Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(–)-(4*R*,5*S*)-4-Methyl-3-[2(*R*)-(4-methylphenyl)propionyl]-5-phenyloxazolidin-2-one

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Key indicators

Single-crystal X-ray study
T = 160 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.078
Data-to-parameter ratio = 7.4

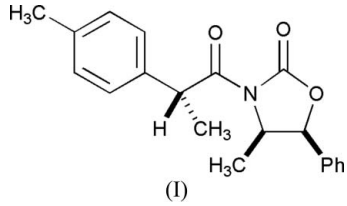
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 27 June 2006
Accepted 12 August 2006

In the title compound, $C_{20}H_{21}NO_3$, formed from enantiomerically pure (+)-(4*R*,5S)-4-methyl-5-phenyl-2-oxazolidinone and racemic 2-(4-methylphenyl)propanoyl chloride, the two carbonyl groups are oriented *anti* to each other, and the methyl group of the (4-methylphenyl)propionyl substituent lies close to the mean plane of the five-membered ring.

Comment

The title compound is the third in a series of structurally related compounds, introduced in our earlier report (Coumbarides, Eames *et al.*, 2006). With R^1 = 4-$(CH_3)C_6H_4$, the reaction shown in that report yielded the *anti–syn* and *syn–syn* diastereomers in 38 and 38% yields, respectively. The title compound, (I), is the *anti–syn* diastereomer (Fig. 1). In the crystal structure, the conformation of the central portion of the molecule is closely comparable with that in the previously reported derivatives (Coumbarides, Eames *et al.*, 2006; Coumbarides, Dingjan *et al.*, 2006); in the twisted five-membered ring, atoms C1 and C2 lie, respectively, 0.245 (4) Å above and −0.202 (4) Å below the plane defined by atoms O1, O2, N1 and C3. The carbonyl groups (C3═O2 and C11═O3) are oriented *anti* to each other, with the torsion angle O3—C11—N1—C3 = −169.3 (2)°. The orientation of the 4-$(CH_3)C_6H_4$ substituent resembles most closely that in the 4-(^{t}Bu)C_6H_4 derivative (Coumbarides, Dingjan *et al.*, 2006), with the C19 methyl group lying close to the mean plane of the five-membered ring [deviating by 0.138 (8) Å from it] and the torsion angle N1—C11—C12—C13 = 78.7 (3)°.



(I)

Experimental

The experimental procedure is comparable with that reported previously (Coumbarides, Eames *et al.*, 2006). The actual quantities used for the preparation of (I) were: *n*-butyllithium (15.45 ml, 2.5 *M* in hexanes, 38.6 mmol) and (*R*,*S*)-oxazolidinone (4.89 g, 27.6 mmol) in 60 ml tetrahydrofuran (THF), combined with a solution of (*rac*)-2-(4-methylphenyl)propanoyl chloride (5.02 g, 27.6 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 (1:1), to give a separable diastereoisomeric mixture in the ratio *anti–syn*:*syn*,*syn* 50:50. The *anti–syn* diastereomer was obtained as

colourless crystals (3.39 g, 38% yield, m.p. 341–343 K, R_F 0.71 [light petroleum (b.p 313–333 K)/diethyl ether, 7:3]. Spectroscopic analysis: $[\alpha]_D^{20}$ = −164.5 ($CHCl_3$, 293 K, concentration 0.18 g per 100 ml); IR ($CHCl_3$, ν_{max}/cm^{-1}): 1779 (C═O), 1710 (C═O); ^1H NMR (270 MHz; $CDCl_3$): δ 7.36–7.24 (9H, *m*, 9 × CH; Ar and Ph), 5.46 (1H, *d*, *J* = 6.9 Hz, CHO), 5.07 (1H, *q*, *J* = 7.1 Hz, ArCH), 4.65 (1H, *m*, $NCHCH_3$), 2.31 (3H, *s*, CH_3; Ar), 1.46 (3H, *d*, *J* = 7.1 Hz, CH_3CH), 0.91 (3H, *d*, *J* = 6.9 Hz, CH_3CHN); ^{13}C NMR (67.5 MHz; $CDCl_3$): δ 174.8 (NC═O), 152.9 (OC═O), 137.7, 137.1, 133.9 (3 × *i*-C; Ar and Ph), 129.7, 129.1, 128.3, 128.3, 126.1 (5 × CH; Ar and Ph), 79.1 (PhCHO), 55.0 (CHN), 43.6 (ArCH), 21.4 (CH_3; Ar), 19.8 (CH_3CH), 14.5 (CH_3CHN); found: MH^+ 324.1187; $C_{20}H_{22}NO_3$ requires 324.1194.

Crystal data

$C_{20}H_{21}NO_3$
M_r = 323.38
Monoclinic, $P2_1$
a = 13.066 (8) Å
b = 9.509 (8) Å
c = 7.201 (4) Å
β = 102.95 (4)°
V = 871.9 (10) Å^3
Z = 2
D_x = 1.232 Mg m^{-3}
Mo *K*α radiation
μ = 0.08 mm^{-1}
T = 160 (2) K
Prism, colourless
0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1743 measured reflections
1630 independent reflections
1417 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
θ_{max} = 25.0°
2 standard reflections
every 100 reflections
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 1.06
1630 reflections
220 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.0761P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-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_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate about their local threefold axes. In the absence of significant anomalous scattering effects, the few measured Friedel pairs have been merged. The absolute configuration is assigned on the basis of the known configuration of the starting material (Coumbarides, Eames *et al.*, 2006).

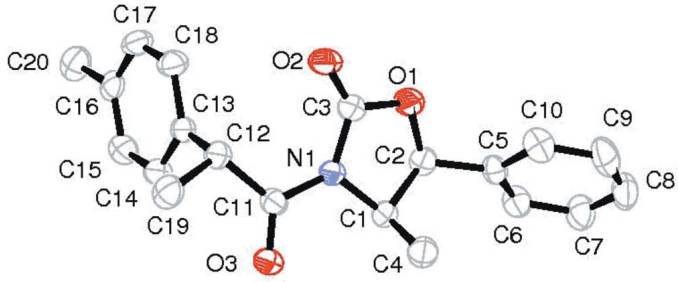


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

Data collection: *CAD-4-PC* (Enraf–Nonius, 1994); cell refinement: *CAD-4-PC*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (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). E**62**, o4037–o4038 [https://doi.org/10.1107/S1600536806031825]

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Crystal data

$C_{20}H_{21}NO_3$
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$V = 871.9\ (10)$ Å^3
$Z = 2$
$F(000) = 344$
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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
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Prism, colourless
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Radiation source: fine-focus sealed tube
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1630 independent reflections
1417 reflections with $I > 2\sigma(I)$
$R_{int} = 0.010$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = 0\rightarrow15$
$k = -2\rightarrow11$
$l = -8\rightarrow8$
2 standard reflections every 100 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.078$
$S = 1.06$
1630 reflections
220 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.0761P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ 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.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
1.7659 (0.0199) *x* + 8.7456 (0.0092) *y* + 2.3685 (0.0098) *z* = 8.8989 (0.0127)
* -0.0015 (0.0008) N1 * 0.0050 (0.0024) C3 * -0.0014 (0.0007) O1 * -0.0020 (0.0010) O2 - 0.2450 (0.0044) C1 0.2015 (0.0043) C2 - 0.1382 (0.0075) C19
Rms deviation of fitted atoms = 0.0029

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.51015 (17)	0.6695 (3)	0.8013 (3)	0.0308 (5)
H1	0.4841	0.7159	0.9065	0.037*
C2	0.49740 (18)	0.7696 (3)	0.6297 (3)	0.0339 (6)
H2	0.4978	0.8686	0.6766	0.041*
C3	0.66853 (19)	0.6938 (3)	0.6989 (3)	0.0393 (6)
C4	0.4596 (2)	0.5268 (3)	0.7589 (4)	0.0407 (7)
H4A	0.4778	0.4676	0.8729	0.061*
H4B	0.4850	0.4825	0.6548	0.061*
H4C	0.3832	0.5377	0.7213	0.061*
C5	0.40230 (19)	0.7494 (3)	0.4694 (3)	0.0325 (6)
C6	0.31243 (19)	0.8228 (3)	0.4763 (4)	0.0409 (7)
H6	0.3128	0.8867	0.5779	0.049*
C7	0.2213 (2)	0.8044 (4)	0.3365 (4)	0.0492 (8)
H7	0.1594	0.8547	0.3433	0.059*
C8	0.2208 (2)	0.7140 (4)	0.1891 (4)	0.0524 (8)
H8	0.1581	0.6999	0.0946	0.063*
C9	0.3109 (3)	0.6431 (4)	0.1769 (4)	0.0547 (8)
H9	0.3106	0.5817	0.0727	0.066*
C10	0.4023 (2)	0.6610 (3)	0.3167 (4)	0.0430 (7)
H10	0.4646	0.6128	0.3076	0.052*
C11	0.67809 (18)	0.6052 (3)	1.0290 (3)	0.0316 (6)
C12	0.79737 (18)	0.6083 (3)	1.0771 (3)	0.0342 (6)
H12	0.8225	0.5842	0.9596	0.041*
C13	0.83601 (17)	0.7545 (3)	1.1413 (3)	0.0320 (6)
C14	0.80485 (19)	0.8201 (3)	1.2912 (3)	0.0378 (6)
H14	0.7535	0.7766	1.3467	0.045*
C15	0.8470 (2)	0.9478 (3)	1.3615 (4)	0.0400 (7)
H15	0.8241	0.9904	1.4644	0.048*
C16	0.92221 (18)	1.0146 (3)	1.2845 (4)	0.0371 (6)
C17	0.9518 (2)	0.9500 (3)	1.1328 (4)	0.0415 (7)
H17	1.0024	0.9943	1.0762	0.050*

C18	0.90949 (19)	0.8226 (3)	1.0614 (4)	0.0381 (6)
H18	0.9311	0.7812	0.9563	0.046*
C19	0.8401 (2)	0.4990 (3)	1.2299 (4)	0.0430 (7)
H19A	0.8174	0.5225	1.3470	0.064*
H19B	0.9170	0.4985	1.2555	0.064*
H19C	0.8133	0.4059	1.1853	0.064*
C20	0.9695 (2)	1.1532 (3)	1.3630 (4)	0.0509 (8)
H20A	0.9370	1.2298	1.2792	0.076*
H20B	1.0453	1.1520	1.3701	0.076*
H20C	0.9569	1.1676	1.4908	0.076*
N1	0.62582 (14)	0.6602 (2)	0.8523 (3)	0.0317 (5)
O1	0.59164 (13)	0.7465 (2)	0.5591 (2)	0.0458 (5)
O2	0.75664 (14)	0.6802 (3)	0.6804 (3)	0.0566 (6)
O3	0.62656 (13)	0.5637 (2)	1.1380 (2)	0.0410 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0269 (12)	0.0347 (14)	0.0304 (12)	0.0006 (11)	0.0059 (10)	0.0005 (11)
C2	0.0341 (12)	0.0297 (15)	0.0364 (13)	0.0000 (11)	0.0047 (10)	0.0028 (11)
C3	0.0340 (13)	0.0503 (18)	0.0333 (13)	−0.0036 (13)	0.0072 (11)	0.0092 (13)
C4	0.0420 (14)	0.0369 (17)	0.0410 (15)	−0.0050 (13)	0.0045 (12)	0.0059 (12)
C5	0.0359 (13)	0.0299 (14)	0.0293 (12)	0.0035 (12)	0.0024 (10)	0.0040 (11)
C6	0.0400 (14)	0.0450 (17)	0.0367 (13)	0.0085 (13)	0.0066 (11)	−0.0018 (13)
C7	0.0388 (15)	0.059 (2)	0.0459 (16)	0.0094 (14)	0.0013 (13)	0.0002 (15)
C8	0.0463 (16)	0.063 (2)	0.0398 (15)	−0.0029 (16)	−0.0075 (13)	0.0010 (15)
C9	0.072 (2)	0.054 (2)	0.0334 (14)	−0.0040 (17)	0.0015 (14)	−0.0114 (14)
C10	0.0502 (15)	0.0382 (16)	0.0402 (14)	0.0102 (14)	0.0089 (12)	−0.0017 (14)
C11	0.0335 (13)	0.0340 (14)	0.0281 (12)	0.0014 (11)	0.0082 (11)	0.0020 (11)
C12	0.0281 (13)	0.0404 (15)	0.0335 (13)	0.0030 (12)	0.0057 (11)	0.0062 (12)
C13	0.0242 (11)	0.0404 (15)	0.0304 (12)	0.0045 (11)	0.0037 (10)	0.0105 (12)
C14	0.0336 (13)	0.0448 (17)	0.0359 (14)	−0.0009 (13)	0.0097 (11)	0.0079 (13)
C15	0.0431 (16)	0.0410 (16)	0.0362 (14)	0.0035 (13)	0.0094 (12)	0.0003 (12)
C16	0.0271 (12)	0.0394 (16)	0.0403 (14)	0.0044 (12)	−0.0022 (11)	0.0101 (13)
C17	0.0312 (13)	0.0447 (17)	0.0499 (15)	−0.0052 (12)	0.0122 (12)	0.0109 (13)
C18	0.0322 (13)	0.0438 (16)	0.0412 (14)	0.0019 (13)	0.0141 (11)	0.0044 (13)
C19	0.0358 (14)	0.0401 (16)	0.0500 (16)	0.0021 (13)	0.0031 (12)	0.0103 (15)
C20	0.0460 (16)	0.0429 (17)	0.0593 (18)	−0.0005 (14)	0.0023 (14)	0.0079 (15)
N1	0.0270 (10)	0.0392 (12)	0.0294 (9)	0.0004 (9)	0.0070 (8)	0.0067 (9)
O1	0.0333 (9)	0.0650 (14)	0.0383 (10)	0.0015 (10)	0.0059 (8)	0.0214 (10)
O2	0.0325 (10)	0.0970 (18)	0.0426 (10)	0.0018 (11)	0.0134 (8)	0.0239 (12)
O3	0.0350 (9)	0.0568 (13)	0.0323 (9)	−0.0019 (9)	0.0098 (8)	0.0099 (9)

Geometric parameters (Å, º)

C1—N1	1.476 (3)	C11—O3	1.210 (3)
C1—C4	1.510 (4)	C11—N1	1.403 (3)
C1—C2	1.539 (3)	C11—C12	1.519 (3)

C1—H1	1.000	C12—C13	1.515 (4)
C2—O1	1.450 (3)	C12—C19	1.525 (4)
C2—C5	1.507 (4)	C12—H12	1.000
C2—H2	1.000	C13—C14	1.385 (4)
C3—O2	1.195 (3)	C13—C18	1.385 (3)
C3—O1	1.349 (3)	C14—C15	1.381 (4)
C3—N1	1.382 (3)	C14—H14	0.950
C4—H4A	0.980	C15—C16	1.386 (4)
C4—H4B	0.980	C15—H15	0.950
C4—H4C	0.980	C16—C17	1.381 (4)
C5—C6	1.377 (4)	C16—C20	1.510 (4)
C5—C10	1.383 (4)	C17—C18	1.382 (4)
C6—C7	1.388 (4)	C17—H17	0.950
C6—H6	0.950	C18—H18	0.950
C7—C8	1.365 (4)	C19—H19A	0.980
C7—H7	0.950	C19—H19B	0.980
C8—C9	1.377 (4)	C19—H19C	0.980
C8—H8	0.950	C20—H20A	0.980
C9—C10	1.389 (4)	C20—H20B	0.980
C9—H9	0.950	C20—H20C	0.980
C10—H10	0.950		

N1—C1—C4	111.9 (2)	N1—C11—C12	117.8 (2)
N1—C1—C2	99.08 (18)	C13—C12—C11	110.0 (2)
C4—C1—C2	115.4 (2)	C13—C12—C19	111.2 (2)
N1—C1—H1	110.0	C11—C12—C19	110.0 (2)
C4—C1—H1	110.0	C13—C12—H12	108.5
C2—C1—H1	110.0	C11—C12—H12	108.5
O1—C2—C5	109.3 (2)	C19—C12—H12	108.5
O1—C2—C1	103.90 (18)	C14—C13—C18	117.7 (3)
C5—C2—C1	117.3 (2)	C14—C13—C12	121.0 (2)
O1—C2—H2	108.7	C18—C13—C12	121.1 (2)
C5—C2—H2	108.7	C15—C14—C13	121.3 (2)
C1—C2—H2	108.7	C15—C14—H14	119.4
O2—C3—O1	122.1 (2)	C13—C14—H14	119.4
O2—C3—N1	129.5 (2)	C14—C15—C16	121.1 (3)
O1—C3—N1	108.4 (2)	C14—C15—H15	119.4
C1—C4—H4A	109.5	C16—C15—H15	119.4
C1—C4—H4B	109.5	C17—C16—C15	117.5 (3)
H4A—C4—H4B	109.5	C17—C16—C20	121.4 (3)
C1—C4—H4C	109.5	C15—C16—C20	121.2 (3)
H4A—C4—H4C	109.5	C16—C17—C18	121.7 (2)
H4B—C4—H4C	109.5	C16—C17—H17	119.2
C6—C5—C10	119.2 (2)	C18—C17—H17	119.2
C6—C5—C2	118.1 (2)	C17—C18—C13	120.8 (3)
C10—C5—C2	122.7 (2)	C17—C18—H18	119.6
C5—C6—C7	120.7 (3)	C13—C18—H18	119.6
C5—C6—H6	119.7	C12—C19—H19A	109.5

C7—C6—H6	119.7	C12—C19—H19B	109.5
C8—C7—C6	119.8 (3)	H19A—C19—H19B	109.5
C8—C7—H7	120.1	C12—C19—H19C	109.5
C6—C7—H7	120.1	H19A—C19—H19C	109.5
C7—C8—C9	120.2 (3)	H19B—C19—H19C	109.5
C7—C8—H8	119.9	C16—C20—H20A	109.5
C9—C8—H8	119.9	C16—C20—H20B	109.5
C8—C9—C10	120.1 (3)	H20A—C20—H20B	109.5
C8—C9—H9	119.9	C16—C20—H20C	109.5
C10—C9—H9	119.9	H20A—C20—H20C	109.5
C5—C10—C9	119.9 (3)	H20B—C20—H20C	109.5
C5—C10—H10	120.1	C3—N1—C11	127.54 (19)
C9—C10—H10	120.1	C3—N1—C1	111.17 (19)
O3—C11—N1	118.8 (2)	C11—N1—C1	120.77 (19)
O3—C11—C12	123.4 (2)	C3—O1—C2	110.07 (18)

N1—C1—C2—O1	25.9 (2)	C12—C13—C14—C15	174.1 (2)
C4—C1—C2—O1	−93.7 (2)	C13—C14—C15—C16	−0.1 (4)
N1—C1—C2—C5	146.7 (2)	C14—C15—C16—C17	1.2 (4)
C4—C1—C2—C5	27.0 (3)	C14—C15—C16—C20	−179.1 (2)
O1—C2—C5—C6	−151.5 (2)	C15—C16—C17—C18	−0.9 (4)
C1—C2—C5—C6	90.6 (3)	C20—C16—C17—C18	179.4 (2)
O1—C2—C5—C10	28.2 (4)	C16—C17—C18—C13	−0.5 (4)
C1—C2—C5—C10	−89.7 (3)	C14—C13—C18—C17	1.5 (4)
C10—C5—C6—C7	2.7 (4)	C12—C13—C18—C17	−173.8 (2)
C2—C5—C6—C7	−177.6 (3)	O2—C3—N1—C11	2.4 (5)
C5—C6—C7—C8	−0.8 (5)	O1—C3—N1—C11	−178.6 (2)
C6—C7—C8—C9	−1.3 (5)	O2—C3—N1—C1	−169.2 (3)
C7—C8—C9—C10	1.3 (5)	O1—C3—N1—C1	9.7 (3)
C6—C5—C10—C9	−2.6 (4)	O3—C11—N1—C3	−169.9 (3)
C2—C5—C10—C9	177.7 (3)	C12—C11—N1—C3	13.2 (4)
C8—C9—C10—C5	0.6 (5)	O3—C11—N1—C1	1.0 (4)
O3—C11—C12—C13	−98.0 (3)	C12—C11—N1—C1	−175.8 (2)
N1—C11—C12—C13	78.7 (3)	C4—C1—N1—C3	99.9 (3)
O3—C11—C12—C19	24.8 (4)	C2—C1—N1—C3	−22.4 (3)
N1—C11—C12—C19	−158.5 (2)	C4—C1—N1—C11	−72.5 (3)
C11—C12—C13—C14	55.6 (3)	C2—C1—N1—C11	165.3 (2)
C19—C12—C13—C14	−66.6 (3)	O2—C3—O1—C2	−171.9 (3)
C11—C12—C13—C18	−129.2 (2)	N1—C3—O1—C2	9.0 (3)
C19—C12—C13—C18	108.7 (3)	C5—C2—O1—C3	−148.9 (2)
C18—C13—C14—C15	−1.3 (4)	C1—C2—O1—C3	−22.9 (3)