) C1-C6 1.383 (3) C15-H15A 0.9600 C1-H1 0.9300 C15-H15B 0.9600 C2-C3 1.355 (4) C16-H16B 0.9600 C3-C4 1.360 (4) C16-H16B 0.9600 C3-C4 1.360 (4) C17-C18 1.395 (3) C4-C5 1.380 (4) C17-C18 1.395 (3) C4-C5 1.380 (4) C17-H17A 0.9700 C5-C6 1.375 (4) C17-H17B 0.9700 C5-H5 0.9300 C18-C23 1.396 (4) C7-C8 1.535 (3) C19-H19 0.3800 C6-C7 1.500 (3) C18-C23 1.369 (4) C7-H7 0.9800 C20-C21 1.369 (4) C7-H7 0.9800 C21-H21 0.9300 C8-C9 1.537 (3) C21-C22 1.369 (4) C8-H8 0.9800 C21-H21 0	07	0.0547 (9)	0.0422(10)	0.0467 (9)	0.0116 (8)	-0.0005(7)	0.0056 (8)
Geometric parameters $(\overline{A}, 9)$ Init (g) </td <td>Geometric parameters $(J, °)$ Intrice Intrice Intrice Intrice Intrice Intrice Cl = C6 1.383 (3) C15—H15A 0.9600 Cl = C2 1.383 (4) C15—H15B 0.9600 C2 = C3 1.355 (4) C16—H16A 0.9600 C3 = C4 1.360 (4) C16—H16B 0.9600 C3 = C4 1.360 (4) C17—C18 1.505 (3) C4 = H4 0.9300 C17—H17A 0.9700 C5 = C6 1.375 (4) C17—H17A 0.9700 C5 = C6 1.375 (4) C17—H17A 0.9700 C5 = C6 1.375 (3) C19—C20 1.369 (4) C7 = C7 1.500 (3) C18—C19 1.380 (3) C7 = C7 1.500 (3) C20—C12 1.364 (4) C8—N2 1.497 (3) C20—C12 1.360 (4) C9—H1 1.472 (3) C21—C22 1.360 (4) C9—H1 1.472 (3) C22—C23 1.380 (4) C9—H1 1.472 (3) C24—C25 1.382 (4) <tr< td=""><td>Cl1</td><td>0.1104 (7)</td><td>0.0618(5)</td><td>0.1454 (9)</td><td>0.0290(5)</td><td>-0.0323(6)</td><td>-0.0224(6)</td></tr<></td>	Geometric parameters $(J, °)$ Intrice Intrice Intrice Intrice Intrice Intrice Cl = C6 1.383 (3) C15—H15A 0.9600 Cl = C2 1.383 (4) C15—H15B 0.9600 C2 = C3 1.355 (4) C16—H16A 0.9600 C3 = C4 1.360 (4) C16—H16B 0.9600 C3 = C4 1.360 (4) C17—C18 1.505 (3) C4 = H4 0.9300 C17—H17A 0.9700 C5 = C6 1.375 (4) C17—H17A 0.9700 C5 = C6 1.375 (4) C17—H17A 0.9700 C5 = C6 1.375 (3) C19—C20 1.369 (4) C7 = C7 1.500 (3) C18—C19 1.380 (3) C7 = C7 1.500 (3) C20—C12 1.364 (4) C8—N2 1.497 (3) C20—C12 1.360 (4) C9—H1 1.472 (3) C21—C22 1.360 (4) C9—H1 1.472 (3) C22—C23 1.380 (4) C9—H1 1.472 (3) C24—C25 1.382 (4) <tr< td=""><td>Cl1</td><td>0.1104 (7)</td><td>0.0618(5)</td><td>0.1454 (9)</td><td>0.0290(5)</td><td>-0.0323(6)</td><td>-0.0224(6)</td></tr<>	Cl1	0.1104 (7)	0.0618(5)	0.1454 (9)	0.0290(5)	-0.0323(6)	-0.0224(6)
Geometric parameters (Å, °) C1—C6 1.383 (3) C15—H15A 0.9600 C1—C2 1.383 (4) C15—H15B 0.9600 C1—H1 0.9300 C15—H15C 0.9600 C2—C3 1.355 (4) C16—H16A 0.9600 C3—C4 1.360 (4) C16—H16C 0.9600 C3—C4 1.360 (4) C17—C18 1.505 (3) C4—C5 1.380 (4) C17—C18 0.9700 C5—C6 1.375 (4) C17—H17A 0.9700 C5—H5 0.9300 C18—C23 1.370 (3) C6—C7 1.500 (3) C18—C19 1.380 (3) C7—O1 1.438 (3) C19—C20 1.369 (4) C7—C8 1.353 (3) C19—L19 0.9300 C8—N2 1.497 (3) C20—C21 1.364 (5) C9 1.537 (3) C21—C22 1.360 (4) C8—H8 0.9800 C21—H21 0.9300 C9—C10 1.522 (3) C24—C29 1.380 (4) C9—C11 1.518 (3)	Geometric parameters (Å. °) C1-C6 1.383 (3) C15-H15A 0.9600 C1-C2 1.383 (4) C15-H15B 0.9600 C1-H1 0.9300 C15-H15B 0.9600 C2-C3 1.355 (4) C16-H16A 0.9600 C2-H2 0.9300 C16-H16B 0.9600 C3-C1 1.360 (4) C16-H16C 0.9600 C3-C1 1.380 (4) C17-C18 1.505 (3) C4-C5 1.380 (4) C17-H17A 0.9700 C5-C6 1.375 (4) C17-H17B 0.9700 C5-C6 1.375 (3) C18-C19 1.380 (3) C7-O1 1.438 (3) C19-C20 1.369 (4) C7-C8 1.551 (3) C19-H19 0.9300 C7-H7 0.9800 C20-C21 1.360 (4) C8-C9 1.537 (3) C21-E22 1.360 (4) C8-N2 1.497 (3) C20-C22 1.360 (4) C8-H8 0.9800 C21-H21 0.9300 C9-H10 1.522 (3) C24-C2		0.1101(7)	0.0010 (0)	0.1101())	0.0290 (0)	0.0525 (0)	0.0221(0)
C1-C6 1.383 (3)C15-H15A 0.9600 C1-C2 1.383 (4)C15-H15B 0.9600 C1-H1 0.9300 C15-H15C 0.9600 C2-C3 1.355 (4)C16-H16A 0.9600 C3-C1 1.355 (4)C16-H16B 0.9600 C3-C1 1.742 (3)C17-O7 1.417 (3)C4-C5 1.380 (4)C17-C18 1.505 (3)C4-H4 0.9300 C17-H17A 0.9700 C5-C6 1.375 (4)C17-H17A 0.9700 C5-C6 1.375 (4)C17-H17B 0.9700 C5-C6 1.375 (3)C18-C19 1.380 (3)C7-C7 1.500 (3)C18-C19 1.380 (3)C7-C8 1.535 (3)C19-H19 0.9300 C7-C7 0.9800 C20-C21 1.364 (5)C8-M2 1.497 (3)C20-H20 0.9300 C8-C9 1.537 (3)C21-H21 0.9300 C9-N1 1.472 (3)C22-C23 1.380 (4)C9-C10 1.522 (3)C23-H22 0.9300 C9-H9 0.9800 C21-H21 0.9300 C9-H9 0.9800 C23-H23 0.9300 C10-C11 1.518 (3)C24-C25 1.382 (4)C10-C11 1.518 (3)C25-G26 1.382 (4)C10-C11 1.516 (3)C25-H25 0.9300 C11-C12 0.9800 C27-H27 0.9300 C11-C12 0.9800 C26-C27 1.374 (4)C12-C13 1.515 (3)C26-C26 1.332 (4)C11-C14 0.9800	C1—C6 1.383 (3) C15—H15A 0.9600 C1—C2 1.383 (4) C15—H15B 0.9600 C2—C3 1.355 (4) C16—H16A 0.9600 C2—C3 1.355 (4) C16—H16B 0.9600 C3—C4 1.360 (4) C16—H16B 0.9600 C3—C4 1.360 (4) C16—H16C 0.9600 C3—C1 1.742 (3) C17—O7 1.417 (3) C4—C5 1.380 (4) C17—H17A 0.9700 C5—C6 1.375 (4) C17—H17B 0.9700 C5—H5 0.9300 C18—C123 1.370 (3) C6—C7 1.500 (3) C18—C19 1.380 (4) C7—C8 1.535 (3) C19—H19 0.9300 C7—H7 0.9800 C20—C21 1.366 (4) C8—N2 1.497 (3) C20—C12 1.360 (4)	Geometric param	neters (Å, °)					
C1-C21.383 (4) $C15-H15B$ 0.9600 $C1-H1$ 0.9300 $C15-H15C$ 0.9600 $C2-C3$ 1.355 (4) $C16-H16A$ 0.9600 $C3-C4$ 1.360 (4) $C16-H16B$ 0.9600 $C3-C4$ 1.360 (4) $C16-H16C$ 0.9600 $C3-C4$ 1.360 (4) $C17-O7$ 1.417 (3) $C4-C5$ 1.380 (4) $C17-C18$ 1.505 (3) $C4-H4$ 0.9300 $C17-H17A$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17A$ 0.9700 $C5-H5$ 0.9300 $C18-C23$ 1.370 (3) $C7-O1$ 1.438 (3) $C19-C20$ 1.369 (4) $C7-O1$ 1.438 (3) $C19-C20$ 1.369 (4) $C7-C8$ 1.535 (3) $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ 1.364 (5) $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-C9$ 1.537 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H10$ 0.9800 $C23-H23$ 0.9300 $C9-H10$ 0.9800 $C24-C29$ 1.378 (3) $C10-O1$ 1.518 (3) $C25-C26$ 1.382 (4) $C10-H10$ 0.9800 $C25-H25$ 0.9300 $C12-C13$ 1.516 (3) $C27-H27$ 0.9300 $C1-H11$ 0.9800 $C25-H25$ 0.9300 $C12-C13$ 1.516 (3) $C25-H26$ 1.382 (4) $C11-O7$ 1.423 (3) $C26-H26$ 0.9300 $C12-C13$ 1.516	C1-C2 1.383 (4) $C15-H15B$ 0.9600 $C1-H1$ 0.9300 $C15-H15C$ 0.9600 $C2-C3$ 1.355 (4) $C16-H16A$ 0.9600 $C3-C4$ 1.300 (4) $C16-H16C$ 0.9600 $C3-C4$ 1.300 (4) $C17-C18$ 1.505 (3) $C4-C5$ 1.380 (4) $C17-C18$ 1.505 (3) $C4-C5$ 1.380 (4) $C17-C18$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17A$ 0.9700 $C5-C6$ 1.530 (3) $C18-C19$ 1.380 (3) $C7-C8$ 1.530 (3) $C19-C20$ 1.369 (4) $C7-C8$ 1.535 (3) $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ 1.364 (5) $C8-N2$ 1.497 (3) $C20-H20$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C9-N1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H19$ 0.9800 $C21-H21$ 0.9300 $C9-H10$ 0.9800 $C21-H21$ 0.9300 $C1-D7$ 1.423 (3) $C24-C29$ 1.378 (3) $C10-C11$ 1.518 (3) $C24-C29$ 1.374 (4) $C1-D7$ 1.423 (3) $C25-H25$ 0.9300 $C1-H11$ 0.9800 $C2-H27$ 1.382 (4) $C11-C12$ 1.516 (3) $C25-H25$ 0.9300 $C1-D7$ 1.423 (3) $C25-H25$ 0.9300 $C12-C13$ 1.515 (3) $C27-C28$ 1.382 (4)<	C1—C6		1.383 (3)	C1	5—H15A	0.960	00
C1-H1 $0,9300$ C15-H15C $0,9600$ C2-G31.355 (4)C16-H16A $0,9600$ C2-H2 $0,9300$ C16-H16B $0,9600$ C3-C41.360 (4)C16-H16C $0,9600$ C3-C111.742 (3)C17-O71.417 (3)C4-C51.380 (4)C17-C181.505 (3)C4-H4 $0,9300$ C18-C231.370 (3)C5-C61.375 (4)C17-H17A $0,9700$ C5-C71.500 (3)C18-C191.380 (3)C7-O11.438 (3)C19-C201.369 (4)C7-C81.535 (3)C19-H19 $0,9300$ C7-H7 $0,9800$ C20-H20 $0,9300$ C8-C91.537 (3)C20-H20 $0,9300$ C8-C91.537 (3)C21-H21 $0,9300$ C9-N11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C22-H22 $0,9300$ C9-H9 $0,9800$ C21-H21 $0,9300$ C9-H9 $0,9800$ C24-C29 $1.378 (3)$ C10-O111.518 (3)C24-C29 $1.378 (3)$ C10-C111.516 (3)C25-C26 $1.382 (4)$ C11-C121.516 (3)C26-C27 $1.374 (4)$ C12-C131.515 (3)C26-C27 $1.374 (4)$ C12-C131.515 (3)C26-H26 $0,9300$ C12-C141.437 (3)C26-H26 $0,9300$ C12-C131.515 (3)C26-H26 $0,9300$ C12-C141.435 (3)C26-H26 $0,9300$ C12-C151.421 (3)C26-H26 $0,9300$	C1—H1 0.9300 C15—H15C 0.9600 C2—C3 1.355 (4) C16—H16A 0.9600 C3—C4 1.360 (4) C16—H16B 0.9600 C3—C1 1.742 (3) C17—O7 1.417 (3) C4—C5 1.380 (4) C17—C18 1.505 (3) C4—H4 0.9300 C17—H17A 0.9700 C5—C6 1.375 (4) C17—H17B 0.9700 C5—C6 1.370 (3) C18—C13 1.380 (3) C7—O1 1.438 (3) C19—H13 0.9300 C7—O1 1.438 (3) C19—H19 0.9300 C7—C8 1.535 (3) C20—H20 1.360 (4) C8—N2 1.497 (3) C20—H20 0.9300 C8—N2 1.497 (3) C21—C22 1.380 (4) C9—C10 1.522 (3) C22—C1 1.380 (4) C9—C10 1.522 (3) C24—C29 1.380 (4) C9—H9 0.9800 C23—H22 0.9300 C9—H9 0.9800 C24—C12 1.381 (3)	C1—C2		1.383 (4)	C1	5—H15B	0.960	00
C2-C31.355 (4) $C16-H16A$ 0.9600 $C2-H2$ 0.9300 $C16-H16B$ 0.9600 $C3-C4$ 1.360 (4) $C16-H16C$ 0.9600 $C3-C11$ 1.742 (3) $C17-O7$ 1.417 (3) $C4-C5$ 1.380 (4) $C17-C18$ 1.505 (3) $C4-H4$ 0.9300 $C17-H17A$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17B$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17B$ 0.9700 $C5-H5$ 0.9300 $C18-C23$ 1.370 (3) $C6-C7$ 1.500 (3) $C18-C19$ 1.380 (3) $C7-O1$ 1.438 (3) $C19-C20$ 1.364 (5) $C8-N2$ 1.497 (3) $C20-H20$ 0.9300 $C7-H7$ 0.9800 $C20-H21$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C9-N1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-C11$ 1.518 (3) $C24-C25$ 1.382 (4) $C10-C11$ 1.518 (3) $C25-C26$ 1.382 (4) $C11-H11$ 0.9800 $C25-H25$ 0.9300 $C12-C13$ 1.515 (3) $C27-C28$ 1.374 (4) $C12-C13$ 1.515 (3) $C27-C28$ 1.374 (4) $C12-C5$ 1.421 (3) $C26-H25$ 0.9300 $C1-H11$ 0.9800 $C27-H27$ 0.9300 $C1-H11$ 0.9800 $C27-H27$ 0.9300 C	C2-C31.355 (4) $C16-H16A$ 0.9600 $C2-H2$ 0.9300 $C16-H16B$ 0.9600 $C3-C4$ 1.360 (4) $C16-H16C$ 0.9600 $C3-C11$ 1.742 (3) $C17-O7$ 1.417 (3) $C4-C5$ 1.380 (4) $C17-C18$ 1.505 (3) $C4-H4$ 0.9300 $C17-H17A$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17B$ 0.9700 $C5-C6$ 1.375 (3) $C18-C19$ 1.380 (3) $C7-C1$ 1.500 (3) $C18-C19$ 1.380 (3) $C7-C8$ 1.533 (3) $C19-C19$ 0.9300 $C7-C8$ 1.533 (3) $C19-H19$ 0.9300 $C7-C8$ 1.537 (3) $C20-C21$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 0.9300 $C8-C9$ 1.537 (3) $C22-C23$ 1.380 (4) $C9-H19$ 0.9800 $C23-H12$ 0.9300 $C9-H19$ 0.9800 $C24-H12$ 0.9300 $C9-H19$ 0.9800 $C24-C29$ 1.378 (3) $C10-C11$ 1.518 (3) $C24-C25$ 1.382 (4) $C10-H10$ 0.9800 $C24-H14$ 1.437 (3) $C11-O7$ 1.423 (3) $C25-C26$ 1.382 (4) $C11-O1$ 1.515 (3) $C26-C17$ 1.374 (4) $C12-C13$ 1.515 (3) $C26-C17$ 1.374 (4) $C12-C13$ 1.515 (3) $C28-C29$ 1.377 (4) $C12-C14$ 0.9800 $C27-H27$ 0.9300 <t< td=""><td>C1—H1</td><td></td><td>0.9300</td><td>C1</td><td>5—H15C</td><td>0.960</td><td>00</td></t<>	C1—H1		0.9300	C1	5—H15C	0.960	00
C2-H20.9300 $C16-H16B$ 0.9600 $C3-C4$ 1.360 (4) $C16-H16C$ 0.9600 $C3-C11$ 1.742 (3) $C17-O7$ 1.417 (3) $C4-C5$ 1.380 (4) $C17-C18$ 1.505 (3) $C4-H4$ 0.9300 $C17-H17A$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17B$ 0.9700 $C5-C6$ 1.375 (4) $C17-H17B$ 0.9700 $C5-C6$ 1.375 (4) $C18-C23$ 1.370 (3) $C6-C7$ 1.500 (3) $C18-C19$ 1.380 (3) $C7-O1$ 1.438 (3) $C19-C20$ 1.369 (4) $C7-C8$ 1.535 (3) $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ 1.364 (5) $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ 1.432 (3) $C24-C25$ 1.382 (4) $C10-H10$ 0.9800 $C24-H1$ 1.437 (3) $C1-C11$ 1.516 (3) $C25-H25$ 0.9300 $C11-H11$ 0.9800 $C2-H27$ 1.374 (4) $C12-C13$ 1.515 (3) $C27-C28$ 1.366 (5) $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C1-C11$ 1.515 (3) $C27-C28$ 1.366 (5) $C1-C13$ 1.515 (3) $C27-C28$ 1.366 (5) $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C1-C13$ 1.5	C2-H2 0,9300 C16-H16B 0,9600 C3-C4 1,360 (4) C16-H16C 0,9600 C3-C11 1,742 (3) C17-O7 1,417 (3) C4-C5 1,380 (4) C17-C18 1,505 (3) C4-H4 0,9300 C17-H17A 0,9700 C5-G6 1,375 (4) C17-H17B 0,9700 C5-H5 0,9300 C18-C19 1,380 (3) C7-O1 1,438 (3) C19-C20 1,369 (4) C7-C8 1,537 (3) C20-C21 1,360 (4) C8-N2 1,497 (3) C20-H20 0,9300 C8-C9 1,537 (3) C21-C22 1,360 (4) C8-M8 0,9800 C21-H21 0,9300 C9-N1 1,472 (3) C22-C33 1,380 (4) C9-N1 1,472 (3) C24-C29 1,378 (3) C10-C11 1,518 (3) C24-C25 0,9300 C10-H10 0,9800 C24-C25 1,382 (4) C11-C12 1,515 (3) C25-C26 1,382 (4)	C2—C3		1.355 (4)	C1	6—H16A	0.960	00
C3-C41.360 (4)C16-H16C0.9600C3-C111.742 (3)C17-O71.417 (3)C4-C51.380 (4)C17-C181.505 (3)C4-H40.9300C17-H17A0.9700C5-C61.375 (4)C17-H17B0.9700C5-H50.9300C18-C231.370 (3)C6-C71.500 (3)C18-C191.380 (3)C7-C81.535 (3)C19-H190.9300C7-C71.535 (3)C19-H190.9300C7-C81.537 (3)C20-C211.364 (5)C8-N21.497 (3)C20-H200.9300C8-C91.537 (3)C21-H210.9300C9-N11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C22-H220.9300C9-H90.9800C23-H230.9300C10-O41.432 (3)C24-C291.378 (3)C10-C111.518 (3)C24-C251.382 (4)C10-H100.9800C24-H11.437 (3)C11-C121.516 (3)C25-G261.382 (4)C11-C141.518 (3)C25-G261.382 (4)C11-C151.515 (3)C26-G271.374 (4)C12-O51.421 (3)C26-H260.9300C13-O61.421 (3)C26-H260.9300C13-O61.421 (3)C28-H280.9300C13-O41.414 (3)C28-H280.9300C13-O41.414 (3)C28-H280.9300C13-O41.412 (3)N1-O11.433 (2)C14-O51.423 (3)N1-O1 </td <td>C3-C41.360 (4)C16-H16C0.9600C3-C111.742 (3)C17-O71.417 (3)C4-C51.380 (4)C17-C181.505 (3)C4-H40.9300C17-H17A0.9700C5-C61.375 (4)C17-H17B0.9700C5-H50.9300C18-C231.370 (3)C6-C71.500 (3)C18-C191.380 (3)C7-O11.438 (3)C19-C201.369 (4)C7-C81.535 (3)C19-L190.9300C7-H70.9800C20-C211.364 (5)C8-N21.497 (3)C20-L221.360 (4)C8-N21.497 (3)C22-C231.380 (4)C9-N11.472 (3)C22-L1220.9300C9-N11.472 (3)C24-C291.380 (4)C9-C101.522 (3)C24-C291.382 (4)C10-C111.518 (3)C24-C251.382 (4)C10-C111.516 (3)C25-C261.382 (4)C11-O71.423 (3)C25-C261.382 (4)C11-C121.516 (3)C26-C271.374 (3)C12-O51.421 (3)C26-C271.374 (4)C12-O51.421 (3)C26-C271.374 (4)C13-O61.405 (3)C28-C291.377 (4)C13-O61.423 (3)C26-C271.374 (3)C13-O61.423 (3)C26-C271.377 (4)C13-O61.423 (3)C26-C271.377 (4)C13-O61.423 (3)N1-O11.433 (2)C14-O51.292 (3)N2-O21.191 (3)C14-O5<</td> <td>С2—Н2</td> <td></td> <td>0.9300</td> <td>C1</td> <td>6—H16B</td> <td>0.960</td> <td>00</td>	C3-C41.360 (4)C16-H16C0.9600C3-C111.742 (3)C17-O71.417 (3)C4-C51.380 (4)C17-C181.505 (3)C4-H40.9300C17-H17A0.9700C5-C61.375 (4)C17-H17B0.9700C5-H50.9300C18-C231.370 (3)C6-C71.500 (3)C18-C191.380 (3)C7-O11.438 (3)C19-C201.369 (4)C7-C81.535 (3)C19-L190.9300C7-H70.9800C20-C211.364 (5)C8-N21.497 (3)C20-L221.360 (4)C8-N21.497 (3)C22-C231.380 (4)C9-N11.472 (3)C22-L1220.9300C9-N11.472 (3)C24-C291.380 (4)C9-C101.522 (3)C24-C291.382 (4)C10-C111.518 (3)C24-C251.382 (4)C10-C111.516 (3)C25-C261.382 (4)C11-O71.423 (3)C25-C261.382 (4)C11-C121.516 (3)C26-C271.374 (3)C12-O51.421 (3)C26-C271.374 (4)C12-O51.421 (3)C26-C271.374 (4)C13-O61.405 (3)C28-C291.377 (4)C13-O61.423 (3)C26-C271.374 (3)C13-O61.423 (3)C26-C271.377 (4)C13-O61.423 (3)C26-C271.377 (4)C13-O61.423 (3)N1-O11.433 (2)C14-O51.292 (3)N2-O21.191 (3)C14-O5<	С2—Н2		0.9300	C1	6—H16B	0.960	00
C3-Cl1 1.742 (3) $C17-O7$ 1.417 (3)C4-C5 1.380 (4) $C17-C18$ 1.505 (3)C4-H4 0.9300 $C17-H17A$ 0.9700 C5-C6 1.375 (4) $C17-H17B$ 0.9700 C5-H5 0.9300 $C18-C23$ 1.370 (3)C6-C7 1.500 (3) $C18-C19$ 1.380 (3)C7-O1 1.438 (3) $C19-C20$ 1.369 (4)C7-C8 1.535 (3) $C19-H19$ 0.9300 C7-H7 0.9800 $C20-C21$ 1.364 (5)C8-N2 1.497 (3) $C20-H20$ 0.9300 C8-C9 1.537 (3) $C21-C22$ 1.360 (4)C8-H8 0.9800 $C21-H21$ 0.9300 C9-H10 1.522 (3) $C22-H22$ 0.9300 C9-H9 0.9800 $C22-H12$ 0.9300 C9-H9 0.9800 $C22-H12$ 0.9300 C10-O4 1.432 (3) $C24-C29$ 1.378 (3)C10-O4 1.432 (3) $C24-C25$ 1.382 (4)C10-H10 0.9800 $C24-H1$ 1.437 (3)C11-O7 1.423 (3) $C25-H25$ 0.9300 C11-O11 1.516 (3) $C25-H25$ 0.9300 C11-C12 1.516 (3) $C25-H25$ 0.9300 C11-H11 0.9800 $C27-H27$ 0.9300 C12-C13 1.515 (3) $C27-C28$ 1.376 (4)C12-O5 1.421 (3) $C26-H26$ 0.9300 C12-H12 0.9800 $C27-H27$ 0.9300 C13-O4 1.4414 (3) $C28-C29$	C3-Cl11.742 (3)C17-O71.417 (3)C4-C51.380 (4)C17-C181.505 (3)C4-H40.9300C17-H17A0.9700C5-C61.375 (4)C17-H17B0.9700C5-H50.9300C18-C231.370 (3)C6-C71.500 (3)C18-C191.380 (3)C7-C81.535 (3)C19-C201.369 (4)C7-C81.535 (3)C19-H190.9300C7-H70.9800C20-C211.360 (4)C8-M21.497 (3)C20-H200.9300C8-C91.537 (3)C21-H210.9300C9-N11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C22-H220.9300C9-H90.9800C23-H230.9300C9-H90.9800C24-C251.382 (4)C10-C111.518 (3)C24-C251.382 (4)C10-H100.9800C24-H11.437 (3)C11-O71.423 (3)C25-C261.382 (4)C11-H110.9800C26-H260.9300C12-C121.516 (3)C26-H260.9300C12-H120.9800C26-H260.9300C12-H110.9800C26-H260.9300C12-H120.9800C27-H270.9300C12-H110.9800C26-H260.9300C12-H120.9800C27-H270.9300C12-H110.9800C26-H260.9300C12-H120.9800C27-H270.9300C12-H110.9800C26-H260.9300 <t< td=""><td>C3—C4</td><td></td><td>1.360 (4)</td><td>C1</td><td>6—H16C</td><td>0.960</td><td>00</td></t<>	C3—C4		1.360 (4)	C1	6—H16C	0.960	00
C4-C5 $1.380 (4)$ $C17-C18$ $1.505 (3)$ $C4-H4$ 0.9300 $C17-H17A$ 0.9700 $C5-C6$ $1.375 (4)$ $C17-H17B$ 0.9700 $C5-H5$ 0.9300 $C18-C23$ $1.370 (3)$ $C6-C7$ $1.500 (3)$ $C18-C19$ $1.380 (3)$ $C7-O1$ $1.438 (3)$ $C19-C20$ $1.369 (4)$ $C7-C8$ $1.535 (3)$ $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ $1.360 (4)$ $C8-C9$ $1.537 (3)$ $C21-C22$ 0.9300 $C8-C9$ $1.537 (3)$ $C21-C22$ 0.9300 $C9-N1$ $1.472 (3)$ $C22-C13$ $1.380 (4)$ $C9-C10$ $1.522 (3)$ $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C9-H9$ 0.9800 $C24-C29$ $1.378 (3)$ $C10-C11$ $1.518 (3)$ $C24-C25$ $1.382 (4)$ $C11-O7$ $1.423 (3)$ $C25-C26$ $1.382 (4)$ $C11-O7$ $1.423 (3)$ $C25-C26$ $1.382 (4)$ $C11-C12$ $1.516 (3)$ $C25-H25$ 0.9300 $C1-H10$ 0.9800 $C24-H26$ 0.9300 $C1-H11$ 0.9800 $C27-H27$ 0.9300 $C12-C13$ $1.515 (3)$ $C27-C28$ $1.377 (4)$ $C12-O5$ $1.421 (3)$ $C28-H28$ 0.9300 $C1-H12$ 0.9800 $C27-H27$ 0.9300 $C1-H12$ 0.9800 $C27-H27$ 0.9300 $C1-H13$ 0.9800 $C27-H28$ 0.9300 $C1-H14$ <	C4—C51.380 (4)C17—C181.505 (3)C4—H40.9300C17—H17A0.9700C5—C61.375 (4)C17—H17B0.9700C5—C61.370 (3)C18—C231.370 (3)C6—C71.500 (3)C18—C191.380 (3)C7—O11.438 (3)C19—C201.369 (4)C7—C81.535 (3)C19—H190.9300C7—H70.9800C20—C211.364 (5)C8—N21.497 (3)C20—H200.9300C8—C91.537 (3)C21—C221.360 (4)C8—H80.9800C21—H210.9300C9—N11.472 (3)C22—C231.380 (4)C9—C101.522 (3)C22—H220.9300C9—H90.9800C23—H230.9300C10—C111.518 (3)C24—C291.378 (3)C10—C111.518 (3)C25—C261.382 (4)C11—C121.516 (3)C25—H250.9300C11—C121.516 (3)C25—H250.9300C11—C121.516 (3)C25—H250.9300C11—C121.516 (3)C25—H250.9300C12—C131.515 (3)C25—H250.9300C14—O61.423 (3)C28—C291.377 (4)C12—O51.421 (3)C28—C291.377 (4)C13—O41.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—O51.429 (3)N2—O21.191 (3)C14—O51.429 (3)N2—O31.203 (3)C14—O51.429 (3)N2—O	C3—C11		1.742 (3)	C1	7—07	1.417	7 (3)
C4-H40.9300C17-H17A0.9700C5-C61.375 (4)C17-H17B0.9700C5-H50.9300C18-C231.370 (3)C6-C71.500 (3)C19-C191.380 (3)C7-O11.438 (3)C19-C201.369 (4)C7-C81.535 (3)C19-H190.9300C7-H70.9800C20-C211.364 (5)C8-N21.497 (3)C20-H200.9300C8-C91.537 (3)C21-C221.360 (4)C9-N11.472 (3)C22-C231.380 (4)C9-N11.472 (3)C22-H220.9300C9-H90.9800C23-H230.9300C9-H90.9800C24-C251.382 (4)C10-C111.518 (3)C25-C261.382 (4)C10-C121.516 (3)C25-C261.382 (4)C11-C121.516 (3)C26-C271.374 (4)C12-C131.515 (3)C26-C271.374 (4)C12-C140.9800C26-H260.9300C12-C151.423 (3)C26-H260.9300C12-H120.9800C27-H270.9300C13-O61.425 (3)C28-C291.377 (4)C13-O41.414 (3)C28-H280.9300C13-O41.414 (3)C28-H280.9300C13-O41.423 (3)NI-O11.433 (2)C13-O41.429 (3)N2-O21.191 (3)C13-O41.429 (3)N2-O21.191 (3)C13-O41.429 (3)N2-O21.191 (3)	C4-H40.9300C17-H17A0.9700C5-C61.375 (4)C17-H17B0.9700C5-H50.9300C18-C231.370 (3)C6-C71.500 (3)C18-C191.380 (3)C7-O11.438 (3)C19-C201.369 (4)C7-C81.535 (3)C19-H190.9300C7-H70.9800C20-C211.364 (5)C8-N21.537 (3)C21-H210.9300C8-C91.537 (3)C21-C221.360 (4)C8-M80.9800C21-H210.9300C9-M11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C24-C290.9300C9-H90.9800C24-H230.9300C10-O41.432 (3)C24-C291.378 (3)C10-C111.518 (3)C24-C251.382 (4)C11-O71.423 (3)C25-H250.9300C11-H100.9800C24-H210.9300C11-O71.423 (3)C25-H250.9300C11-H110.9800C26-C271.374 (4)C12-O51.515 (3)C27-C281.366 (5)C12-H120.9800C27-H270.9300C13-O41.405 (3)C28-C291.377 (4)C13-O41.421 (3)C28-H280.9300C13-H130.9800C29-H1290.9300C13-H130.9800C29-H290.9300C13-H130.9800C28-H280.9300C14-O61.423 (3)N1-O11.433 (2)C14-O51.429 (3)N2-O21.191 (3) <td>C4—C5</td> <td></td> <td>1.380 (4)</td> <td>C1</td> <td>7—C18</td> <td>1.505</td> <td>5 (3)</td>	C4—C5		1.380 (4)	C1	7—C18	1.505	5 (3)
CSC6 $1.375 (4)$ $C17$ H17B 0.9700 CSH5 0.9300 $C18$ C23 $1.370 (3)$ C6C7 $1.500 (3)$ $C18$ C19 $1.380 (3)$ C701 $1.438 (3)$ $C19$ C20 $1.369 (4)$ C7C8 $1.535 (3)$ $C19$ H19 0.9300 C7H7 0.9800 $C20$ C21 $1.364 (5)$ C8N2 $1.497 (3)$ $C20$ H20 0.9300 C8C9 $1.537 (3)$ $C21$ C22 $1.360 (4)$ C8H8 0.9800 $C21$ H21 0.9300 C9N1 $1.472 (3)$ $C22$ C23 $1.380 (4)$ C9C10 $1.522 (3)$ $C24$ C29 0.9300 C9H9 0.9800 $C23$ H23 0.9300 C10C4 $1.432 (3)$ $C24$ C29 $1.378 (3)$ C10-C11 $1.518 (3)$ $C24$ C25 $1.382 (4)$ C10-C11 $1.518 (3)$ $C25$ C26 $1.382 (4)$ C10-C11 0.9800 $C26$ H25 0.9300 C11C12 $1.516 (3)$ $C25$ C26 $1.382 (4)$ C12O5 $1.421 (3)$ $C26$ H26 0.9300 C12C13 $1.515 (3)$ $C27$ C28 0.9300 C12C13 $1.515 (3)$ $C27$ H27 0.9300 C12H12 0.9800 $C27$ -H27 0.9300 C1306 $1.405 (3)$ $C28$ H28 0.9300 C1304 $1.414 (3)$ $C28$ -H28 0.9300 C1304 $1.423 (3)$ N -O1 $1.433 (2)$ C1405 $1.429 (3)$ $N2$ -O2 $1.191 (3)$ <	CS-C6 1.375 (4)C17-H17B 0.9700 C5-H5 0.9300 C18-C23 1.370 (3)C6-C7 1.500 (3)C18-C19 1.380 (3)C7-C01 1.438 (3)C19-C20 1.369 (4)C7-C8 1.355 (3)C19-H19 0.9300 C7-H7 0.9800 C20-C21 1.364 (5)C8-N2 1.497 (3)C20-H20 0.9300 C8-C9 1.537 (3)C21-H21 0.9300 C8-H8 0.9800 C21-H21 0.9300 C9-N1 1.472 (3)C22-C23 1.380 (4)C9-C10 1.522 (3)C22-H22 0.9300 C9-H9 0.9800 C23-H23 0.9300 C10-O4 1.432 (3)C24-C29 1.378 (3)C10-C11 1.518 (3)C24-C25 1.382 (4)C10-H10 0.9800 C24-N1 1.437 (3)C11-O7 1.423 (3)C25-C26 1.382 (4)C11-H11 0.9800 C26-H25 0.9300 C12-O5 1.421 (3)C26-H26 0.9300 C12-C13 1.515 (3)C27-C28 1.366 (5)C12-H12 0.9800 C27-H27 0.9300 C13-O6 1.405 (3)C28-H28 0.9300 C13-H13 0.9800 C27-H27 0.9300 C13-H13 0.9800 C27-H27 0.9300 C13-H13 0.9800 C27-H29 0.9300 C13-H13 0.9800 C29-H29 0.9300 C13-H13 0.9800 C29-H29 0.9300 C14-C15 1.500 (4)<	C4—H4		0.9300	C1	7—H17A	0.970	00
CS-H5 0.9300 $C18-C23$ $1.370 (3)$ C6-C7 $1.500 (3)$ $C18-C19$ $1.380 (3)$ C7-O1 $1.438 (3)$ $C19-C20$ $1.369 (4)$ C7-C8 $1.535 (3)$ $C19-H19$ 0.9300 C7-H7 0.9800 $C20-C21$ $1.364 (5)$ C8-N2 $1.497 (3)$ $C20-H20$ 0.9300 C8-C9 $1.537 (3)$ $C21-C22$ $1.360 (4)$ C8-H8 0.9800 $C21-H21$ 0.9300 C9-N1 $1.472 (3)$ $C22-C23$ $1.380 (4)$ C9-C10 $1.522 (3)$ $C22-H22$ 0.9300 C9-H9 0.9800 $C23-H23$ 0.9300 C10-C11 $1.518 (3)$ $C24-C25$ $1.382 (4)$ C10-C11 $1.518 (3)$ $C24-C25$ $1.382 (4)$ C10-C11 $1.518 (3)$ $C25-L26$ $1.382 (4)$ C11-C12 $1.516 (3)$ $C25-L26$ $1.382 (4)$ C11-C12 $1.516 (3)$ $C25-L26$ $1.382 (4)$ C12-C5 $1.421 (3)$ $C26-L27$ $1.374 (4)$ C12-O5 $1.421 (3)$ $C27-L28$ 0.9300 C12-C13 $1.515 (3)$ $C27-C28$ $1.366 (5)$ C12-C13 $1.515 (3)$ $C27-C28$ $1.377 (4)$ C13-O6 $1.405 (3)$ $C28-L29$ $1.377 (4)$ C13-O4 $1.414 (3)$ $C28-H28$ 0.9300 C13-O4 $1.414 (3)$ $C28-H28$ 0.9300 C13-O4 $1.423 (3)$ $N1-O1$ $1.433 (2)$ C14-O5 $1.429 (3)$ $N2-O3$ $1.903 (3)$	CS-H50.9300C18-C231.370 (3)C6-C71.500 (3)C18-C191.380 (3)C7-O11.438 (3)C19-C201.369 (4)C7-C81.535 (3)C19-H190.9300C7-H70.9800C20-C211.364 (5)C8-N21.497 (3)C20-H200.9300C8-C91.537 (3)C21-C221.360 (4)C8-H80.9800C21-H210.9300C9-N11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C22-H230.9300C9-H90.9800C23-H230.9300C10-O41.432 (3)C24-C291.378 (3)C10-C111.518 (3)C24-C251.382 (4)C10-H100.9800C24-N11.437 (3)C11-O71.423 (3)C25-C261.382 (4)C11-H110.9800C26-C271.374 (4)C12-O51.421 (3)C26-C281.366 (5)C12-H120.9800C27-H270.9300C13-O61.405 (3)C28-C291.377 (4)C13-O41.414 (3)C28-C291.377 (4)C13-O41.414 (3)C28-C291.377 (4)C13-O41.414 (3)C28-C291.377 (4)C13-O51.421 (3)C28-C291.377 (4)C13-O61.405 (3)C28-C291.377 (4)C13-O61.423 (3)N1-O11.433 (2)C14-O51.429 (3)N2-O21.191 (3)C14-O51.429 (3)N2-O31.203 (3)C14-O51.429 (3)	C5—C6		1.375 (4)	C1	7—H17B	0.970	00
C6-C7 $1.500 (3)$ $C18-C19$ $1.380 (3)$ $C7-O1$ $1.438 (3)$ $C19-C20$ $1.369 (4)$ $C7-C8$ $1.535 (3)$ $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ $1.364 (5)$ $C8-N2$ $1.497 (3)$ $C20-H20$ 0.9300 $C8-C9$ $1.537 (3)$ $C21-C22$ $1.360 (4)$ $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ $1.472 (3)$ $C22-C23$ $1.380 (4)$ $C9-C10$ $1.522 (3)$ $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ $1.432 (3)$ $C24-C29$ $1.378 (3)$ $C10-C11$ $1.518 (3)$ $C24-C25$ $1.382 (4)$ $C10-H10$ 0.9800 $C24-N1$ $1.437 (3)$ $C11-O7$ $1.423 (3)$ $C25-C26$ $1.382 (4)$ $C11-O7$ $1.423 (3)$ $C26-C27$ $1.374 (4)$ $C12-C13$ $1.515 (3)$ $C27-C28$ $1.366 (5)$ $C12-C13$ $1.515 (3)$ $C28-H26$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ $1.405 (3)$ $C28-H28$ 0.9300 $C13-O4$ $1.414 (3)$ $C28-H28$ 0.9300 $C13-O4$ $1.414 (3)$ $C28-H28$ 0.9300 $C13-O4$ $1.429 (3)$ $N1-O1$ $1.433 (2)$ $C14-O5$ $1.429 (3)$ $N2-O2$ $1.191 (3)$ <	C6-C7 $1.500 (3)$ $C18-C19$ $1.380 (3)$ $C7-O1$ $1.438 (3)$ $C19-C20$ $1.369 (4)$ $C7-C8$ $1.535 (3)$ $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ $1.364 (5)$ $C8-N2$ $1.497 (3)$ $C20-H20$ 0.9300 $C8-C9$ $1.537 (3)$ $C21-C22$ $1.360 (4)$ $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-H1$ $1.472 (3)$ $C22-C23$ $1.380 (4)$ $C9-C10$ $1.522 (3)$ $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C9-H9$ 0.9800 $C24-C29$ $1.378 (3)$ $C10-C11$ $1.518 (3)$ $C24-C25$ $1.382 (4)$ $C1-C11$ $1.518 (3)$ $C25-C26$ $1.382 (4)$ $C1-C12$ $1.516 (3)$ $C25-H25$ 0.9300 $C11-H11$ 0.9800 $C26-C27$ $1.374 (4)$ $C12-O5$ $1.421 (3)$ $C26-H26$ 0.9300 $C1-H11$ 0.9800 $C27-H27$ 0.9300 $C12-C13$ $1.515 (3)$ $C27-C28$ $1.366 (5)$ $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ $1.405 (3)$ $C28-H28$ 0.9300 $C13-O4$ $1.414 (3)$ $C28-H28$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C14-O5$ $1.429 (3)$ $N1-O1$ $1.433 (2)$ $C14-O5$ $1.429 (3)$ $N2-O2$ $1.191 (3)$ $C1$	С5—Н5		0.9300	C1	8—C23	1.370) (3)
C7-O1 $1.438(3)$ $C19-C20$ $1.369(4)$ $C7-C8$ $1.535(3)$ $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ $1.364(5)$ $C8-N2$ $1.497(3)$ $C20-H20$ 0.9300 $C8-C9$ $1.537(3)$ $C21-C22$ $1.360(4)$ $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ $1.472(3)$ $C22-C23$ $1.380(4)$ $C9-C10$ $1.522(3)$ $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ $1.432(3)$ $C24-C29$ $1.378(3)$ $C10-C11$ $1.518(3)$ $C24-C25$ $1.382(4)$ $C1-C12$ $1.516(3)$ $C25-C26$ $1.382(4)$ $C11-O7$ $1.423(3)$ $C25-C26$ $1.382(4)$ $C11-C12$ $1.516(3)$ $C25-H25$ 0.9300 $C11-H11$ 0.9800 $C26-C27$ $1.374(4)$ $C12-O5$ $1.421(3)$ $C26-H26$ 0.9300 $C1-H12$ 0.9800 $C27-H27$ 0.9300 $C12-C13$ $1.515(3)$ $C27-C28$ $1.366(5)$ $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ $1.405(3)$ $C28-C29$ $1.377(4)$ $C13-O4$ $1.414(3)$ $C28-H28$ 0.9300 $C13-O4$ $1.414(3)$ $C28-H28$ 0.9300 $C14-O5$ $1.429(3)$ $N-O2$ $1.191(3)$ $C14-O5$ $1.429(3)$ $N2-O2$ $1.191(3)$	C7-O1 1.438 (3) $C19-C20$ 1.369 (4) $C7-C8$ 1.535 (3) $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ 1.364 (5) $C8-N2$ 1.497 (3) $C20-H20$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-C41$ 1.432 (3) $C24-C29$ 1.378 (3) $C10-C11$ 1.518 (3) $C24-C25$ 1.382 (4) $C11-P10$ 0.9800 $C24-N1$ 1.437 (3) $C11-P10$ 0.9800 $C26-C27$ 1.374 (4) $C12-O5$ 1.421 (3) $C26-H26$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C29-H29$ 0.9300 $C13-O6$ 1.405 (3) $C28-C29$ 1.377 (4) $C13-O4$ 1.414 (3) $C28-H28$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C14-O5$ 1.429 (3) $N1-O1$ 1.433 (2) $C14-O5$ 1.429 (3) $N2-O2$ 1.911 (3) $C14-O5$ 1.429 (3) $N2-O2$ 1.911 (3) $C14-O5$ 1.429 (3) $N2-O2$ 1.995 $C4-C1-$	С6—С7		1.500 (3)	C1	8—C19	1.380) (3)
C7-C8 $1.535 (3)$ $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ $1.364 (5)$ $C8-N2$ $1.497 (3)$ $C20-H20$ 0.9300 $C8-C9$ $1.537 (3)$ $C21-C22$ $1.360 (4)$ $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ $1.472 (3)$ $C22-C23$ $1.380 (4)$ $C9-C10$ $1.522 (3)$ $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ $1.432 (3)$ $C24-C29$ $1.378 (3)$ $C10-C11$ $1.518 (3)$ $C24-C25$ $1.382 (4)$ $C11-O7$ $1.423 (3)$ $C25-C26$ $1.382 (4)$ $C11-O7$ $1.423 (3)$ $C25-H25$ 0.9300 $C11-H11$ 0.9800 $C26-C27$ $1.374 (4)$ $C12-O5$ $1.421 (3)$ $C26-H26$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ $1.405 (3)$ $C28-C29$ $1.377 (4)$ $C13-O4$ $1.414 (3)$ $C28-H28$ 0.9300 $C13-O4$ $1.414 (3)$ $C28-H28$ 0.9300 $C13-O4$ $1.423 (3)$ $N1-O1$ $1.433 (2)$ $C14-O5$ $1.429 (3)$ $N2-O3$ $1.203 (3)$	C7-C81.535 (3) $C19-H19$ 0.9300 $C7-H7$ 0.9800 $C20-C21$ 1.364 (5) $C8-N2$ 1.497 (3) $C20-H20$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ 1.432 (3) $C24-C29$ 1.378 (3) $C10-C11$ 1.518 (3) $C24-C25$ 1.382 (4) $C10-H10$ 0.9800 $C24-N11$ 1.437 (3) $C1-O7$ 1.423 (3) $C25-C26$ 1.382 (4) $C11-C12$ 1.516 (3) $C25-H25$ 0.9300 $C1-H11$ 0.9800 $C26-C27$ 1.374 (4) $C12-O5$ 1.421 (3) $C26-C26$ 1.382 (4) $C12-C13$ 1.515 (3) $C27-C28$ 1.366 (5) $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ 1.405 (3) $C28-C29$ 1.377 (4) $C13-O4$ 1.414 (3) $C28-H28$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C14-O5$ 1.429 (3) $N1-O1$ 1.433 (2) $C14-O5$ 1.429 (3) $N2-O2$ 1.191 (3) $C14-O5$ 1.205 (3) $C14-C15-H15R$ 109.5 $C-C-I-H1$ 1.98 $(14-C15-H15B$ 109.5 <td>C7—O1</td> <td></td> <td>1.438 (3)</td> <td>C1</td> <td>9—C20</td> <td>1.369</td> <td>9(4)</td>	C7—O1		1.438 (3)	C1	9—C20	1.369	9(4)
C7-H70.9800 $C20-C21$ 1.364 (5) $C8-N2$ 1.497 (3) $C20-H20$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-N1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ 1.432 (3) $C24-C29$ 1.378 (3) $C10-C11$ 1.518 (3) $C24-C25$ 1.382 (4) $C10-H10$ 0.9800 $C24-N1$ 1.437 (3) $C11-O7$ 1.423 (3) $C25-C26$ 1.382 (4) $C11-C12$ 1.516 (3) $C26-C27$ 1.374 (4) $C12-O5$ 1.421 (3) $C26-H26$ 0.9300 $C12-C13$ 1.515 (3) $C27-C28$ 1.366 (5) $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ 1.405 (3) $C28-C29$ 1.377 (4) $C13-O4$ 1.414 (3) $C28-H28$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C13-H13$ 0.9800 $C29-H29$ 0.9300 $C14-O6$ 1.423 (3)N1-O11.433 (2) $C14-O5$ 1.429 (3)N2-O21.191 (3) $C14-O5$ 1.429 (3)N2-O31.203 (3)	C7-H70.9800 $C20-C21$ 1.364 (5) $C8-N2$ 1.497 (3) $C20-H20$ 0.9300 $C8-C9$ 1.537 (3) $C21-C22$ 1.360 (4) $C8-H8$ 0.9800 $C21-H21$ 0.9300 $C9-H1$ 1.472 (3) $C22-C23$ 1.380 (4) $C9-C10$ 1.522 (3) $C22-H22$ 0.9300 $C9-H9$ 0.9800 $C23-H23$ 0.9300 $C10-O4$ 1.432 (3) $C24-C29$ 1.378 (3) $C10-C11$ 1.518 (3) $C24-C25$ 1.382 (4) $C10-H10$ 0.9800 $C24-N1$ 1.437 (3) $C1-C12$ 1.516 (3) $C25-H25$ 0.9300 $C1-C12$ 1.516 (3) $C25-H25$ 0.9300 $C1-C12$ 1.516 (3) $C25-H25$ 0.9300 $C11-H11$ 0.9800 $C26-C27$ 1.374 (4) $C12-C13$ 1.515 (3) $C27-C28$ 1.366 (5) $C12-H12$ 0.9800 $C27-H27$ 0.9300 $C13-O6$ 1.405 (3) $C28-C29$ 1.377 (4) $C13-O4$ 1.414 (3) $C28-H28$ 0.9300 $C13-O4$ 1.414 (3) $C28-H28$ 0.9300 $C13-O4$ 1.423 (3)N1-O11.433 (2) $C14-O5$ 1.429 (3)N2-O21.191 (3) $C14-O5$ 1.429 (3)N2-O21.191 (3) $C14-O5$ 1.429 (3)N2-O31.203 (3) $C14-C15-H15A$ 109.5 $C6-C1-H1$ 1.98(14-C15-H15B $C9-C1-H1$ 1.98H15A-C15-H15B109.5	С7—С8		1.535 (3)	C1	9—H19	0.930	00
C8-N21.497 (3)C20-H200.9300C8-C91.537 (3)C21-C221.360 (4)C8-H80.9800C21-H210.9300C9-N11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C22-H220.9300C9-H90.9800C23-H230.9300C10-O41.432 (3)C24-C291.378 (3)C10-C111.518 (3)C24-C251.382 (4)C10-H100.9800C24-N11.437 (3)C11-O71.423 (3)C25-C261.382 (4)C11-C121.516 (3)C26-C271.374 (4)C12-O51.421 (3)C26-H260.9300C12-C131.515 (3)C27-C281.366 (5)C12-H120.9800C27-H270.9300C13-O61.405 (3)C28-C291.377 (4)C13-O41.414 (3)C28-H280.9300C13-H130.9800C29-H290.9300C14-O61.423 (3)N1-O11.433 (2)C14-O51.429 (3)N2-O31.203 (3)	C8-N2 $1.497 (3)$ C20-H20 0.9300 C8-C9 $1.537 (3)$ C21-C22 $1.360 (4)$ C8-H8 0.9800 C21-H21 0.9300 C9-N1 $1.472 (3)$ C22-C23 $1.380 (4)$ C9-C10 $1.522 (3)$ C23-H22 0.9300 C9-H9 0.9800 C23-H23 0.9300 C10-O4 $1.432 (3)$ C24-C29 $1.378 (3)$ C10-C11 $1.518 (3)$ C24-C25 $1.382 (4)$ C10-H10 0.9800 C24-N1 $1.437 (3)$ C11-O7 $1.423 (3)$ C25-C26 $1.382 (4)$ C11-C12 $1.516 (3)$ C25-H25 0.9300 C11-H11 0.9800 C26-C27 $1.374 (4)$ C12-O5 $1.421 (3)$ C26-H26 0.9300 C12-C13 $1.515 (3)$ C27-C28 $1.366 (5)$ C12-H12 0.9800 C27-H27 0.9300 C13-O6 $1.405 (3)$ C28-H28 0.9300 C13-O4 $1.414 (3)$ C28-H28 0.9300 C13-O4 $1.423 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.429 (3)$ N2-O2 $1.191 (3)$ C14-O6 $1.423 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.500 (4)$ N2-O3 $1.203 (3)$ C14-C16 $1.500 (4)$ C11-O2 ⁱ $3.111 (3)$ C6-C1-H1 119.8 $C14-C15-H15B$ 109.5	С7—Н7		0.9800	C2	c0—C21	1.364	4 (5)
C8-C9 $1.537 (3)$ C21-C22 $1.360 (4)$ C8-H8 0.9800 C21-H21 0.9300 C9-N1 $1.472 (3)$ C22-C23 $1.380 (4)$ C9-C10 $1.522 (3)$ C22-H22 0.9300 C9-H9 0.9800 C23-H23 0.9300 C10-O4 $1.432 (3)$ C24-C29 $1.378 (3)$ C10-C11 $1.518 (3)$ C24-C25 $1.382 (4)$ C10-H10 0.9800 C24-N1 $1.437 (3)$ C11-O7 $1.423 (3)$ C25-C26 $1.382 (4)$ C11-C12 $1.516 (3)$ C25-H25 0.9300 C11-H11 0.9800 C26-C27 $1.374 (4)$ C12-O5 $1.421 (3)$ C26-H26 0.9300 C12-C13 $1.515 (3)$ C27-C28 $1.366 (5)$ C12-H12 0.9800 C27-H27 0.9300 C13-O6 $1.405 (3)$ C28-C29 $1.377 (4)$ C13-O4 $1.414 (3)$ C28-H28 0.9300 C13-H13 0.9800 C29-H29 0.9300 C14-O5 $1.429 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.429 (3)$ N2-O2 $1.191 (3)$	C8-C9 $1.537 (3)$ C21C22 $1.360 (4)$ C8-H8 0.9800 C21H21 0.9300 C9-N1 $1.472 (3)$ C22C23 $1.380 (4)$ C9-C10 $1.522 (3)$ C23H22 0.9300 C9-H9 0.9800 C23H23 0.9300 C10-O4 $1.432 (3)$ C24C29 $1.378 (3)$ C10-C11 $1.518 (3)$ C24C25 $1.382 (4)$ C10-H10 0.9800 C24N1 $1.437 (3)$ C11-O7 $1.423 (3)$ C25C26 $1.382 (4)$ C11-C12 $1.516 (3)$ C25H25 0.9300 C11-H11 0.9800 C26C27 $1.374 (4)$ C12-O5 $1.421 (3)$ C26H26 0.9300 C12-C13 $1.515 (3)$ C27C28 $1.366 (5)$ C12-H12 0.9800 C27-H27 0.9300 C13-O4 $1.414 (3)$ C28-H28 0.9300 C13-O4 $1.414 (3)$ C28-H28 0.9300 C13-H13 0.9800 C29-H29 0.9300 C14-O5 $1.429 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.429 (3)$ N2-O2 $1.191 (3)$ C14-C15 $1.500 (4)$ N2-O3 $1.203 (3)$ C14-C16 $1.500 (4)$ C11-O2 ⁱ $3.111 (3)$ C6-C1-C2 $120.5 (3)$ C14-C15-H15B 109.5 C2-C1-H1 119.8 $C14-C15-H15B$ 109.5	C8—N2		1.497 (3)	C2	ю—H20	0.930	00
C8—H80.9800C21—H210.9300C9—N1 1.472 (3)C22—C23 1.380 (4)C9—C10 1.522 (3)C22—H220.9300C9—H90.9800C23—H230.9300C10—O4 1.432 (3)C24—C29 1.378 (3)C10—C11 1.518 (3)C24—C25 1.382 (4)C10—H100.9800C24—N1 1.437 (3)C11—O7 1.423 (3)C25—C26 1.382 (4)C11—C12 1.516 (3)C25—H250.9300C11—H110.9800C26—C27 1.374 (4)C12—O5 1.421 (3)C26—H260.9300C12—C13 1.515 (3)C27—C28 1.366 (5)C12—H120.9800C27—H270.9300C13—O4 1.414 (3)C28—C29 1.377 (4)C13—O4 1.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O5 1.429 (3)N1—O1 1.433 (2)C14—O5 1.429 (3)N2—O2 1.191 (3)C14—C15 1.500 (4)N2—O3 1.203 (3)	C8—H80.9800C21—H210.9300C9—N11.472 (3)C22—C231.380 (4)C9—C101.522 (3)C22—H220.9300C9—H90.9800C23—H230.9300C10—O41.432 (3)C24—C291.378 (3)C10—C111.518 (3)C24—C251.382 (4)C10—H100.9800C24—N11.437 (3)C11—O71.423 (3)C25—C261.382 (4)C11—C121.516 (3)C25—H250.9300C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—O41.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—O51.500 (4)N2—O31.203 (3)C14—C161.500 (4)N2—O31.203 (3)C14—C161.500 (4)C1—O2 ⁱ 3.111 (3)C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	С8—С9		1.537 (3)	C2	L1—C22	1.360) (4)
C9-N11.472 (3)C22-C231.380 (4)C9-C101.522 (3)C22-H220.9300C9-H90.9800C23-H230.9300C10-O41.432 (3)C24-C291.378 (3)C10-C111.518 (3)C24-C251.382 (4)C10-H100.9800C24-N11.437 (3)C11-O71.423 (3)C25-C261.382 (4)C11-C121.516 (3)C25-H250.9300C11-H110.9800C26-C271.374 (4)C12-O51.421 (3)C26-H260.9300C12-C131.515 (3)C27-C281.366 (5)C12-H120.9800C27-H270.9300C13-O61.405 (3)C28-C291.377 (4)C13-O41.414 (3)C28-H280.9300C13-H130.9800C29-H290.9300C14-O51.429 (3)N1-O11.433 (2)C14-O51.429 (3)N2-O21.191 (3)C14-C151.500 (4)N2-O31.203 (3)	C9-N1 $1.472 (3)$ C22C23 $1.380 (4)$ C9-C10 $1.522 (3)$ C22H22 0.9300 C9-H9 0.9800 C23H23 0.9300 C10-O4 $1.432 (3)$ C24C29 $1.378 (3)$ C10-C11 $1.518 (3)$ C24C25 $1.382 (4)$ C10-H10 0.9800 C24N1 $1.437 (3)$ C11-O7 $1.423 (3)$ C25C26 $1.382 (4)$ C11-C12 $1.516 (3)$ C25H25 0.9300 C11-H11 0.9800 C26C27 $1.374 (4)$ C12-O5 $1.421 (3)$ C26H26 0.9300 C12-C13 $1.515 (3)$ C27C28 $1.366 (5)$ C13-O4 $1.414 (3)$ C28C29 $1.377 (4)$ C13-O4 $1.414 (3)$ C28H28 0.9300 C13-H13 0.9800 C29H29 0.9300 C14-O5 $1.429 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.429 (3)$ N2-O2 $1.191 (3)$ C14-C16 $1.500 (4)$ C11-O2 ⁱ $3.111 (3)$ C6-C1-H1 $1.9.5 (3)$ C14C15H15B 109.5 C2-C1-H1 119.8 $H15AC15-H15B$ 109.5	С8—Н8		0.9800	C2	L1—H21	0.930	00
C9—C10 $1.522 (3)$ C22—H22 0.9300 C9—H9 0.9800 C23—H23 0.9300 C10—O4 $1.432 (3)$ C24—C29 $1.378 (3)$ C10—C11 $1.518 (3)$ C24—C25 $1.382 (4)$ C10—H10 0.9800 C24—N1 $1.437 (3)$ C11—O7 $1.423 (3)$ C25—C26 $1.382 (4)$ C11—C12 $1.516 (3)$ C25—H25 0.9300 C11—H11 0.9800 C26—C27 $1.374 (4)$ C12—O5 $1.421 (3)$ C26—H26 0.9300 C12—C13 $1.515 (3)$ C27—C28 $1.366 (5)$ C13—O6 $1.405 (3)$ C28—C29 $1.377 (4)$ C13—O4 $1.414 (3)$ C28—H28 0.9300 C13—H13 0.9800 C29—H29 0.9300 C14—O6 $1.423 (3)$ N1—O1 $1.433 (2)$ C14—O5 $1.429 (3)$ N2—O2 $1.191 (3)$ C14—C15 $1.500 (4)$ N2—O3 $1.203 (3)$	C9-C10 $1.522 (3)$ C22-H22 0.9300 C9-H9 0.9800 C23-H23 0.9300 C10-O4 $1.432 (3)$ C24-C29 $1.378 (3)$ C10-C11 $1.518 (3)$ C24-C25 $1.382 (4)$ C10-H10 0.9800 C24-N1 $1.437 (3)$ C11-O7 $1.423 (3)$ C25-C26 $1.382 (4)$ C11-C12 $1.516 (3)$ C25-H25 0.9300 C11-H11 0.9800 C26-C27 $1.374 (4)$ C12-O5 $1.421 (3)$ C26-H26 0.9300 C12-C13 $1.515 (3)$ C27-C28 $1.366 (5)$ C12-H12 0.9800 C27-H27 0.9300 C13-O6 $1.405 (3)$ C28-C29 $1.377 (4)$ C13-O4 $1.414 (3)$ C28-H28 0.9300 C13-H13 0.9800 C29-H29 0.9300 C14-O5 $1.429 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.500 (4)$ N2-O3 $1.203 (3)$ C14-C16 $1.500 (4)$ C11-O2 ¹ $3.111 (3)$ C6-C1-C2 $120.5 (3)$ C14-C15-H15B 109.5 C2-C1-H1 119.8 H15A-C15-H15B 109.5	C9—N1		1.472 (3)	C2	2—C23	1.380) (4)
C9—H90.9800C23—H230.9300C10—O41.432 (3)C24—C291.378 (3)C10—C111.518 (3)C24—C251.382 (4)C10—H100.9800C24—N11.437 (3)C11—O71.423 (3)C25—C261.382 (4)C11—C121.516 (3)C25—H250.9300C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O51.429 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)	C9—H90.9800C23—H230.9300C10—O41.432 (3)C24—C291.378 (3)C10—C111.518 (3)C24—C251.382 (4)C10—H100.9800C24—N11.437 (3)C11—O71.423 (3)C25—C261.382 (4)C11—C121.516 (3)C25—H250.9300C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O51.429 (3)N1—O11.433 (2)C14—O51.500 (4)N2—O21.191 (3)C14—C161.500 (4)C11—O2 ¹ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C9—C10		1.522 (3)	C2	2—H22	0.930	00
C1004 $1.432 (3)$ C24C29 $1.378 (3)$ C10C11 $1.518 (3)$ C24C25 $1.382 (4)$ C10H10 0.9800 C24N1 $1.437 (3)$ C11O7 $1.423 (3)$ C25C26 $1.382 (4)$ C11C12 $1.516 (3)$ C25H25 0.9300 C11H11 0.9800 C26C27 $1.374 (4)$ C12O5 $1.421 (3)$ C26H26 0.9300 C12C13 $1.515 (3)$ C27C28 $1.366 (5)$ C13O6 $1.405 (3)$ C28C29 $1.377 (4)$ C13O4 $1.414 (3)$ C28H28 0.9300 C13H13 0.9800 C29H29 0.9300 C14O6 $1.423 (3)$ N1O1 $1.433 (2)$ C14O5 $1.429 (3)$ N2O2 $1.191 (3)$ C14C15 $1.500 (4)$ N2O3 $1.203 (3)$	C1004 $1.432 (3)$ C24C29 $1.378 (3)$ C10C11 $1.518 (3)$ C24C25 $1.382 (4)$ C10H10 0.9800 C24N1 $1.437 (3)$ C11O7 $1.423 (3)$ C25C26 $1.382 (4)$ C11C12 $1.516 (3)$ C25H25 0.9300 C11H11 0.9800 C26C27 $1.374 (4)$ C12O5 $1.421 (3)$ C26H26 0.9300 C12C13 $1.515 (3)$ C27C28 $1.366 (5)$ C12H12 0.9800 C27H27 0.9300 C13O6 $1.405 (3)$ C28C29 $1.377 (4)$ C13O4 $1.414 (3)$ C28H28 0.9300 C13H13 0.9800 C29H29 0.9300 C14O5 $1.429 (3)$ N1O1 $1.433 (2)$ C14O5 $1.500 (4)$ N2O2 $1.191 (3)$ C14C16 $1.500 (4)$ C11O2 ⁱ $3.111 (3)$ C6C1C2 $120.5 (3)$ C14C15H15B 109.5 C2C1H1 119.8 H15AC15H15B 109.5	С9—Н9		0.9800	C2	3—Н23	0.930	00
C10—C11 $1.518 (3)$ C24—C25 $1.382 (4)$ C10—H10 0.9800 C24—N1 $1.437 (3)$ C11—O7 $1.423 (3)$ C25—C26 $1.382 (4)$ C11—C12 $1.516 (3)$ C25—H25 0.9300 C11—H11 0.9800 C26—C27 $1.374 (4)$ C12—O5 $1.421 (3)$ C26—H26 0.9300 C12—C13 $1.515 (3)$ C27—C28 $1.366 (5)$ C12—H12 0.9800 C27—H27 0.9300 C13—O6 $1.405 (3)$ C28—C29 $1.377 (4)$ C13—O4 $1.414 (3)$ C28—H28 0.9300 C13—H13 0.9800 C29—H29 0.9300 C14—O6 $1.423 (3)$ N1—O1 $1.433 (2)$ C14—O5 $1.429 (3)$ N2—O2 $1.191 (3)$ C14—C15 $1.500 (4)$ N2—O3 $1.203 (3)$	C10—C111.518 (3)C24—C251.382 (4)C10—H100.9800C24—N11.437 (3)C11—O71.423 (3)C25—C261.382 (4)C11—C121.516 (3)C25—H250.9300C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.500 (4)N2—O21.191 (3)C14—C161.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C10—O4		1.432 (3)	C2	24—C29	1.378	3 (3)
C10—H10 0.9800 C24—N1 $1.437 (3)$ C11—O7 $1.423 (3)$ C25—C26 $1.382 (4)$ C11—C12 $1.516 (3)$ C25—H25 0.9300 C11—H11 0.9800 C26—C27 $1.374 (4)$ C12—O5 $1.421 (3)$ C26—H26 0.9300 C12—C13 $1.515 (3)$ C27—C28 $1.366 (5)$ C12—H12 0.9800 C27—H27 0.9300 C13—O6 $1.405 (3)$ C28—C29 $1.377 (4)$ C13—O4 $1.414 (3)$ C28—H28 0.9300 C13—H13 0.9800 C29—H29 0.9300 C14—O6 $1.423 (3)$ N1—O1 $1.433 (2)$ C14—O5 $1.429 (3)$ N2—O2 $1.191 (3)$ C14—C15 $1.500 (4)$ N2—O3 $1.203 (3)$	C10—H100.9800C24—N11.437 (3)C11—O71.423 (3)C25—C261.382 (4)C11—C121.516 (3)C25—H250.9300C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C161.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8H15A—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C10-C11		1.518 (3)	C2	4—C25	1.382	2 (4)
C11O7 $1.423 (3)$ C25C26 $1.382 (4)$ C11C12 $1.516 (3)$ C25H25 0.9300 C11H11 0.9800 C26C27 $1.374 (4)$ C12O5 $1.421 (3)$ C26H26 0.9300 C12C13 $1.515 (3)$ C27C28 $1.366 (5)$ C12H12 0.9800 C27H27 0.9300 C13O6 $1.405 (3)$ C28C29 $1.377 (4)$ C13O4 $1.414 (3)$ C28H28 0.9300 C13H13 0.9800 C29H29 0.9300 C14O6 $1.423 (3)$ N1O1 $1.433 (2)$ C14O5 $1.429 (3)$ N2O2 $1.191 (3)$ C14C15 $1.500 (4)$ N2O3 $1.203 (3)$	C1107 $1.423 (3)$ C25C26 $1.382 (4)$ C11C12 $1.516 (3)$ C25H25 0.9300 C11H11 0.9800 C26C27 $1.374 (4)$ C12O5 $1.421 (3)$ C26H26 0.9300 C12C13 $1.515 (3)$ C27C28 $1.366 (5)$ C12H12 0.9800 C27H27 0.9300 C13O6 $1.405 (3)$ C28C29 $1.377 (4)$ C13O4 $1.414 (3)$ C28H28 0.9300 C13H13 0.9800 C29H29 0.9300 C14O6 $1.423 (3)$ N1O1 $1.433 (2)$ C14O5 $1.429 (3)$ N2O2 $1.191 (3)$ C14C16 $1.500 (4)$ C11O2 ⁱ $3.111 (3)$ C6C1C2 $120.5 (3)$ C14C15H15A 109.5 C6C1H1 119.8 C14C15H15B 109.5	C10—H10		0.9800	C2	24—N1	1.437	7 (3)
C11—C12 $1.516 (3)$ C25—H25 0.9300 C11—H11 0.9800 C26—C27 $1.374 (4)$ C12—O5 $1.421 (3)$ C26—H26 0.9300 C12—C13 $1.515 (3)$ C27—C28 $1.366 (5)$ C12—H12 0.9800 C27—H27 0.9300 C13—O6 $1.405 (3)$ C28—C29 $1.377 (4)$ C13—O4 $1.414 (3)$ C28—H28 0.9300 C13—H13 0.9800 C29—H29 0.9300 C14—O6 $1.423 (3)$ N1—O1 $1.433 (2)$ C14—O5 $1.429 (3)$ N2—O2 $1.191 (3)$ C14—C15 $1.500 (4)$ N2—O3 $1.203 (3)$	C11—C121.516 (3)C25—H250.9300C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.500 (4)N2—O21.191 (3)C14—C151.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C2—C1—H1119.8H15A—C15—H15B109.5	C11—O7		1.423 (3)	C2	5—C26	1.382	2 (4)
C11—H11 0.9800 C26—C27 $1.374 (4)$ C12—O5 $1.421 (3)$ C26—H26 0.9300 C12—C13 $1.515 (3)$ C27—C28 $1.366 (5)$ C12—H12 0.9800 C27—H27 0.9300 C13—O6 $1.405 (3)$ C28—C29 $1.377 (4)$ C13—O4 $1.414 (3)$ C28—H28 0.9300 C13—H13 0.9800 C29—H29 0.9300 C14—O6 $1.423 (3)$ N1—O1 $1.433 (2)$ C14—O5 $1.429 (3)$ N2—O2 $1.191 (3)$ C14—C15 $1.500 (4)$ N2—O3 $1.203 (3)$	C11—H110.9800C26—C271.374 (4)C12—O51.421 (3)C26—H260.9300C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C2—C1—H1119.8H15A—C15—H15B109.5	C11—C12		1.516 (3)	C2	5—H25	0.930	00
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C12O51.421 (3)C26H260.9300C12C131.515 (3)C27C281.366 (5)C12H120.9800C27H270.9300C13O61.405 (3)C28C291.377 (4)C13O41.414 (3)C28H280.9300C13H130.9800C29H290.9300C14O61.423 (3)N1O11.433 (2)C14O51.429 (3)N2O21.191 (3)C14C151.500 (4)N2O31.203 (3)C14C161.500 (4)C11O2 ⁱ 3.111 (3)C6C1C2120.5 (3)C14C15H15A109.5C2C1H1119.8H15AC15H15B109.5	C11—H11		0.9800	C2	.6—C27	1.374	4 (4)
C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)	C12—C131.515 (3)C27—C281.366 (5)C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C2—C1—H1119.8H15A—C15—H15B109.5	C12—O5		1.421 (3)	C2	e6—H26	0.930	00
C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)	C12—H120.9800C27—H270.9300C13—O61.405 (3)C28—C291.377 (4)C13—O41.414 (3)C28—H280.9300C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C2—C1—H1119.8H15A—C15—H15B109.5	C12—C13		1.515 (3)	C2	27—C28	1.360	5 (5)
C13O61.405 (3)C28C291.377 (4)C13O41.414 (3)C28H280.9300C13H130.9800C29H290.9300C14O61.423 (3)N1O11.433 (2)C14O51.429 (3)N2O21.191 (3)C14C151.500 (4)N2O31.203 (3)	C13-O6 $1.405 (3)$ C28-C29 $1.377 (4)$ C13-O4 $1.414 (3)$ C28-H28 0.9300 C13-H13 0.9800 C29-H29 0.9300 C14-O6 $1.423 (3)$ N1-O1 $1.433 (2)$ C14-O5 $1.429 (3)$ N2-O2 $1.191 (3)$ C14-C15 $1.500 (4)$ N2-O3 $1.203 (3)$ C14-C16 $1.500 (4)$ C11-O2 ⁱ $3.111 (3)$ C6-C1-C2 $120.5 (3)$ C14-C15-H15A 109.5 C2-C1-H1 119.8 H15A-C15-H15B 109.5	C12—H12		0.9800	C2	27—H27	0.930	00
C13-O41.414 (3)C28-H280.9300C13-H130.9800C29-H290.9300C14-O61.423 (3)N1-O11.433 (2)C14-O51.429 (3)N2-O21.191 (3)C14-C151.500 (4)N2-O31.203 (3)	C13-O41.414 (3)C28-H280.9300C13-H130.9800C29-H290.9300C14-O61.423 (3)N1-O11.433 (2)C14-O51.429 (3)N2-O21.191 (3)C14-C151.500 (4)N2-O31.203 (3)C14-C161.500 (4)C11-O2 ⁱ 3.111 (3)C6-C1-C2120.5 (3)C14-C15-H15A109.5C6-C1-H1119.8C14-C15-H15B109.5C2-C1-H1119.8H15A-C15-H15B109.5	C13—O6		1.405 (3)	C2	.8—C29	1.37	7 (4)
C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)	C13—H130.9800C29—H290.9300C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)C11—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8H15A—C15—H15B109.5	C13—O4		1.414 (3)	C2	8—H28	0.930	00
C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31 203 (3)	C14—O61.423 (3)N1—O11.433 (2)C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)Cl1—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	С13—Н13		0.9800	C2	9—Н29	0.930	00
C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)	C14—O51.429 (3)N2—O21.191 (3)C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)Cl1—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C14—O6		1.423 (3)	N1	01	1.433	3 (2)
C14—C15 1.500 (4) N2—O3 1.203 (3)	C14—C151.500 (4)N2—O31.203 (3)C14—C161.500 (4)Cl1—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C14—O5		1.429 (3)	N2	2—02	1.191	l (3)
	C14—C161.500 (4)Cl1—O2 ⁱ 3.111 (3)C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C14—C15		1.500 (4)	N2	2—03	1.203	3 (3)
C14—C16 1.500 (4) C11—O2 ⁱ 3.111 (3)	C6—C1—C2120.5 (3)C14—C15—H15A109.5C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C14—C16		1.500 (4)	Cl	1—02 ⁱ	3.111	(3)
C6—C1—C2 120.5 (3) C14—C15—H15A 109.5	C6—C1—H1119.8C14—C15—H15B109.5C2—C1—H1119.8H15A—C15—H15B109.5	C6—C1—C2		120.5 (3)	C1	4—C15—H15A	109.5	5
C6—C1—H1 119.8 C14—C15—H15B 109.5	C2—C1—H1 119.8 H15A—C15—H15B 109.5	C6-C1-H1		119.8	C1	4—C15—H15B	109.5	5
C2—C1—H1 119.8 H15A—C15—H15B 109.5		C2-C1-H1		119.8	H1	5A—C15—H15B	109.5	5
$C_{2} = C_{2} = C_{1} = 110.8 (2)$ $C_{14} = C_{15} = 115.0 = 100.5$	C3—C2—C1 119.8 (3) C14—C15—H15C 109.5	C3—C2—C1		119.8 (3)	C1	4—C15—H15C	109.5	5

С3—С2—Н2	120.1	H15A—C15—H15C	109.5
C1—C2—H2	120.1	H15B—C15—H15C	109.5
C2—C3—C4	120.8 (3)	C14—C16—H16A	109.5
C2—C3—Cl1	120.2 (2)	C14—C16—H16B	109.5
C4—C3—Cl1	119.0 (3)	H16A—C16—H16B	109.5
C3—C4—C5	119.6 (3)	C14—C16—H16C	109.5
C3—C4—H4	120.2	H16A—C16—H16C	109.5
С5—С4—Н4	120.2	H16B—C16—H16C	109.5
C6—C5—C4	121.0 (3)	O7—C17—C18	110.8 (2)
С6—С5—Н5	119.5	O7—C17—H17A	109.5
С4—С5—Н5	119.5	С18—С17—Н17А	109.5
C5—C6—C1	118.3 (2)	O7—C17—H17B	109.5
C5—C6—C7	119.3 (2)	С18—С17—Н17В	109.5
C1—C6—C7	122.3 (2)	H17A—C17—H17B	108.1
O1—C7—C6	109.53 (18)	C23—C18—C19	118.9 (2)
O1—C7—C8	102.22 (18)	C23—C18—C17	123.0 (2)
C6—C7—C8	114.67 (18)	C19—C18—C17	118.2 (2)
O1—C7—H7	110.0	C20—C19—C18	120.0 (3)
С6—С7—Н7	110.0	С20—С19—Н19	120.0
С8—С7—Н7	110.0	C18—C19—H19	120.0
N2—C8—C7	110.11 (18)	C21—C20—C19	120.8 (3)
N2—C8—C9	111.63 (19)	C21—C20—H20	119.6
С7—С8—С9	104.23 (17)	С19—С20—Н20	119.6
N2—C8—H8	110.2	C22—C21—C20	119.7 (3)
С7—С8—Н8	110.2	C22—C21—H21	120.2
С9—С8—Н8	110.2	C20-C21-H21	120.2
N1—C9—C10	108.61 (18)	C21—C22—C23	120.0 (3)
N1—C9—C8	105.42 (17)	C21—C22—H22	120.0
C10—C9—C8	111.29 (18)	С23—С22—Н22	120.0
N1—C9—H9	110.5	C18—C23—C22	120.6 (3)
С10—С9—Н9	110.5	C18—C23—H23	119.7
С8—С9—Н9	110.5	С22—С23—Н23	119.7
O4—C10—C11	104.21 (17)	C29—C24—C25	120.1 (2)
O4—C10—C9	107.70 (18)	C29—C24—N1	121.5 (2)
C11—C10—C9	115.70 (18)	C25—C24—N1	118.0 (2)
O4—C10—H10	109.7	C24—C25—C26	119.1 (3)
С11—С10—Н10	109.7	C24—C25—H25	120.4
С9—С10—Н10	109.7	C26—C25—H25	120.4
O7—C11—C12	110.55 (18)	C27—C26—C25	121.1 (3)
O7—C11—C10	108.43 (18)	C27—C26—H26	119.5
C12—C11—C10	101.32 (17)	С25—С26—Н26	119.5
O7—C11—H11	112.0	C28—C27—C26	119.0 (3)
C12—C11—H11	112.0	С28—С27—Н27	120.5
C10—C11—H11	112.0	С26—С27—Н27	120.5
O5—C12—C13	104.04 (18)	C27—C28—C29	121.2 (3)
O5—C12—C11	109.12 (19)	C27—C28—H28	119.4
C13—C12—C11	103.89 (18)	C29—C28—H28	119.4
O5—C12—H12	113.0	C28—C29—C24	119.5 (3)
C13—C12—H12	113.0	С28—С29—Н29	120.2

C11—C12—H12	113.0	С24—С29—Н29	120.2
O6—C13—O4	110.77 (19)	O1—N1—C24	112.06 (18)
O6—C13—C12	105.37 (18)	O1—N1—C9	104.32 (16)
O4—C13—C12	107.62 (17)	C24—N1—C9	118.42 (18)
O6—C13—H13	111.0	O2—N2—O3	123.5 (3)
O4—C13—H13	111.0	O2—N2—C8	118.8 (2)
С12—С13—Н13	111.0	O3—N2—C8	117.8 (2)
O6—C14—O5	105.13 (18)	N1—O1—C7	106.94 (16)
O6—C14—C15	108.9 (2)	C13—O4—C10	108.40 (16)
O5—C14—C15	108.9 (2)	C12	107.88 (17)
O6—C14—C16	109.5 (2)	C13—O6—C14	110.31 (18)
O5—C14—C16	110.3 (2)	C17—O7—C11	113.41 (18)
C15—C14—C16	113.8 (3)	C3—Cl1—O2 ⁱ	160.74 (11)
C6—C1—C2—C3	1.9 (4)	C17—C18—C23—C22	-179.1 (3)
C1—C2—C3—C4	-3.4 (4)	C21—C22—C23—C18	0.3 (4)
C1—C2—C3—Cl1	175.3 (2)	C29—C24—C25—C26	-1.4 (4)
C2—C3—C4—C5	1.6 (4)	N1—C24—C25—C26	-174.0(2)
Cl1—C3—C4—C5	-177.2 (2)	C24—C25—C26—C27	1.5 (4)
C_{3} — C_{4} — C_{5} — C_{6}	1.8 (4)	C25-C26-C27-C28	-1.2(5)
C4-C5-C6-C1	-32(4)	$C_{26} = C_{27} = C_{28} = C_{29}$	10(5)
C4-C5-C6-C7	1734(2)	$C_{27} = C_{28} = C_{29} = C_{24}$	-0.9(4)
C_{2} C_{1} C_{6} C_{5}	1 4 (4)	$C_{25} = C_{24} = C_{29} = C_{28}$	11(4)
C_{2}^{-} C_{1}^{-} C_{6}^{-} C_{7}^{-}	-1751(2)	N1 - C24 - C29 - C28	1735(2)
$C_{5} - C_{6} - C_{7} - O_{1}$	160.2(2)	$C_{29} - C_{24} - N_{1} - O_{1}$	163(3)
C1 - C6 - C7 - O1	-233(3)	$C_{25} = C_{24} = N_1 = 0_1$	-1712(2)
C_{5} C_{6} C_{7} C_{8}	-85.6(3)	$C_{29} - C_{24} - N_{1} - C_{9}$	137.8(2)
C1 - C6 - C7 - C8	90.9 (3)	$C_{25} = C_{24} = N_1 = C_{9}$	-497(3)
01 - C7 - C8 - N2	-143.01(19)	C10-C9-N1-O1	-95.32(19)
C6-C7-C8-N2	98.6 (2)	C8 - C9 - N1 - O1	240(2)
01 - 07 - 08 - 09	-232(2)	C10-C9-N1-C24	1393(2)
C_{6} C_{7} C_{8} C_{9}	-1416(2)	C8 - C9 - N1 - C24	-1013(2)
$N_{2}^{2} = C_{8}^{2} = C_{9}^{2} = N_{1}^{2}$	1185(2)	C7 - C8 - N2 - O2	68 6 (3)
C7 - C8 - C9 - N1	-0.3(2)	$C_{9} = C_{8} = N_{2} = O_{2}^{2}$	-46.6(3)
$N^2 - C^8 - C^9 - C^{10}$	-1240(2)	C7 - C8 - N2 - O3	-110.8(2)
C7-C8-C9-C10	117 22 (19)	C9 - C8 - N2 - O3	133.9(2)
N1-C9-C10-O4	166.62 (17)	$C_{24} = N_{1} = O_{1} = C_{7}$	88.2 (2)
C8—C9—C10—O4	51.0 (2)	C9 - N1 - O1 - C7	-41.12 (19)
N1—C9—C10—C11	-77.3 (2)	C6—C7—O1—N1	161.96 (16)
C8—C9—C10—C11	167.08 (18)	C8—C7—O1—N1	39.96 (19)
O4—C10—C11—O7	78.2 (2)	O6—C13—O4—C10	101.9 (2)
C9—C10—C11—O7	-39.9 (2)	C12—C13—O4—C10	-12.8 (2)
O4—C10—C11—C12	-38.2 (2)	C11—C10—O4—C13	32.4 (2)
C9—C10—C11—C12	-156.24 (19)	C9—C10—O4—C13	155.77 (18)
O7—C11—C12—O5	164.63 (18)	C13—C12—O5—C14	26.3 (2)
C10-C11-C12-O5	-80.6 (2)	C11—C12—O5—C14	136.67 (19)
07—C11—C12—C13	-84.9 (2)	O6—C14—O5—C12	-26.7 (3)
C10-C11-C12-C13	29.9 (2)	C15—C14—O5—C12	-143.2 (2)
O5—C12—C13—O6	-15.9 (2)	C16—C14—O5—C12	91.3 (2)

C11—C12—C13—O6	-130.13 (19)	O4—C13—O6—C14	-116.2 (2)		
O5-C12-C13-O4	102.3 (2)	C12-C13-O6-C14	-0.1 (3)		
C11—C12—C13—O4	-11.9 (2)	O5-C14-O6-C13	16.1 (3)		
O7—C17—C18—C23	-4.6 (3)	C15—C14—O6—C13	132.6 (2)		
O7—C17—C18—C19	176.1 (2)	C16-C14-O6-C13	-102.4 (2)		
C23-C18-C19-C20	-0.3 (4)	C18—C17—O7—C11	-178.33 (18)		
C17—C18—C19—C20	179.0 (3)	C12-C11-O7-C17	-83.7 (2)		
C18—C19—C20—C21	-0.1 (5)	C10-C11-O7-C17	166.09 (18)		
C19—C20—C21—C22	0.6 (5)	C2—C3—Cl1—O2 ⁱ	-90.1 (5)		
C20—C21—C22—C23	-0.7 (5)	C4—C3—Cl1—O2 ⁱ	88.7 (5)		
C19—C18—C23—C22	0.2 (4)				
Symmetry codes: (i) $x-1/2, -y+3/2, -z+1$.					

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	$H \cdots A$	$D \cdots A$	$D\!\!-\!\!\mathrm{H}^{\dots}\!A$
C13—H13···O2 ⁱⁱ	0.98	2.54	3.298 (3)	134
C17—H17B···O1 ⁱⁱⁱ	0.97	2.46	3.218 (3)	135
C21—H21···Cg1 ⁱⁱ	0.93	2.75	3.598 (1)	152
Symmetry codes: (ii) $x-1/2$, $-y+1/2$, $-z+1$; (iii) $-x+1$,	y - 1/2, -z + 3/2.			

Fig. 1







