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(+)-(4*R*,5*S*)-4-Methyl-3-[2(*R*)-phenoxypropionyl]-5-phenyloxazolidin-2-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.089
Data-to-parameter ratio = 7.6

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

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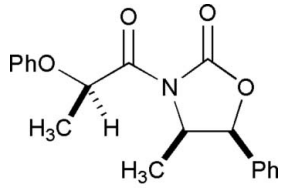
In the title compound, $C_{19}H_{19}NO_4$, formed from enantiomerically pure (+)-(4*R*,5*S*)-4-methyl-5-phenyl-2-oxazolidinone and racemic 2-phenoxypropanoyl chloride, the two carbonyl groups are oriented *anti* to each other, and the two methyl groups are oriented *anti* to each other.

Comment

The title compound, (I), is the fifth in a series of structurally related compounds, introduced in our earlier report (Coumbarides *et al.*, 2006). With R^1 = C_6H_5O, the reaction shown in that report yielded the *anti–syn* and *syn–syn* diastereomers in 44 and 45% yields, respectively. The title compound, (I), is the *syn–syn* diastereomer.



(I)

The conformation of (I) (Fig. 1) is closely comparable with that of the phenylpropionyl derivative (Coumbarides *et al.*, 2006). The five-membered ring displays a twist conformation in which atoms C1 and C2 lie, respectively, 0.286 (5) Å above and 0.291 (5) Å below the plane defined by atoms O1, O2, N1 and C3. The two methyl groups (C4 and C19) lie *anti* to each other, on either side of the five-membered ring. The carbonyl groups (C3═O2 and C11═O3) are also oriented *anti* to each other [torsion angle O3—C11—N1—C3 = −171.2 (3)°], avoiding electrostatic repulsion between the two O atoms. The shortest intermolecular contacts (Fig. 2) are C—H···O interactions [H16···O2^{i} = 2.66 Å; symmetry code: (i) $\frac{1}{2}-x, 2-y, \frac{1}{2}+z$] and edge-to-face C—H···π interactions [H9···centroid(C13–C18) = 2.92 Å; symmetry code: (ii) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$].

Experimental

The experimental procedure is comparable with that reported previously (Coumbarides *et al.*, 2006). The actual quantities used for preparation of (I) were: *n*-butyllithium (12.42 ml, 2.5 *M* in hexanes, 31.0 mmol) and (*R*,*S*)-oxazolidinone (5.00 g, 28.2 mmol) in 60 ml tetrahydrofuran (THF), combined with a solution of (*rac*)-2-phenoxypropanoyl chloride (5.71 g, 31.0 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 approximate ratio *anti–syn*:*syn–syn* 50:50. The *syn–syn* diastereomer was isolated as colourless crystals {4.13 g, 45% yield, m.p. 403–404 K, R_F 0.42 [light petroleum b.p 313–333 K/diethyl ether, 1:1]}. Spectroscopic analysis: $[\alpha]_D^{22}$ = +69.8 ($CHCl_3$, 295 K, concentration 1.9 g per 100 ml); IR ($CHCl_3$, ν_{max}, cm^{-1}): 1770 (C═O), 1712 (C═O); ^1H NMR (250 MHz; $CDCl_3$): δ 7.44–7.21 (7H, *m*, 7 × CH; Ph_a and Ph_b), 6.99–6.84 (3H, *t*, *J* = 7.3 Hz, 3 × CH; Ph_a and/or Ph_b), 6.02 (1H, *q*, *J* = 6.6 Hz, PhCH), 5.75 (1H, *d*, *J* = 7.2 Hz, PhCHO), 5.69 (1H, *m*, CHN), 1.68 (3H, *d*, *J* = 6.6 Hz, CH_3CHCO), 0.90 (3H, *d*, *J* = 6.8 Hz, CH_3CHN); ^{13}C NMR (67.9 MHz; $CDCl_3$): δ 172.2 (NC═O), 157.3 (*i*-CO; Ph), 152.9 (OC═O), 132.9 (*i*-C; Ph), 129.7, 129.1, 128.9, 125.7, 121.6, 115.0 (6 × CH; Ph_a and Ph_b), 80.8 (PhCHO), 71.7 (PhCH), 55.2 (CHN), 18.6 (CH_3), 14.5 (CH_3); found: MH^+ 326.1393; $C_{19}H_{20}NO_4$ requires 326.1392.

Crystal data

$C_{19}H_{19}NO_4$	Z = 4
M_r = 325.35	D_x = 1.302 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
a = 16.915 (12) Å	μ = 0.09 mm^{-1}
b = 10.634 (5) Å	T = 293 (2) K
c = 9.226 (6) Å	Prism, colourless
V = 1659.5 (18) $Å^3$	0.40 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	1115 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	R_{int} = 0.032
Absorption correction: none	θ_{max} = 25.0°
3072 measured reflections	2 standard reflections
1681 independent reflections	every 100 reflections
	intensity decay: 3%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.089	$\Delta\rho_{max}$ = 0.14 e $Å^{-3}$
S = 1.01	$\Delta\rho_{min}$ = −0.14 e $Å^{-3}$
1681 reflections	Extinction correction: *SHELXL97*
220 parameters	Extinction coefficient: 0.017 (2)
H-atom parameters constrained	

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 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 *et al.*, 2006).

Data collection: *CAD-4-PC* Software (Enraf–Nonius, 1994); cell refinement: *CAD-4-PC* Software; 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).

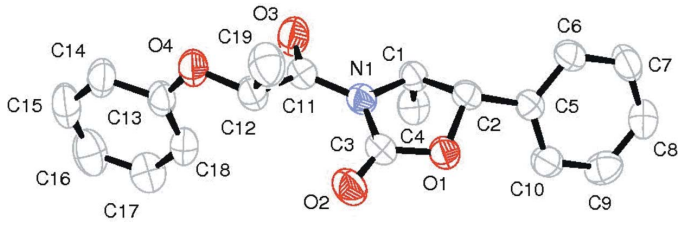


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

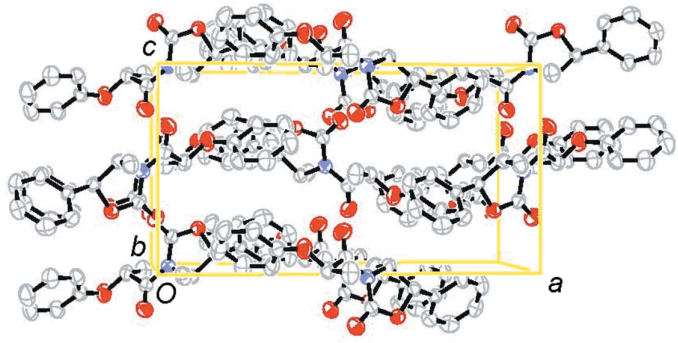


Figure 2
A view of (I) along the *b*-axis direction. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

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References

Coumbarides, G. S., Eames, J., Motevalli, M., Malatesti, N. & Yohannes, Y. (2006). *Acta Cryst.* E**62**, o4032–o4034.
Enraf–Nonius (1994). *CAD-4-PC* Software. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

supporting information

Acta Cryst. (2006). E**62**, o4041–o4042 [https://doi.org/10.1107/S1600536806031862]

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$c = 9.226$ (6) Å
$V = 1659.5$ (18) Å^3
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$D_x = 1.302$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10.1$–$12.0°$
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Prism, colourless
0.40 × 0.30 × 0.30 mm

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Graphite monochromator
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3072 measured reflections
1681 independent reflections
1115 reflections with $I > 2\sigma(I)$
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$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -13\rightarrow20$
$k = -12\rightarrow12$
$l = -10\rightarrow10$
2 standard reflections every 100 reflections
intensity decay: 3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.089$
$S = 1.02$
1681 reflections
220 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
$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.017 (2)
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)
- 7.0724 (0.0216) *x* + 9.3149 (0.0101) *y* - 2.2196 (0.0144) *z* = 2.7468 (0.0234)
* 0.0012 (0.0008) O1 * 0.0017 (0.0011) O2 * 0.0013 (0.0008) N1 * -0.0042 (0.0027) C3 0.2866 (0.0047) C1 - 0.2905 (0.0047) C2
Rms deviation of fitted atoms = 0.0024

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	0.60109 (17)	1.0289 (3)	1.0360 (4)	0.0451 (8)
H1	0.6180	1.0100	1.1353	0.054*
C2	0.66484 (18)	0.9896 (3)	0.9279 (3)	0.0433 (8)
H2	0.6900	0.9130	0.9648	0.052*
C3	0.54789 (19)	0.9118 (3)	0.8452 (4)	0.0480 (8)
C4	0.5737 (2)	1.1638 (3)	1.0245 (4)	0.0612 (10)
H4A	0.5586	1.1815	0.9263	0.092*
H4B	0.6159	1.2190	1.0528	0.092*
H4C	0.5291	1.1766	1.0873	0.092*
C5	0.72911 (18)	1.0811 (3)	0.8882 (3)	0.0411 (8)
C6	0.79914 (19)	1.0795 (3)	0.9648 (4)	0.0557 (10)
H6	0.8054	1.0222	1.0401	0.067*
C7	0.8600 (2)	1.1609 (4)	0.9322 (4)	0.0644 (11)
H7	0.9062	1.1596	0.9866	0.077*
C8	0.8522 (2)	1.2433 (4)	0.8204 (4)	0.0616 (10)
H8	0.8933	1.2978	0.7975	0.074*
C9	0.7834 (2)	1.2456 (3)	0.7413 (4)	0.0651 (11)
H9	0.7782	1.3017	0.6646	0.078*
C10	0.7218 (2)	1.1650 (3)	0.7748 (4)	0.0538 (9)
H10	0.6754	1.1673	0.7208	0.065*
C11	0.47944 (19)	0.8982 (3)	1.0836 (4)	0.0497 (9)
C12	0.42713 (19)	0.7910 (3)	1.0310 (4)	0.0531 (9)
H12	0.4052	0.8107	0.9353	0.064*
C13	0.2992 (2)	0.8435 (3)	1.1255 (4)	0.0525 (9)
C14	0.2365 (2)	0.8044 (4)	1.2099 (4)	0.0633 (11)
H14	0.2415	0.7329	1.2673	0.076*
C15	0.1666 (2)	0.8706 (4)	1.2094 (5)	0.0774 (13)
H15	0.1246	0.8436	1.2663	0.093*
C16	0.1586 (3)	0.9763 (4)	1.1254 (5)	0.0811 (13)
H16	0.1112	1.0206	1.1245	0.097*
C17	0.2208 (2)	1.0158 (4)	1.0433 (4)	0.0700 (11)

H17	0.2155	1.0876	0.9867	0.084*
C18	0.2916 (2)	0.9507 (4)	1.0429 (4)	0.0591 (10)
H18	0.3337	0.9791	0.9871	0.071*
C19	0.4742 (2)	0.6684 (3)	1.0253 (4)	0.0710 (11)
H19A	0.4856	0.6409	1.1222	0.106*
H19B	0.5228	0.6821	0.9740	0.106*
H19C	0.4437	0.6053	0.9763	0.106*
N1	0.53871 (15)	0.9397 (2)	0.9892 (3)	0.0462 (7)
O1	0.61905 (12)	0.9558 (2)	0.8006 (2)	0.0493 (6)
O2	0.50324 (15)	0.8593 (2)	0.7646 (3)	0.0645 (7)
O3	0.47462 (14)	0.9432 (2)	1.2024 (3)	0.0683 (7)
O4	0.36534 (14)	0.7686 (2)	1.1322 (3)	0.0626 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0422 (19)	0.0472 (19)	0.0460 (19)	−0.0033 (16)	−0.0029 (15)	−0.0047 (16)
C2	0.0408 (18)	0.0457 (18)	0.0435 (18)	0.0051 (17)	−0.0025 (16)	−0.0019 (16)
C3	0.042 (2)	0.051 (2)	0.051 (2)	0.0015 (18)	−0.0084 (18)	−0.0023 (19)
C4	0.057 (2)	0.054 (2)	0.073 (3)	0.0023 (19)	0.009 (2)	−0.012 (2)
C5	0.0383 (18)	0.0417 (18)	0.0433 (19)	0.0068 (16)	0.0022 (15)	−0.0071 (17)
C6	0.047 (2)	0.058 (2)	0.062 (2)	0.0069 (19)	−0.0058 (19)	0.014 (2)
C7	0.038 (2)	0.075 (3)	0.080 (3)	−0.005 (2)	−0.005 (2)	0.003 (2)
C8	0.048 (2)	0.061 (2)	0.076 (3)	−0.0053 (19)	0.010 (2)	0.000 (2)
C9	0.082 (3)	0.051 (2)	0.062 (3)	−0.007 (2)	−0.001 (2)	0.013 (2)
C10	0.052 (2)	0.0544 (19)	0.055 (2)	−0.0025 (19)	−0.0085 (19)	0.005 (2)
C11	0.041 (2)	0.057 (2)	0.051 (2)	0.0007 (17)	−0.0029 (18)	0.0033 (19)
C12	0.042 (2)	0.057 (2)	0.060 (2)	−0.0032 (18)	−0.0020 (18)	0.0000 (19)
C13	0.046 (2)	0.058 (2)	0.054 (2)	−0.0165 (19)	−0.0003 (18)	−0.007 (2)
C14	0.053 (2)	0.068 (2)	0.069 (3)	−0.021 (2)	0.007 (2)	0.000 (2)
C15	0.049 (2)	0.099 (3)	0.084 (3)	−0.024 (3)	0.015 (2)	−0.021 (3)
C16	0.056 (3)	0.078 (3)	0.109 (4)	0.001 (2)	0.008 (3)	−0.025 (3)
C17	0.065 (3)	0.060 (2)	0.085 (3)	0.003 (2)	0.003 (2)	−0.005 (2)
C18	0.045 (2)	0.061 (2)	0.071 (3)	−0.009 (2)	0.0103 (19)	−0.002 (2)
C19	0.058 (2)	0.059 (2)	0.096 (3)	0.000 (2)	0.001 (2)	0.003 (2)
N1	0.0423 (16)	0.0529 (17)	0.0434 (17)	−0.0035 (14)	−0.0015 (13)	−0.0044 (14)
O1	0.0416 (13)	0.0606 (13)	0.0458 (12)	−0.0018 (12)	0.0011 (11)	−0.0088 (12)
O2	0.0515 (14)	0.0824 (16)	0.0595 (15)	−0.0106 (15)	−0.0097 (12)	−0.0144 (15)
O3	0.0592 (17)	0.0874 (18)	0.0583 (16)	−0.0187 (15)	0.0101 (13)	−0.0113 (16)
O4	0.0437 (14)	0.0670 (16)	0.0770 (18)	−0.0058 (13)	0.0026 (14)	0.0161 (14)

Geometric parameters (Å, º)

C1—N1	1.483 (4)	C10—H10	0.930
C1—C4	1.511 (5)	C11—O3	1.198 (4)
C1—C2	1.527 (4)	C11—N1	1.400 (4)
C1—H1	0.980	C11—C12	1.522 (5)
C2—O1	1.452 (4)	C12—O4	1.422 (4)

C2—C5	1.504 (4)	C12—C19	1.528 (4)
C2—H2	0.980	C12—H12	0.980
C3—O2	1.198 (4)	C13—O4	1.375 (4)
C3—O1	1.355 (4)	C13—C18	1.377 (5)
C3—N1	1.370 (4)	C13—C14	1.379 (5)
C4—H4A	0.960	C14—C15	1.377 (5)
C4—H4B	0.960	C14—H14	0.930
C4—H4C	0.960	C15—C16	1.371 (6)
C5—C6	1.379 (5)	C15—H15	0.930
C5—C10	1.380 (4)	C16—C17	1.362 (6)
C6—C7	1.378 (5)	C16—H16	0.930
C6—H6	0.930	C17—C18	1.383 (5)
C7—C8	1.360 (5)	C17—H17	0.930
C7—H7	0.930	C18—H18	0.930
C8—C9	1.373 (5)	C19—H19A	0.960
C8—H8	0.930	C19—H19B	0.960
C9—C10	1.384 (5)	C19—H19C	0.960
C9—H9	0.930		

N1—C1—C4	111.6 (3)	O3—C11—N1	119.5 (3)
N1—C1—C2	97.9 (2)	O3—C11—C12	123.5 (3)
C4—C1—C2	115.5 (3)	N1—C11—C12	117.0 (3)
N1—C1—H1	110.4	O4—C12—C11	110.1 (3)
C4—C1—H1	110.4	O4—C12—C19	105.2 (3)
C2—C1—H1	110.4	C11—C12—C19	110.3 (3)
O1—C2—C5	110.4 (3)	O4—C12—H12	110.4
O1—C2—C1	102.7 (2)	C11—C12—H12	110.4
C5—C2—C1	119.5 (3)	C19—C12—H12	110.4
O1—C2—H2	107.9	O4—C13—C18	125.5 (3)
C5—C2—H2	107.9	O4—C13—C14	115.2 (3)
C1—C2—H2	107.9	C18—C13—C14	119.3 (4)
O2—C3—O1	122.2 (3)	C15—C14—C13	120.3 (4)
O2—C3—N1	129.2 (3)	C15—C14—H14	119.9
O1—C3—N1	108.7 (3)	C13—C14—H14	119.9
C1—C4—H4A	109.5	C16—C15—C14	120.4 (4)
C1—C4—H4B	109.5	C16—C15—H15	119.8
H4A—C4—H4B	109.5	C14—C15—H15	119.8
C1—C4—H4C	109.5	C17—C16—C15	119.4 (4)
H4A—C4—H4C	109.5	C17—C16—H16	120.3
H4B—C4—H4C	109.5	C15—C16—H16	120.3
C6—C5—C10	118.2 (3)	C16—C17—C18	121.0 (4)
C6—C5—C2	119.2 (3)	C16—C17—H17	119.5
C10—C5—C2	122.6 (3)	C18—C17—H17	119.5
C7—C6—C5	121.4 (3)	C13—C18—C17	119.6 (3)
C7—C6—H6	119.3	C13—C18—H18	120.2
C5—C6—H6	119.3	C17—C18—H18	120.2
C8—C7—C6	119.9 (3)	C12—C19—H19A	109.5
C8—C7—H7	120.1	C12—C19—H19B	109.5

C6—C7—H7	120.1	H19A—C19—H19B	109.5
C7—C8—C9	119.8 (4)	C12—C19—H19C	109.5
C7—C8—H8	120.1	H19A—C19—H19C	109.5
C9—C8—H8	120.1	H19B—C19—H19C	109.5
C8—C9—C10	120.5 (3)	C3—N1—C11	128.1 (3)
C8—C9—H9	119.8	C3—N1—C1	109.9 (3)
C10—C9—H9	119.8	C11—N1—C1	122.0 (3)
C5—C10—C9	120.2 (3)	C3—O1—C2	108.3 (2)
C5—C10—H10	119.9	C13—O4—C12	118.1 (3)
C9—C10—H10	119.9		

N1—C1—C2—O1	33.8 (3)	C15—C16—C17—C18	0.3 (6)
C4—C1—C2—O1	−84.8 (3)	O4—C13—C18—C17	178.3 (3)
N1—C1—C2—C5	156.3 (3)	C14—C13—C18—C17	−1.4 (5)
C4—C1—C2—C5	37.7 (4)	C16—C17—C18—C13	0.7 (6)
O1—C2—C5—C6	−148.7 (3)	O2—C3—N1—C11	10.0 (6)
C1—C2—C5—C6	92.6 (4)	O1—C3—N1—C11	−170.9 (3)
O1—C2—C5—C10	29.4 (4)	O2—C3—N1—C1	−167.7 (3)
C1—C2—C5—C10	−89.2 (4)	O1—C3—N1—C1	11.4 (3)
C10—C5—C6—C7	1.4 (5)	O3—C11—N1—C3	−171.2 (3)
C2—C5—C6—C7	179.7 (3)	C12—C11—N1—C3	12.3 (5)
C5—C6—C7—C8	−1.4 (6)	O3—C11—N1—C1	6.2 (5)
C6—C7—C8—C9	0.6 (6)	C12—C11—N1—C1	−170.2 (3)
C7—C8—C9—C10	0.2 (6)	C4—C1—N1—C3	93.1 (3)
C6—C5—C10—C9	−0.6 (5)	C2—C1—N1—C3	−28.4 (3)
C2—C5—C10—C9	−178.8 (3)	C4—C1—N1—C11	−84.8 (4)
C8—C9—C10—C5	−0.2 (5)	C2—C1—N1—C11	153.7 (3)
O3—C11—C12—O4	9.6 (5)	O2—C3—O1—C2	−168.2 (3)
N1—C11—C12—O4	−174.1 (3)	N1—C3—O1—C2	12.6 (3)
O3—C11—C12—C19	−106.0 (4)	C5—C2—O1—C3	−158.8 (2)
N1—C11—C12—C19	70.3 (4)	C1—C2—O1—C3	−30.3 (3)
O4—C13—C14—C15	−178.6 (3)	C18—C13—O4—C12	−9.8 (5)
C18—C13—C14—C15	1.1 (5)	C14—C13—O4—C12	169.9 (3)
C13—C14—C15—C16	−0.1 (6)	C11—C12—O4—C13	82.5 (3)
C14—C15—C16—C17	−0.6 (6)	C19—C12—O4—C13	−158.7 (3)