organic papers

(+)-(4R,5S)-4-Methyl-5-phenyl-3-[2(S)-phenyl-propionyl]oxazolidin-2-one

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In the title compound, $C_{19}H_{19}NO_3$, formed from enantiomerically pure (+)-(4R,5S)-4-methyl-5-phenyl-2-oxazolidinone and racemic 2-phenylpropanoyl chloride, the two carbonyl groups are oriented *anti* to each other, and the two methyl groups are oriented *anti* to each other.

Comment

The development of predictable and efficient resolution methodology is becoming increasingly important for academia and industry alike. With this aim in mind, we have recently focused our attention on the resolution of profens (Sonawane *et al.*, 1992; Fuji *et al.*, 1989; Larsen *et al.*, 1989), such as ibuprofen (Alper & Hamel, 1990; Piccolo *et al.*, 1991) and naproxen (Stille & Parrinello, 1993; Ohta *et al.*, 1987; Kumar *et al.*, 1991), using a novel parallel kinetic resolution methodology (Coumbarides, Dingjan, Eames, Flinn *et al.*, 2006; Coumbarides, Dingjan *et al.*, 2005; Coumbarides, Eames *et al.*, 2005). For this project, we were required to determine the relative and absolute configurations of a series of related profen adducts derived from (+)-(4R,5S)-4-methyl-5-phenyl-2-oxazolidinone, (1). The compounds were obtained in each case by addition of racemic 2-(R^1)-propanoyl chloride (where R^1 is a substituent group) to a solution of lithiated oxazolidinone, the latter being derived from the addition of *n*-BuLi to the (R,S)-oxazolidinone (1) in tetrahydrofuran at 195 K (see reaction scheme).
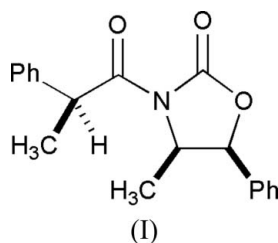

The reaction provided in each case a separable mixture of diastereoisomeric *anti–syn* and *syn–syn* oxazolidinone adducts. In the following series of reports (Chavda *et al.* 2006a,b; Coumbarides, Dingjan, Eames, Motevalli & Malatesti *et al.*, 2006; Chavda *et al.*, 2006; Coumbarides, Eames, Motevalli, Malatesti & Yohannes, 2006), we describe the crystal structures of six of these related compounds.

With $R^1 = C_6H_5$, the reaction shown in the scheme yielded the *anti–syn* and *syn–syn* diastereomers in 23 and 25% yields, respectively. The title compound, (I), is the *syn–syn* diastereomer (Fig. 1).

In the crystal structure of (I), the five-membered ring displays a twist conformation in which atoms O1, O2, N1 and C3 lie in an approximate plane, and C1 and C2 lie, respectively,

0.248 (3) Å above and 0.262 (3) Å below that plane. The two methyl groups (C4 and C19) lie *anti* to each other, on either side of the central five-membered ring. The carbonyl groups (C3=O2 and C11=O3) are also oriented *anti* to each other [torsion angle O3−C11−N1−C3 = −169.3 (2)°], avoiding electrostatic repulsion between the two O atoms. The electrostatic factor also appears to be important for determining the molecular packing (Fig. 2), whereby adjacent molecules approach each other in a 'side-on' manner. The shortest intermolecular contacts to each O atom are made by H atoms [H4A···O2^i = 2.66 Å, H2···O3^{ii} = 2.63 Å; symmetry codes: (i) $1 - x, \frac{1}{2} + y, 2 - z$; (ii) $1 - x, -\frac{1}{2} + y, 1 - z$].

Figure 2
The crystal packing of (I), viewed along the *b* axis. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

m, 10 × CH; Ph$_a$ and Ph$_b$), 5.64 (1H, d, J = 7.2 Hz, OCHPh), 5.08 (1H, q, J = 7.1 Hz, PhCH), 4.82 (1H, m, CHN), 1.51 (3H, d, J = 7.1 Hz, CH$_3$CHCO), 0.74 (3H, d, J = 6.6 Hz, CH$_3$CHN); ^{13}C NMR (62.9 MHz; CDCl$_3$): δ 174.3 (NC=O), 152.5 (OC=O), 140.3 (*i*-C; Ph$_a$), 133.5 (*i*-C; Ph$_b$), 128.9, 128.8, 128.6, 128.1, 127.1, 125.7 (6 × CH; Ph$_a$ and Ph$_b$), 78.8 (OCHPh), 54.7 (CH$_3$CHO), 43.6 (PhCH), 19.4 (CH$_3$), 14.1 (CH$_3$); MS m/z: MH$^+$ 310.1460; C$_{19}$H$_{20}$NO$_3$ requires 310.1443.

Experimental

The following procedure is representative for the reaction sequence depicted in the reaction scheme. *n*-Butyllithium (6.33 ml, 2.5 M in hexanes, 15.8 mmol) was added dropwise to a stirred solution of (*R,S*)-oxazolidinone, (1) (2 g, 11.3 mmol), in tetrahydrofuran (20 ml) at 195 K. The resulting solution was stirred at 195 K for 1 h. A solution of racemic 2-phenylpropanoyl chloride (1.90 g, 11.3 mmol) in tetrahydrofuran (5 ml) was added dropwise and the resulting solution was stirred at 195 K for 2 h. The reaction was quenched by the addition of water (10 ml), extracted with CH$_2$Cl$_2$ (3 × 10 ml) and dried over MgSO$_4$. The combined organic layers were evaporated under reduced pressure. 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) of the title compound; *anti–syn* diastereomer (0.80 g, 23%), *syn–syn* diastereomer (0.87 g, 25%). The latter was obtained as colourless crystals suitable for X-ray analysis [m.p. 394–396 K, R_F 0.63 (light petroleum (b.p 313–333 K)/diethyl ether, 1:1].

Spectroscopic analysis for (I): $[\alpha]_D^{20}$ = 122.9 (CHCl$_3$, 293 K, concentration 0.81 g per 100 ml); IR (CHCl$_3$, ν_{max}, cm^{-1}): 1774 (C=O), 1701 (C=O); ^{1}H NMR (250 MHz, CDCl$_3$): δ 7.40–7.17 (10H,
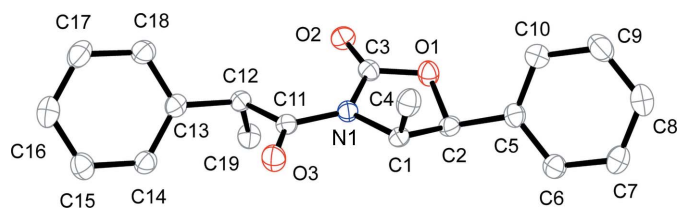

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.
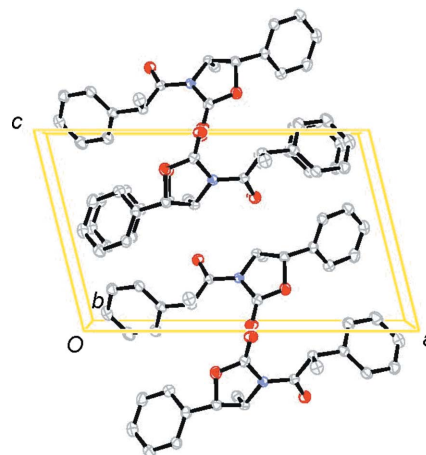
Crystal data

C$_{19}$H$_{19}$NO$_3$	Z = 2
M_r = 309.35	D_x = 1.298 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
a = 14.757 (2) Å	μ = 0.09 mm^{-1}
b = 6.069 (2) Å	T = 160 (2) K
c = 9.109 (4) Å	Prism, colourless
β = 104.02 (6)°	0.40 × 0.30 × 0.20 mm
V = 791.5 (5) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	1449 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	R_{int} = 0.009
Absorption correction: none	θ_{max} = 25.1°
1623 measured reflections	4 standard reflections
1521 independent reflections	every 100 reflections
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.028	$+ 0.119P]$
$wR(F^2)$ = 0.075	where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
1521 reflections	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
210 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
H-atom parameters constrained	

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 were merged. The absolute configuration is assigned on the basis of the known configuration of (1) (Evans *et al.*, 1985).

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supporting information

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(+)-(4*R*,5*S*)-4-Methyl-5-phenyl-3-[-2(*S*)-phenylpropionyl]- oxazolidin-2-one

Crystal data

$C_{19}H_{19}NO_3$	$F(000) = 328$
$M_r = 309.35$	$D_x = 1.298$ Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2yb	Cell parameters from 25 reflections
$a = 14.757$ (2) Å	$\theta = 9.7–13.0°$
$b = 6.069$ (2) Å	$\mu = 0.09$ mm^{-1}
$c = 9.109$ (4) Å	$T = 160$ K
$\beta = 104.02$ (6)°	Prism, colourless
$V = 791.5$ (5) Å^3	$0.40 \times 0.30 \times 0.20$ mm
$Z = 2$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.009$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.1°$, $\theta_{min} = 1.4°$
Graphite monochromator	$h = -16 \rightarrow 17$
$\omega/2\theta$ scans	$k = 0 \rightarrow 7$
1623 measured reflections	$l = -10 \rightarrow 0$
1521 independent reflections	4 standard reflections every 100 reflections
1449 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.028$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.075$	H-atom parameters constrained
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
1521 reflections	
210 parameters	$(\Delta/\sigma)_{max} < 0.001$
1 restraint	$\Delta\rho_{max} = 0.13$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{min} = -0.23$ 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)
- 3.1511 (0.0161) x + 5.4484 (0.0064) y + 3.8763 (0.0094) z = 1.0707 (0.0091)
* 0.0004 (0.0005) O1 * 0.0006 (0.0007) O2 * 0.0004 (0.0005) N1 * -0.0014 (0.0018) C3 0.2480 (0.0033) C1 - 0.2624 (0.0030) C2
Rms deviation of fitted atoms = 0.0008

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.49725 (10)	−0.0506 (3)	0.75171 (16)	0.0223 (4)
O1	0.36438 (9)	−0.1645 (3)	0.80375 (14)	0.0288 (3)
O2	0.49467 (11)	−0.2176 (3)	0.98430 (16)	0.0292 (3)
O3	0.61111 (9)	0.1127 (3)	0.66406 (15)	0.0304 (4)
C1	0.42346 (13)	0.0405 (3)	0.6275 (2)	0.0228 (4)
H1A	0.4394	0.0154	0.5282	0.027*
C2	0.34228 (13)	−0.1103 (3)	0.6418 (2)	0.0241 (4)
H2A	0.3448	−0.2483	0.5830	0.029*
C3	0.45794 (13)	−0.1511 (4)	0.8604 (2)	0.0240 (4)
C4	0.40795 (14)	0.2829 (4)	0.6495 (2)	0.0290 (5)
H4A	0.4663	0.3634	0.6553	0.043*
H4B	0.3879	0.3045	0.7435	0.043*
H4C	0.3596	0.3383	0.5639	0.043*
C5	0.24509 (13)	−0.0169 (4)	0.5956 (2)	0.0249 (4)
C6	0.19350 (13)	−0.0559 (4)	0.4484 (2)	0.0271 (4)
H6A	0.2190	−0.1435	0.3818	0.033*
C7	0.10495 (14)	0.0336 (4)	0.3992 (2)	0.0317 (5)
H7A	0.0700	0.0079	0.2985	0.038*
C8	0.06702 (14)	0.1605 (4)	0.4963 (2)	0.0343 (5)
H8A	0.0064	0.2221	0.4619	0.041*
C9	0.11767 (14)	0.1972 (4)	0.6431 (3)	0.0359 (5)
H9A	0.0916	0.2836	0.7096	0.043*
C10	0.20617 (14)	0.1087 (4)	0.6934 (2)	0.0316 (5)
H10A	0.2405	0.1333	0.7946	0.038*
C11	0.59155 (12)	−0.0054 (3)	0.7605 (2)	0.0227 (4)
C12	0.66371 (13)	−0.1199 (4)	0.8843 (2)	0.0241 (4)
H12A	0.6446	−0.1038	0.9818	0.029*
C13	0.75975 (13)	−0.0172 (3)	0.9030 (2)	0.0241 (4)
C14	0.81250 (13)	−0.0474 (4)	0.7946 (2)	0.0275 (4)
H14A	0.7872	−0.1311	0.7060	0.033*
C15	0.90074 (13)	0.0432 (4)	0.8157 (2)	0.0311 (5)

H15A	0.9355	0.0216	0.7417	0.037*
C16	0.93844 (13)	0.1653 (4)	0.9444 (2)	0.0335 (5)
H16A	0.9991	0.2273	0.9592	0.040*
C17	0.88689 (14)	0.1966 (4)	1.0521 (2)	0.0349 (5)
H17A	0.9124	0.2813	1.1402	0.042*
C18	0.79813 (14)	0.1048 (4)	1.0317 (2)	0.0302 (5)
H18A	0.7638	0.1258	1.1063	0.036*
C19	0.66362 (14)	−0.3671 (4)	0.8450 (2)	0.0311 (5)
H19D	0.6039	−0.4327	0.8507	0.047*
H19A	0.7146	−0.4411	0.9171	0.047*
H19B	0.6723	−0.3845	0.7423	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0212 (7)	0.0260 (9)	0.0195 (7)	−0.0001 (7)	0.0047 (6)	0.0030 (7)
O1	0.0235 (7)	0.0334 (8)	0.0295 (7)	−0.0010 (7)	0.0067 (5)	0.0069 (7)
O2	0.0333 (7)	0.0314 (8)	0.0229 (7)	0.0022 (7)	0.0065 (5)	0.0082 (7)
O3	0.0266 (7)	0.0378 (9)	0.0270 (7)	−0.0020 (7)	0.0071 (5)	0.0087 (7)
C1	0.0219 (9)	0.0297 (10)	0.0163 (9)	0.0025 (8)	0.0035 (7)	0.0015 (8)
C2	0.0254 (10)	0.0244 (11)	0.0217 (9)	−0.0001 (8)	0.0039 (7)	−0.0035 (8)
C3	0.0251 (9)	0.0205 (9)	0.0271 (10)	0.0007 (8)	0.0081 (8)	−0.0011 (9)
C4	0.0274 (10)	0.0289 (11)	0.0284 (10)	−0.0003 (9)	0.0023 (8)	0.0060 (9)
C5	0.0226 (9)	0.0239 (10)	0.0283 (9)	−0.0035 (8)	0.0066 (7)	−0.0001 (9)
C6	0.0253 (9)	0.0266 (11)	0.0298 (9)	−0.0039 (9)	0.0072 (8)	−0.0026 (9)
C7	0.0264 (10)	0.0334 (12)	0.0320 (10)	−0.0044 (9)	0.0004 (8)	−0.0008 (10)
C8	0.0239 (9)	0.0338 (12)	0.0445 (11)	0.0018 (10)	0.0071 (8)	0.0047 (11)
C9	0.0299 (10)	0.0377 (13)	0.0431 (11)	0.0031 (10)	0.0147 (9)	−0.0054 (11)
C10	0.0290 (10)	0.0373 (13)	0.0288 (10)	0.0006 (10)	0.0076 (8)	−0.0030 (10)
C11	0.0234 (9)	0.0247 (11)	0.0201 (9)	0.0007 (8)	0.0053 (7)	−0.0005 (9)
C12	0.0232 (9)	0.0273 (11)	0.0213 (9)	0.0013 (8)	0.0045 (7)	0.0018 (8)
C13	0.0236 (9)	0.0222 (10)	0.0241 (9)	0.0051 (8)	0.0014 (7)	0.0025 (9)
C14	0.0260 (9)	0.0297 (11)	0.0249 (9)	0.0017 (9)	0.0028 (7)	−0.0011 (9)
C15	0.0259 (10)	0.0333 (11)	0.0343 (11)	0.0037 (9)	0.0077 (8)	0.0034 (10)
C16	0.0246 (9)	0.0299 (11)	0.0424 (11)	−0.0010 (10)	0.0013 (8)	0.0012 (11)
C17	0.0311 (10)	0.0329 (13)	0.0362 (11)	−0.0017 (9)	−0.0007 (9)	−0.0089 (10)
C18	0.0288 (10)	0.0315 (13)	0.0290 (10)	0.0041 (9)	0.0046 (8)	−0.0037 (9)
C19	0.0303 (10)	0.0255 (11)	0.0367 (11)	0.0013 (9)	0.0067 (8)	−0.0001 (10)

Geometric parameters (Å, º)

N1—C11	1.402 (2)	C8—H8A	0.950
N1—C3	1.403 (3)	C9—C10	1.384 (3)
N1—C1	1.475 (2)	C9—H9A	0.950
O1—C3	1.354 (2)	C10—H10A	0.950
O1—C2	1.469 (2)	C11—C12	1.519 (3)
O2—C3	1.197 (2)	C12—C13	1.520 (3)
O3—C11	1.222 (2)	C12—C19	1.542 (3)

C1—C4	1.510 (3)	C12—H12A	1.000
C1—C2	1.538 (3)	C13—C18	1.386 (3)
C1—H1A	1.000	C13—C14	1.409 (3)
C2—C5	1.504 (3)	C14—C15	1.383 (3)
C2—H2A	1.000	C14—H14A	0.950
C4—H4A	0.980	C15—C16	1.385 (3)
C4—H4B	0.980	C15—H15A	0.950
C4—H4C	0.980	C16—C17	1.392 (3)
C5—C6	1.393 (3)	C16—H16A	0.950
C5—C10	1.397 (3)	C17—C18	1.394 (3)
C6—C7	1.385 (3)	C17—H17A	0.950
C6—H6A	0.950	C18—H18A	0.950
C7—C8	1.389 (3)	C19—H19D	0.980
C7—H7A	0.950	C19—H19A	0.980
C8—C9	1.383 (3)	C19—H19B	0.980
C11—N1—C3	128.28 (16)	C8—C9—H9A	119.9
C11—N1—C1	120.59 (16)	C10—C9—H9A	119.9
C3—N1—C1	110.48 (14)	C9—C10—C5	120.09 (19)
C3—O1—C2	109.10 (15)	C9—C10—H10A	120.0
N1—C1—C4	111.80 (18)	C5—C10—H10A	120.0
N1—C1—C2	99.06 (15)	O3—C11—N1	118.56 (17)
C4—C1—C2	115.00 (17)	O3—C11—C12	123.87 (16)
N1—C1—H1A	110.2	N1—C11—C12	117.44 (17)
C4—C1—H1A	110.2	C11—C12—C13	111.25 (17)
C2—C1—H1A	110.2	C11—C12—C19	108.15 (16)
O1—C2—C5	109.26 (16)	C13—C12—C19	111.92 (17)
O1—C2—C1	103.31 (15)	C11—C12—H12A	108.5
C5—C2—C1	117.49 (17)	C13—C12—H12A	108.5
O1—C2—H2A	108.8	C19—C12—H12A	108.5
C5—C2—H2A	108.8	C18—C13—C14	118.69 (18)
C1—C2—H2A	108.8	C18—C13—C12	119.50 (18)
O2—C3—O1	121.74 (19)	C14—C13—C12	121.78 (18)
O2—C3—N1	129.92 (18)	C15—C14—C13	120.80 (19)
O1—C3—N1	108.34 (16)	C15—C14—H14A	119.6
C1—C4—H4A	109.5	C13—C14—H14A	119.6
C1—C4—H4B	109.5	C14—C15—C16	120.12 (19)
H4A—C4—H4B	109.5	C14—C15—H15A	119.9
C1—C4—H4C	109.5	C16—C15—H15A	119.9
H4A—C4—H4C	109.5	C15—C16—C17	119.58 (19)
H4B—C4—H4C	109.5	C15—C16—H16A	120.2
C6—C5—C10	119.57 (18)	C17—C16—H16A	120.2
C6—C5—C2	117.84 (18)	C16—C17—C18	120.5 (2)
C10—C5—C2	122.59 (17)	C16—C17—H17A	119.7
C7—C6—C5	119.84 (19)	C18—C17—H17A	119.7
C7—C6—H6A	120.1	C13—C18—C17	120.31 (19)
C5—C6—H6A	120.1	C13—C18—H18A	119.8
C6—C7—C8	120.37 (19)	C17—C18—H18A	119.8

C6—C7—H7A	119.8	C12—C19—H19D	109.5
C8—C7—H7A	119.8	C12—C19—H19A	109.5
C9—C8—C7	119.9 (2)	H19D—C19—H19A	109.5
C9—C8—H8A	120.1	C12—C19—H19B	109.5
C7—C8—H8A	120.1	H19D—C19—H19B	109.5
C8—C9—C10	120.2 (2)	H19A—C19—H19B	109.5
C11—N1—C1—C4	−75.0 (2)	C7—C8—C9—C10	0.3 (4)
C3—N1—C1—C4	96.5 (2)	C8—C9—C10—C5	0.5 (4)
C11—N1—C1—C2	163.36 (17)	C6—C5—C10—C9	−1.3 (3)
C3—N1—C1—C2	−25.2 (2)	C2—C5—C10—C9	177.6 (2)
C3—O1—C2—C5	−152.44 (17)	C3—N1—C11—O3	−169.1 (2)
C3—O1—C2—C1	−26.6 (2)	C1—N1—C11—O3	0.8 (3)
N1—C1—C2—O1	29.82 (18)	C3—N1—C11—C12	15.0 (3)
C4—C1—C2—O1	−89.5 (2)	C1—N1—C11—C12	−175.22 (18)
N1—C1—C2—C5	150.16 (16)	O3—C11—C12—C13	17.3 (3)
C4—C1—C2—C5	30.9 (3)	N1—C11—C12—C13	−166.97 (16)
C2—O1—C3—O2	−169.2 (2)	O3—C11—C12—C19	−106.0 (2)
C2—O1—C3—N1	11.1 (2)	N1—C11—C12—C19	69.7 (2)
C11—N1—C3—O2	1.1 (4)	C11—C12—C13—C18	109.8 (2)
C1—N1—C3—O2	−169.5 (2)	C19—C12—C13—C18	−129.1 (2)
C11—N1—C3—O1	−179.17 (19)	C11—C12—C13—C14	−72.0 (2)
C1—N1—C3—O1	10.2 (2)	C19—C12—C13—C14	49.1 (2)
O1—C2—C5—C6	−148.48 (18)	C18—C13—C14—C15	−0.2 (3)
C1—C2—C5—C6	94.3 (2)	C12—C13—C14—C15	−178.4 (2)
O1—C2—C5—C10	32.6 (3)	C13—C14—C15—C16	0.0 (3)
C1—C2—C5—C10	−84.6 (2)	C14—C15—C16—C17	−0.2 (3)
C10—C5—C6—C7	1.3 (3)	C15—C16—C17—C18	0.5 (4)
C2—C5—C6—C7	−177.71 (19)	C14—C13—C18—C17	0.5 (3)
C5—C6—C7—C8	−0.5 (3)	C12—C13—C18—C17	178.76 (19)
C6—C7—C8—C9	−0.3 (4)	C16—C17—C18—C13	−0.7 (3)