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Key indicators

Single-crystal X-ray study
 T = 160 K
 Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
 R factor = 0.047
 wR factor = 0.105
 Data-to-parameter ratio = 8.2

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

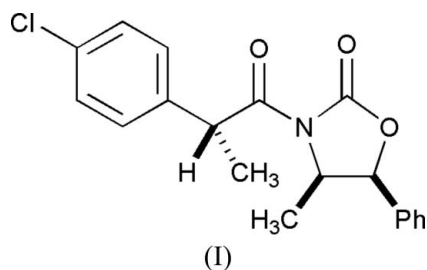
(-)-(4*R*,5*S*)-3-[2(*R*)-(4-Chlorophenyl)propionyl]-4-methyl-5-phenyloxazolidin-2-one

The title compound, $\text{C}_{19}\text{H}_{18}\text{ClNO}_3$, is formed from enantiomerically pure (+)-(4*R*,5*S*)-4-methyl-5-phenyl-2-oxazolidinone and racemic 2-(4-chlorophenyl)propanoyl chloride. The crystal structure resembles closely that of the comparable (4-methylphenyl)propionyl derivative, although the two structures differ in the nature of the intermolecular contacts to the Cl atom and methyl group.

Received 27 June 2006
 Accepted 12 August 2006

Comment

The title compound, (I), is the fourth in a series of structurally related compounds, introduced in our earlier report (Coumbarides *et al.*, 2006). With $R^1 = 4\text{-(Cl)C}_6\text{H}_4$, the reaction shown in that report yielded the *anti-syn* and *syn-syn* diastereomers in 38 and 39% yields, respectively. The title compound, (I), is the *anti-syn* diastereomer (Fig. 1). In the crystal structure, the conformation of the molecule is essentially indistinguishable from that of the (4-methylphenyl)propionyl derivative (Chavda *et al.*, 2006).



The crystal structure of (I) is closely related to that of the (4-methylphenyl)propionyl derivative. The two structures contain essentially identical two-dimensional layers, lying in the (010) planes for (I) and in the (100) planes for the methyl derivative (Fig. 2). In the methyl derivative, adjacent layers are related by translation along *a*, bringing the methyl groups of the 4-(CH_3) C_6H_4 substituent into the vicinity of O2 [$\text{H}20\text{B} \cdots \text{O}2 = 2.71 \text{ \AA}$]. In (I), adjacent layers are related by 2_1 screw axes, and Cl1 forms its shortest intermolecular contacts between layers to the methyl group C19 [$\text{H}19\text{B} \cdots \text{Cl}1^i = 3.35 \text{ \AA}$; symmetry code: (i) $-\frac{1}{2} + x, \frac{3}{2} + y, \frac{3}{2} - z$]. Thus, chloro/methyl interchange (Edwards *et al.*, 2006) does not lead to isostructurality in this instance, and this can be attributed to the influence of the different charge distributions of the Cl atom and CH_3 group.

Experimental

The experimental procedure is comparable with that reported previously (Coumbarides *et al.*, 2006). The actual quantities used for

the preparation of (I) were: *n*-butyllithium (15.81 ml, 2.5 M in hexanes, 39.5 mmol) and (*R,S*)-oxazolidinone (5.00 g, 28.2 mmol) in 60 ml tetrahydrofuran (THF), combined with a solution of (*rac*)-2-(4-chlorophenyl)propanoyl chloride (5.73 g, 28.2 mmol) in 10 ml THF. The crude residue was purified by flash column chromatography on silica gel, eluting with light petroleum (b.p. 313–333 K)/diethyl ether (7:3), to give a separable diastereoisomeric mixture in the approximate ratio *anti-syn*:*syn-syn* 50:50. The *anti-syn* diastereomer was obtained as colourless crystals [3.68 g, 38% yield, m.p. 362–364 K, R_F 0.58 [light petroleum (b.p. 313–333 K)/diethyl ether, 7:3]]. Spectroscopic analysis: $[\alpha]_D^{22} = -60.0$ (CHCl₃, 293 K, concentration 0.60 g per 100 ml); IR (CHCl₃, $\nu_{\max}/\text{cm}^{-1}$): 1779 (C=O), 1713 (C=O); ¹H NMR (270 MHz; CDCl₃): 7.36–7.20 (9H, *m*, 9 × CH; Ar and Ph), 5.62 (1H, *d*, *J* = 6.4 Hz, CHPh), 5.01 (1H, *q*, *J* = 6.9 Hz, ArCH), 4.79 (1H, *m*, CHN), 1.48 (3H, *d*, *J* = 6.9 Hz, CH₃CH), 0.86 (3H, *d*, *J* = 6.4 Hz, CH₃CHN); ¹³C NMR (100 MHz; CDCl₃): δ 173.9 (NC=O), 152.5 (OC=O), 138.9 (*i*-CCl; Ar), 133.2, 133.1 (2 × *i*-C; Ar and Ph), 129.5, 128.9, 128.8, 128.7, 125.6 (5 × CH; Ar and Ph), 78.7 (PhCHO), 55.4 (CHN), 42.7 (ArCH), 19.2 (CH₃CH), 14.4 (CH₃CHN); found: MNH₄⁺ 361.1307; C₁₉H₂₂ClN₂O₃ requires 361.1313.

Crystal data

C ₁₉ H ₁₈ ClNO ₃	Z = 4
$M_r = 343.79$	$D_x = 1.307 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 7.105$ (3) Å	$\mu = 0.24 \text{ mm}^{-1}$
$b = 25.662$ (12) Å	$T = 160$ (2) K
$c = 9.580$ (8) Å	Prism, colourless
$V = 1746.7$ (18) Å ³	0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	1083 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$R_{\text{int}} = 0.044$
Absorption correction: none	$\theta_{\text{max}} = 25.0^\circ$
2316 measured reflections	2 standard reflections
1794 independent reflections	frequency: 60 min
	intensity decay: 2%

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2]$
$wR(F^2) = 0.105$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{\text{max}} < 0.001$
1794 reflections	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
219 parameters	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$

H atoms were placed in geometrically idealised positions and constrained to ride on their parent atoms, with C–H = 0.95–1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The methyl groups were allowed to rotate about their local threefold axes. The absolute configuration could not be established and is assigned on the basis of the known configuration of the starting material (Coumbarides *et al.*, 2006).

Data collection: CAD-4 EXPRESS (Enraf–Nonius, 1994); cell refinement: CAD-4 EXPRESS; data reduction: XCAD4 (Harms & Wocadlo, 1995); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97

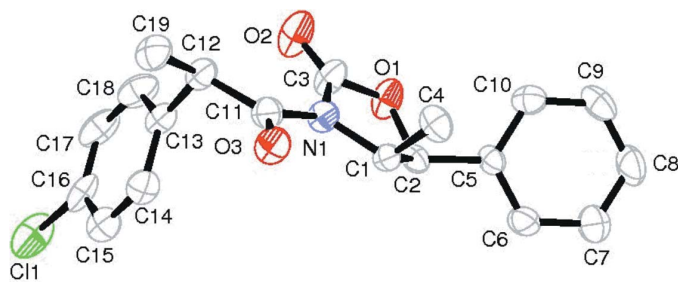


Figure 1

The molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

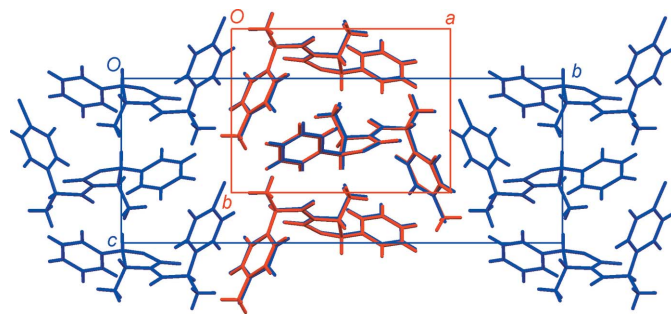


Figure 2

Overlay of the unit-cell contents of (I) (blue) and the (4-methylphenyl)propionyl derivative (red) (Chavda *et al.*, 2006), showing essentially identical layers of molecules in the (010) planes of (I) and (100) planes of the methyl derivative.

(Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

We are grateful to the Royal Society and the University of London Central Research Fund for their financial support to JE, and the EPSRC National Mass Spectrometry Service (Swansea) for accurate mass determination.

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supporting information

Acta Cryst. (2006). E62, o4039–o4040 [https://doi.org/10.1107/S1600536806031837]

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Crystal data

C₁₉H₁₈ClNO₃

M_r = 343.79

Orthorhombic, *P*2₁2₁2₁

Hall symbol: P 2ac 2ab

a = 7.105 (3) Å

b = 25.662 (12) Å

c = 9.580 (8) Å

V = 1746.7 (18) Å³

Z = 4

F(000) = 720

D_x = 1.307 Mg m⁻³

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 25 reflections

θ = 8.2–11.9°

μ = 0.24 mm⁻¹

T = 160 K

Prism, colourless

0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω/2θ scans

2316 measured reflections

1794 independent reflections

1083 reflections with *I* > 2σ(*I*)

*R*_{int} = 0.044

θ_{max} = 25.0°, θ_{min} = 1.6°

h = –7→8

k = –29→30

l = –9→11

2 standard reflections every 60 min

intensity decay: 2%

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.047

wR(*F*²) = 0.105

S = 1.04

1794 reflections

219 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

w = 1/[σ²(*F*_o²) + (0.0394*P*)²]

where *P* = (*F*_o² + 2*F*_c²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.21 e Å⁻³

Δρ_{min} = –0.22 e Å⁻³

Absolute structure: assigned on the basis of
known starting material

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > 2\sigma(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.0521 (7)	0.99165 (16)	0.6453 (5)	0.0297 (11)
H1	0.1699	1.0054	0.6015	0.036*
C2	-0.1152 (6)	0.99826 (18)	0.5432 (5)	0.0313 (12)
H2	-0.0641	0.9989	0.4459	0.038*
C3	-0.1139 (7)	0.9124 (2)	0.6137 (6)	0.0431 (15)
C4	0.0255 (7)	1.01583 (19)	0.7868 (5)	0.0392 (14)
H4A	-0.0933	1.0036	0.8273	0.059*
H4B	0.0221	1.0539	0.7777	0.059*
H4C	0.1302	1.0058	0.8478	0.059*
C5	-0.2390 (7)	1.04543 (19)	0.5625 (5)	0.0316 (12)
C6	-0.1982 (7)	1.0901 (2)	0.4914 (5)	0.0438 (14)
H6	-0.0943	1.0908	0.4291	0.053*
C7	-0.3074 (9)	1.1346 (2)	0.5092 (7)	0.0571 (17)
H7	-0.2767	1.1657	0.4602	0.069*
C8	-0.4585 (9)	1.1337 (2)	0.5972 (6)	0.0546 (17)
H8	-0.5331	1.1641	0.6094	0.065*
C9	-0.5026 (7)	1.0886 (2)	0.6681 (5)	0.0504 (15)
H9	-0.6070	1.0882	0.7300	0.061*
C10	-0.3963 (7)	1.0440 (2)	0.6502 (5)	0.0399 (13)
H10	-0.4298	1.0127	0.6969	0.048*
C11	0.2150 (7)	0.9084 (2)	0.7053 (5)	0.0382 (13)
C12	0.2189 (7)	0.84953 (18)	0.6971 (5)	0.0371 (13)
H12	0.0913	0.8361	0.7222	0.045*
C13	0.2654 (7)	0.83165 (18)	0.5505 (5)	0.0346 (13)
C14	0.4216 (7)	0.85110 (19)	0.4812 (5)	0.0389 (13)
H14	0.4948	0.8777	0.5240	0.047*
C15	0.4732 (8)	0.83257 (19)	0.3506 (5)	0.0438 (14)
H15	0.5781	0.8470	0.3029	0.053*
C16	0.3700 (9)	0.79294 (19)	0.2913 (5)	0.0459 (15)
C17	0.2146 (9)	0.7732 (2)	0.3574 (6)	0.0539 (17)
H17	0.1434	0.7462	0.3148	0.065*
C18	0.1616 (9)	0.7925 (2)	0.4861 (6)	0.0513 (16)
H18	0.0530	0.7789	0.5311	0.062*
C19	0.3609 (8)	0.8280 (2)	0.8017 (5)	0.0443 (14)
H19A	0.4877	0.8396	0.7760	0.066*

H19B	0.3560	0.7898	0.8009	0.066*
H19C	0.3302	0.8407	0.8954	0.066*
C11	0.4415 (3)	0.76689 (5)	0.13160 (15)	0.0697 (6)
N1	0.0589 (6)	0.93434 (14)	0.6506 (4)	0.0346 (10)
O1	-0.2233 (5)	0.95084 (13)	0.5604 (4)	0.0455 (10)
O2	-0.1685 (5)	0.86858 (14)	0.6235 (5)	0.0629 (13)
O3	0.3457 (5)	0.93430 (12)	0.7494 (4)	0.0425 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.021 (3)	0.032 (3)	0.036 (3)	0.000 (2)	-0.003 (3)	0.007 (2)
C2	0.026 (3)	0.038 (3)	0.030 (3)	0.003 (2)	0.001 (2)	0.000 (2)
C3	0.033 (3)	0.034 (3)	0.063 (4)	-0.002 (3)	-0.019 (3)	0.009 (3)
C4	0.030 (3)	0.052 (3)	0.036 (3)	0.008 (3)	-0.006 (3)	-0.002 (3)
C5	0.026 (3)	0.040 (3)	0.029 (3)	0.009 (2)	-0.001 (3)	0.004 (2)
C6	0.031 (3)	0.048 (3)	0.053 (4)	0.003 (3)	0.008 (3)	0.010 (3)
C7	0.047 (4)	0.052 (4)	0.072 (4)	0.014 (3)	0.008 (4)	0.007 (3)
C8	0.044 (4)	0.056 (4)	0.064 (4)	0.023 (3)	0.005 (4)	-0.001 (3)
C9	0.029 (3)	0.072 (4)	0.050 (4)	0.010 (3)	0.008 (3)	-0.003 (3)
C10	0.034 (3)	0.046 (3)	0.040 (3)	-0.003 (3)	-0.003 (3)	0.010 (3)
C11	0.032 (3)	0.041 (3)	0.041 (3)	0.002 (3)	-0.001 (3)	0.006 (3)
C12	0.028 (3)	0.033 (3)	0.050 (3)	-0.002 (2)	-0.008 (3)	0.008 (3)
C13	0.029 (3)	0.031 (3)	0.044 (3)	-0.005 (2)	-0.013 (3)	0.007 (2)
C14	0.034 (3)	0.034 (3)	0.049 (3)	-0.008 (3)	-0.011 (3)	-0.005 (3)
C15	0.040 (3)	0.044 (3)	0.046 (3)	-0.002 (3)	-0.011 (3)	0.004 (3)
C16	0.069 (4)	0.024 (3)	0.045 (3)	0.004 (3)	-0.021 (4)	0.006 (3)
C17	0.073 (5)	0.033 (3)	0.055 (4)	-0.018 (3)	-0.028 (4)	0.004 (3)
C18	0.052 (4)	0.046 (3)	0.056 (4)	-0.016 (3)	-0.017 (3)	0.012 (3)
C19	0.041 (3)	0.048 (3)	0.044 (3)	0.003 (3)	-0.010 (3)	0.012 (3)
C11	0.1206 (16)	0.0473 (9)	0.0412 (8)	0.0003 (10)	-0.0178 (11)	-0.0029 (7)
N1	0.022 (2)	0.038 (2)	0.044 (3)	0.000 (2)	-0.009 (2)	0.006 (2)
O1	0.034 (2)	0.036 (2)	0.067 (3)	0.0029 (18)	-0.023 (2)	0.0009 (19)
O2	0.036 (2)	0.039 (2)	0.114 (4)	-0.0045 (19)	-0.028 (3)	0.004 (2)
O3	0.026 (2)	0.040 (2)	0.061 (2)	-0.0048 (17)	-0.012 (2)	0.0033 (18)

Geometric parameters (Å, °)

C1—N1	1.472 (5)	C9—H9	0.950
C1—C4	1.503 (6)	C10—H10	0.950
C1—C2	1.548 (6)	C11—O3	1.217 (6)
C1—H1	1.000	C11—N1	1.396 (6)
C2—O1	1.449 (5)	C11—C12	1.513 (7)
C2—C5	1.508 (6)	C12—C13	1.514 (7)
C2—H2	1.000	C12—C19	1.526 (6)
C3—O2	1.194 (6)	C12—H12	1.000
C3—O1	1.355 (6)	C13—C14	1.387 (7)
C3—N1	1.396 (6)	C13—C18	1.391 (7)

C4—H4A	0.980	C14—C15	1.388 (6)
C4—H4B	0.980	C14—H14	0.950
C4—H4C	0.980	C15—C16	1.377 (7)
C5—C6	1.364 (7)	C15—H15	0.950
C5—C10	1.399 (7)	C16—C17	1.370 (8)
C6—C7	1.392 (7)	C16—C11	1.745 (6)
C6—H6	0.950	C17—C18	1.381 (8)
C7—C8	1.365 (8)	C17—H17	0.950
C7—H7	0.950	C18—H18	0.950
C8—C9	1.378 (7)	C19—H19A	0.980
C8—H8	0.950	C19—H19B	0.980
C9—C10	1.383 (7)	C19—H19C	0.980
N1—C1—C4	112.7 (4)	C5—C10—H10	120.4
N1—C1—C2	99.0 (4)	O3—C11—N1	118.4 (5)
C4—C1—C2	115.3 (4)	O3—C11—C12	123.3 (5)
N1—C1—H1	109.8	N1—C11—C12	118.1 (5)
C4—C1—H1	109.8	C13—C12—C11	110.8 (4)
C2—C1—H1	109.8	C13—C12—C19	110.8 (4)
O1—C2—C5	110.5 (4)	C11—C12—C19	109.9 (4)
O1—C2—C1	104.1 (3)	C13—C12—H12	108.4
C5—C2—C1	117.3 (4)	C11—C12—H12	108.4
O1—C2—H2	108.2	C19—C12—H12	108.4
C5—C2—H2	108.2	C14—C13—C18	118.2 (5)
C1—C2—H2	108.2	C14—C13—C12	120.6 (5)
O2—C3—O1	121.9 (5)	C18—C13—C12	121.0 (5)
O2—C3—N1	130.2 (5)	C13—C14—C15	121.3 (5)
O1—C3—N1	107.9 (4)	C13—C14—H14	119.3
C1—C4—H4A	109.5	C15—C14—H14	119.3
C1—C4—H4B	109.5	C16—C15—C14	119.0 (5)
H4A—C4—H4B	109.5	C16—C15—H15	120.5
C1—C4—H4C	109.5	C14—C15—H15	120.5
H4A—C4—H4C	109.5	C17—C16—C15	120.7 (5)
H4B—C4—H4C	109.5	C17—C16—C11	119.9 (4)
C6—C5—C10	119.5 (5)	C15—C16—C11	119.4 (5)
C6—C5—C2	119.3 (5)	C16—C17—C18	120.0 (5)
C10—C5—C2	121.2 (4)	C16—C17—H17	120.0
C5—C6—C7	120.7 (5)	C18—C17—H17	120.0
C5—C6—H6	119.7	C17—C18—C13	120.7 (6)
C7—C6—H6	119.7	C17—C18—H18	119.6
C8—C7—C6	120.0 (6)	C13—C18—H18	119.6
C8—C7—H7	120.0	C12—C19—H19A	109.5
C6—C7—H7	120.0	C12—C19—H19B	109.5
C7—C8—C9	119.8 (5)	H19A—C19—H19B	109.5
C7—C8—H8	120.1	C12—C19—H19C	109.5
C9—C8—H8	120.1	H19A—C19—H19C	109.5
C8—C9—C10	120.7 (5)	H19B—C19—H19C	109.5
C8—C9—H9	119.7	C11—N1—C3	127.0 (4)

C10—C9—H9	119.7	C11—N1—C1	121.0 (4)
C9—C10—C5	119.3 (5)	C3—N1—C1	111.4 (4)
C9—C10—H10	120.4	C3—O1—C2	110.4 (4)
N1—C1—C2—O1	25.6 (4)	C12—C13—C14—C15	175.7 (5)
C4—C1—C2—O1	-94.8 (5)	C13—C14—C15—C16	-2.1 (7)
N1—C1—C2—C5	148.1 (4)	C14—C15—C16—C17	2.3 (8)
C4—C1—C2—C5	27.7 (6)	C14—C15—C16—C11	-176.4 (4)
O1—C2—C5—C6	-149.4 (4)	C15—C16—C17—C18	-1.0 (8)
C1—C2—C5—C6	91.5 (6)	C11—C16—C17—C18	177.7 (4)
O1—C2—C5—C10	29.6 (6)	C16—C17—C18—C13	-0.6 (8)
C1—C2—C5—C10	-89.5 (5)	C14—C13—C18—C17	0.8 (8)
C10—C5—C6—C7	2.4 (8)	C12—C13—C18—C17	-174.3 (5)
C2—C5—C6—C7	-178.6 (5)	O3—C11—N1—C3	-170.2 (5)
C5—C6—C7—C8	-0.9 (9)	C12—C11—N1—C3	14.2 (8)
C6—C7—C8—C9	0.0 (9)	O3—C11—N1—C1	0.4 (7)
C7—C8—C9—C10	-0.7 (8)	C12—C11—N1—C1	-175.3 (4)
C8—C9—C10—C5	2.2 (8)	O2—C3—N1—C11	2.3 (10)
C6—C5—C10—C9	-3.0 (7)	O1—C3—N1—C11	-177.8 (4)
C2—C5—C10—C9	178.0 (4)	O2—C3—N1—C1	-169.0 (6)
O3—C11—C12—C13	-99.3 (6)	O1—C3—N1—C1	10.9 (6)
N1—C11—C12—C13	76.1 (6)	C4—C1—N1—C11	-72.3 (6)
O3—C11—C12—C19	23.4 (7)	C2—C1—N1—C11	165.3 (4)
N1—C11—C12—C19	-161.1 (4)	C4—C1—N1—C3	99.6 (5)
C11—C12—C13—C14	51.5 (6)	C2—C1—N1—C3	-22.8 (5)
C19—C12—C13—C14	-70.7 (6)	O2—C3—O1—C2	-172.4 (5)
C11—C12—C13—C18	-133.5 (5)	N1—C3—O1—C2	7.7 (6)
C19—C12—C13—C18	104.3 (6)	C5—C2—O1—C3	-148.7 (4)
C18—C13—C14—C15	0.5 (7)	C1—C2—O1—C3	-21.9 (5)
