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

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In the title compound, $C_{23}H_{27}NO_3$, formed from enantiomerically pure (+)-(4*R*,5*S*)-4-methyl-5-phenyl-2-oxazolidinone and racemic 2-(4-isobutylphenyl)propanoyl chloride, the two carbonyl groups are oriented *anti* to each other, and the methyl group of the (4-isobutylphenyl)propionyl substituent lies close to the mean plane of the five-membered ring.

Comment

The title compound, (I), is the second in a series of structurally related compounds, introduced in our previous report (Coumbarides *et al.*, 2006). With R^1 = 4-(*i*Bu)C₆H₄, the reaction shown in that report yielded the *anti–syn* and *syn–syn* diastereomers in 34 and 32% yields, respectively. The title compound, (I), is the *syn–syn* diastereomer (Fig. 1). In the crystal structure, the conformation of the central portion of the molecule is closely comparable with that in the phenyl derivative (Coumbarides *et al.*, 2006). The conformation of the five-membered ring is similar, with atoms C1 and C2 lying respectively 0.170 (6) Å above and 0.298 (6) 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 = −179.7 (4)°. The principal difference between the conformations of (I) and the phenyl derivative lies in the orientation of the (4-isobutylphenyl)propionyl substituent with respect to the remainder of the molecule: in (I), the torsion angle N1—C11—C12—C13 = −90.2 (4)° compared with −166.97 (16)° for the comparable measurement in the phenyl derivative. Thus, the C19 methyl group lies closer to the plane of the five-membered ring in (I), in contrast with the *anti* arrangement observed for the C4 and C19 methyl groups in the phenyl derivative.

(I)
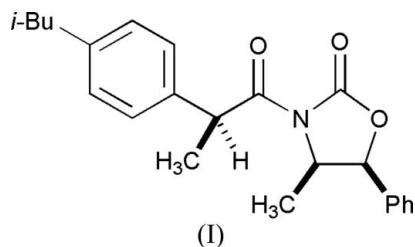
Experimental

The experimental procedure is comparable with that reported previously (Coumbarides *et al.*, 2006). The actual quantities used for preparation of (I) were: *n*-butyllithium (0.22 ml, 2.5 *M* in hexanes, 0.56 mmol) and (*R*,*S*)-oxazolidinone (0.1 g, 0.56 mmol) in 10 ml tetrahydrofuran (THF), combined with a solution of (*rac*)-2-(4-

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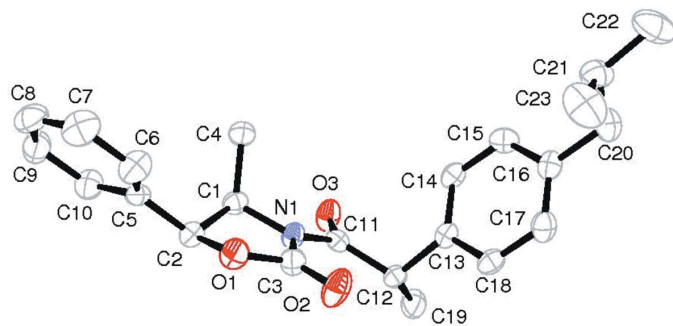
Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted.

isobutylphenyl)propanoyl chloride (0.125 g, 0.56 mmol) in 1 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 54:46). The syn–syn diastereomer was obtained as colourless crystals {67 mg, 32% yield, m.p. 394–396 K, R_F 0.55 [light petroleum (b.p 313–333 K)/diethyl ether, 1:1]}. Spectroscopic analysis: $[\alpha]_D^{25} = +98.1$ (CHCl$_3$, 293 K, concentration 1.3 g per 100 ml); IR (CHCl$_3$, ν_{max}, cm^{-1}): 1770 (C=O), 1699 (C=O); ^{1}H NMR (250 MHz; CDCl$_3$): δ 7.38–7.16 (7H, m, 7 × CH; Ar and Ph), 7.08 (2H, d, J = 8.2 Hz, 2 × CH; Ar), 5.63 (1H, d, J = 7.4 Hz, CHO), 5.05 (1H, q, J = 7.1 Hz, ArCH), 4.81 (1H, m, CHN), 2.43 (2H, d, J = 7.2 Hz, CH$_2$), 1.89–1.79 (1H, m, CH(CH$_3$)$_2$)), 1.48 (3H, d, J = 7.1 Hz, CH$_3$CHAr), 0.88 (3H, d, J = 6.7 Hz, CH$_3^a$CHCH$_3^b$), 0.87 (3H, d, J = 6.7 Hz, CH$_3^a$CHCH$_3^b$), 0.72 (3H, d, J = 6.7 Hz, CH$_3$CHN); ^{13}C NMR (100.6 MHz; CDCl$_3$): δ 174.6 (NC=O), 152.6 (OC=O), 140.5 (i-C; Ar), 137.5 (i-C; Ar), 133.6 (i-C; Ph), 129.3, 127.7 (2 × CH; Ar), 129.1, 128.7 and 125.8 (3 × CH; Ph), 78.8 (OCHPh), 54.7 (CHN), 45.1 [CH(CH$_3$)$_2$], 42.2 (ArCH), 30.1 (CH$_2$), 22.5 (CH$_3^a$CHCH$_3^b$; isobutylphenyl), 19.4 (CH$_3$CH), 14.2 (CH$_3$CHN); found: M 365.1986; C$_{23}$H$_{27}$NO$_3$ requires 365.1985.

Crystal data

C$_{23}$H$_{27}$NO$_3$
$M_r = 365.46$
Orthorhombic, $P2_12_12_1$
$a = 7.194\ (4)$ Å
$b = 14.208\ (8)$ Å
$c = 20.049\ (11)$ Å
$V = 2049\ (2)$ Å^3

$Z = 4$
$D_x = 1.185$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 160\ (2)$ K
Block, colourless
$0.63 \times 0.38 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2141 measured reflections
2079 independent reflections

1340 reflections with $I > 2\sigma(I)$
$R_{int} = 0.004$
$\theta_{max} = 25.0°$
2 standard reflections
  frequency: 60 min
  intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.101$
$S = 1.00$
2079 reflections
248 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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, 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 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* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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supporting information

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

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Crystal data

$C_{23}H_{27}NO_3$	$F(000) = 784$
$M_r = 365.46$	$D_x = 1.185$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 25 reflections
$a = 7.194$ (4) Å	$\theta = 10.0$–$12.3°$
$b = 14.208$ (8) Å	$\mu = 0.08$ mm^{-1}
$c = 20.049$ (11) Å	$T = 160$ K
$V = 2049$ (2) Å^3	Block, colourless
$Z = 4$	$0.63 \times 0.38 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.004$
	$\theta_{max} = 25.0°$, $\theta_{min} = 1.8°$
Radiation source: Enraf Nonius FR590	$h = 0 \rightarrow 8$
Graphite monochromator	$k = 0 \rightarrow 16$
$\omega/2\theta$ scans	$l = 0 \rightarrow 23$
2141 measured reflections	2 standard reflections every 60 min
2079 independent reflections	intensity decay: 1%
1340 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.101$	
$S = 1.00$	H-atom parameters constrained
2079 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2]$
248 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.18$ e Å^{-3}
	$\Delta\rho_{min} = -0.20$ 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)
0.2684 (0.0131) x + 8.7530 (0.0193) y + 15.7745 (0.0224) z = 7.3649 (0.0082)
* 0.0000 (0.0010) O1 * 0.0000 (0.0013) O2 * 0.0000 (0.0010) N1 * 0.0001 (0.0033) C3 0.1698 (0.0055) C1 - 0.2981 (0.0059) C2 - 1.3428 (0.0082) C19
Rms deviation of fitted atoms = 0.0001

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	0.2227 (5)	0.2446 (2)	0.33816 (18)	0.0277 (9)
H1	0.1236	0.2379	0.3035	0.033*
C2	0.2850 (5)	0.1467 (2)	0.36175 (18)	0.0289 (9)
H2	0.2635	0.1007	0.3248	0.035*
C3	0.5476 (6)	0.2262 (3)	0.3321 (2)	0.0339 (10)
C4	0.1573 (5)	0.3102 (3)	0.39234 (18)	0.0363 (10)
H4A	0.2470	0.3099	0.4291	0.054*
H4B	0.0358	0.2894	0.4087	0.054*
H4C	0.1465	0.3742	0.3744	0.054*
C5	0.1927 (5)	0.1101 (3)	0.42366 (18)	0.0296 (9)
C6	0.2798 (6)	0.1061 (3)	0.48455 (17)	0.0426 (11)
H6	0.4049	0.1266	0.4887	0.051*
C7	0.1862 (7)	0.0723 (3)	0.5399 (2)	0.0517 (13)
H7	0.2468	0.0705	0.5820	0.062*
C8	0.0071 (6)	0.0417 (3)	0.5342 (2)	0.0450 (12)
H8	−0.0566	0.0179	0.5721	0.054*
C9	−0.0809 (6)	0.0453 (3)	0.4732 (2)	0.0446 (11)
H9	−0.2062	0.0250	0.4692	0.053*
C10	0.0126 (6)	0.0783 (3)	0.4181 (2)	0.0373 (11)
H10	−0.0476	0.0792	0.3759	0.045*
C11	0.3942 (5)	0.3446 (2)	0.25742 (16)	0.0267 (8)
C12	0.5717 (5)	0.3735 (3)	0.22302 (17)	0.0286 (9)
H12	0.6590	0.3187	0.2229	0.034*
C13	0.6625 (5)	0.4547 (2)	0.25974 (18)	0.0260 (9)
C14	0.5624 (5)	0.5283 (3)	0.28743 (17)	0.0286 (9)
H14	0.4305	0.5263	0.2866	0.034*
C15	0.6509 (5)	0.6051 (3)	0.31640 (18)	0.0322 (9)
H15	0.5786	0.6539	0.3358	0.039*
C16	0.8434 (5)	0.6115 (3)	0.31736 (17)	0.0308 (9)
C17	0.9411 (5)	0.5378 (3)	0.28901 (19)	0.0362 (10)
H17	1.0730	0.5402	0.2888	0.043*

C18	0.8537 (5)	0.4608 (3)	0.26105 (18)	0.0329 (9)
H18	0.9262	0.4115	0.2425	0.039*
C19	0.5285 (6)	0.4009 (3)	0.15034 (17)	0.0415 (10)
H19A	0.4710	0.3473	0.1274	0.062*
H19B	0.6441	0.4181	0.1276	0.062*
H19C	0.4429	0.4545	0.1498	0.062*
C20	0.9382 (6)	0.6947 (3)	0.34867 (18)	0.0409 (11)
H20A	0.8716	0.7526	0.3352	0.049*
H20B	1.0664	0.6989	0.3310	0.049*
C21	0.9471 (6)	0.6910 (3)	0.4245 (2)	0.0435 (11)
H21	0.8188	0.6785	0.4415	0.052*
C22	1.0109 (7)	0.7844 (3)	0.4524 (2)	0.0663 (15)
H22A	1.0057	0.7825	0.5012	0.099*
H22B	0.9295	0.8346	0.4359	0.099*
H22C	1.1389	0.7967	0.4380	0.099*
C23	1.0722 (7)	0.6124 (3)	0.4485 (2)	0.0656 (15)
H23A	1.2000	0.6246	0.4340	0.098*
H23B	1.0297	0.5525	0.4297	0.098*
H23C	1.0678	0.6092	0.4973	0.098*
N1	0.3962 (4)	0.27652 (19)	0.30671 (13)	0.0269 (7)
O1	0.4839 (3)	0.15713 (18)	0.37146 (13)	0.0376 (7)
O2	0.7093 (4)	0.2401 (2)	0.32159 (15)	0.0477 (8)
O3	0.2465 (4)	0.38040 (17)	0.24285 (12)	0.0381 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0224 (19)	0.032 (2)	0.0284 (19)	0.0008 (18)	0.0002 (17)	−0.0020 (17)
C2	0.027 (2)	0.032 (2)	0.027 (2)	−0.0007 (17)	−0.0009 (18)	0.0006 (17)
C3	0.034 (3)	0.033 (2)	0.035 (2)	−0.002 (2)	0.0005 (19)	0.003 (2)
C4	0.036 (2)	0.032 (2)	0.041 (2)	0.0037 (19)	0.010 (2)	−0.0010 (18)
C5	0.036 (2)	0.026 (2)	0.027 (2)	0.0018 (19)	0.0077 (18)	−0.0020 (18)
C6	0.037 (2)	0.059 (3)	0.032 (2)	−0.005 (2)	−0.003 (2)	0.003 (2)
C7	0.056 (3)	0.067 (3)	0.032 (2)	0.007 (3)	−0.006 (2)	0.009 (2)
C8	0.051 (3)	0.050 (3)	0.033 (2)	0.008 (3)	0.010 (2)	0.007 (2)
C9	0.042 (3)	0.048 (3)	0.044 (2)	−0.007 (2)	0.004 (2)	0.003 (2)
C10	0.039 (3)	0.046 (3)	0.027 (2)	−0.005 (2)	−0.003 (2)	0.0012 (19)
C11	0.029 (2)	0.0208 (17)	0.030 (2)	0.0013 (18)	−0.0017 (19)	−0.0009 (17)
C12	0.023 (2)	0.030 (2)	0.033 (2)	0.0011 (17)	0.0050 (17)	−0.0012 (17)
C13	0.021 (2)	0.030 (2)	0.027 (2)	0.0019 (17)	−0.0012 (17)	0.0052 (19)
C14	0.021 (2)	0.036 (2)	0.029 (2)	0.0017 (19)	−0.0005 (17)	0.0073 (19)
C15	0.034 (2)	0.033 (2)	0.029 (2)	0.009 (2)	−0.0019 (19)	−0.001 (2)
C16	0.031 (2)	0.036 (2)	0.025 (2)	−0.001 (2)	−0.0042 (18)	0.007 (2)
C17	0.023 (2)	0.041 (2)	0.045 (3)	−0.003 (2)	−0.0041 (19)	0.005 (2)
C18	0.023 (2)	0.039 (2)	0.037 (2)	0.0060 (19)	0.0014 (19)	0.001 (2)
C19	0.046 (2)	0.046 (2)	0.032 (2)	−0.015 (2)	0.003 (2)	−0.002 (2)
C20	0.040 (3)	0.040 (2)	0.043 (2)	−0.006 (2)	−0.011 (2)	0.004 (2)
C21	0.036 (2)	0.056 (3)	0.038 (2)	0.001 (2)	−0.007 (2)	−0.012 (2)

C22	0.061 (3)	0.066 (3)	0.072 (3)	0.007 (3)	−0.025 (3)	−0.032 (3)
C23	0.084 (4)	0.060 (3)	0.053 (3)	−0.002 (3)	−0.032 (3)	0.005 (3)
N1	0.0198 (16)	0.0300 (17)	0.0310 (16)	0.0022 (14)	0.0008 (15)	0.0051 (14)
O1	0.0325 (17)	0.0388 (15)	0.0414 (16)	0.0045 (13)	−0.0004 (13)	0.0083 (14)
O2	0.0227 (16)	0.061 (2)	0.0593 (19)	0.0015 (14)	0.0004 (15)	0.0207 (16)
O3	0.0244 (14)	0.0374 (14)	0.0524 (17)	0.0030 (14)	−0.0007 (14)	0.0149 (14)

Geometric parameters (Å, º)

C1—N1	1.470 (4)	C12—C19	1.540 (5)
C1—C4	1.507 (5)	C12—H12	1.000
C1—C2	1.536 (5)	C13—C18	1.378 (5)
C1—H1	1.000	C13—C14	1.386 (5)
C2—O1	1.452 (4)	C14—C15	1.390 (5)
C2—C5	1.500 (5)	C14—H14	0.950
C2—H2	1.000	C15—C16	1.388 (5)
C3—O2	1.198 (4)	C15—H15	0.950
C3—O1	1.340 (4)	C16—C17	1.383 (5)
C3—N1	1.399 (5)	C16—C20	1.502 (5)
C4—H4A	0.980	C17—C18	1.380 (5)
C4—H4B	0.980	C17—H17	0.950
C4—H4C	0.980	C18—H18	0.950
C5—C6	1.373 (5)	C19—H19A	0.980
C5—C10	1.377 (5)	C19—H19B	0.980
C6—C7	1.384 (5)	C19—H19C	0.980
C6—H6	0.950	C20—C21	1.522 (5)
C7—C8	1.365 (6)	C20—H20A	0.990
C7—H7	0.950	C20—H20B	0.990
C8—C9	1.377 (5)	C21—C22	1.512 (6)
C8—H8	0.950	C21—C23	1.513 (6)
C9—C10	1.376 (5)	C21—H21	1.000
C9—H9	0.950	C22—H22A	0.980
C10—H10	0.950	C22—H22B	0.980
C11—O3	1.214 (4)	C22—H22C	0.980
C11—N1	1.383 (4)	C23—H23A	0.980
C11—C12	1.508 (5)	C23—H23B	0.980
C12—C13	1.517 (5)	C23—H23C	0.980
N1—C1—C4	112.5 (3)	C14—C13—C12	123.0 (3)
N1—C1—C2	99.5 (3)	C13—C14—C15	121.5 (3)
C4—C1—C2	115.5 (3)	C13—C14—H14	119.3
N1—C1—H1	109.7	C15—C14—H14	119.3
C4—C1—H1	109.7	C16—C15—C14	120.9 (4)
C2—C1—H1	109.7	C16—C15—H15	119.5
O1—C2—C5	111.1 (3)	C14—C15—H15	119.5
O1—C2—C1	103.6 (3)	C17—C16—C15	116.9 (4)
C5—C2—C1	116.1 (3)	C17—C16—C20	122.5 (3)
O1—C2—H2	108.6	C15—C16—C20	120.7 (4)

C5—C2—H2	108.6	C18—C17—C16	122.3 (4)
C1—C2—H2	108.6	C18—C17—H17	118.8
O2—C3—O1	123.8 (4)	C16—C17—H17	118.8
O2—C3—N1	127.4 (4)	C13—C18—C17	120.8 (4)
O1—C3—N1	108.8 (3)	C13—C18—H18	119.6
C1—C4—H4A	109.5	C17—C18—H18	119.6
C1—C4—H4B	109.5	C12—C19—H19A	109.5
H4A—C4—H4B	109.5	C12—C19—H19B	109.5
C1—C4—H4C	109.5	H19A—C19—H19B	109.5
H4A—C4—H4C	109.5	C12—C19—H19C	109.5
H4B—C4—H4C	109.5	H19A—C19—H19C	109.5
C6—C5—C10	119.2 (4)	H19B—C19—H19C	109.5
C6—C5—C2	123.2 (3)	C16—C20—C21	114.2 (3)
C10—C5—C2	117.6 (4)	C16—C20—H20A	108.7
C5—C6—C7	120.4 (4)	C21—C20—H20A	108.7
C5—C6—H6	119.8	C16—C20—H20B	108.7
C7—C6—H6	119.8	C21—C20—H20B	108.7
C8—C7—C6	120.1 (4)	H20A—C20—H20B	107.6
C8—C7—H7	119.9	C22—C21—C23	110.5 (3)
C6—C7—H7	119.9	C22—C21—C20	110.6 (4)
C7—C8—C9	119.8 (4)	C23—C21—C20	111.6 (3)
C7—C8—H8	120.1	C22—C21—H21	108.0
C9—C8—H8	120.1	C23—C21—H21	108.0
C10—C9—C8	120.1 (4)	C20—C21—H21	108.0
C10—C9—H9	120.0	C21—C22—H22A	109.5
C8—C9—H9	120.0	C21—C22—H22B	109.5
C9—C10—C5	120.4 (4)	H22A—C22—H22B	109.5
C9—C10—H10	119.8	C21—C22—H22C	109.5
C5—C10—H10	119.8	H22A—C22—H22C	109.5
O3—C11—N1	118.3 (3)	H22B—C22—H22C	109.5
O3—C11—C12	121.1 (3)	C21—C23—H23A	109.5
N1—C11—C12	120.6 (3)	C21—C23—H23B	109.5
C11—C12—C13	110.5 (3)	H23A—C23—H23B	109.5
C11—C12—C19	109.3 (3)	C21—C23—H23C	109.5
C13—C12—C19	110.7 (3)	H23A—C23—H23C	109.5
C11—C12—H12	108.7	H23B—C23—H23C	109.5
C13—C12—H12	108.7	C11—N1—C3	128.7 (3)
C19—C12—H12	108.7	C11—N1—C1	120.9 (3)
C18—C13—C14	117.6 (4)	C3—N1—C1	110.3 (3)
C18—C13—C12	119.2 (3)	C3—O1—C2	109.5 (3)
N1—C1—C2—O1	27.6 (3)	C14—C15—C16—C17	−0.7 (6)
C4—C1—C2—O1	−93.0 (4)	C14—C15—C16—C20	179.9 (3)
N1—C1—C2—C5	149.7 (3)	C15—C16—C17—C18	−0.2 (6)
C4—C1—C2—C5	29.1 (5)	C20—C16—C17—C18	179.1 (3)
O1—C2—C5—C6	12.4 (5)	C14—C13—C18—C17	0.0 (6)
C1—C2—C5—C6	−105.7 (4)	C12—C13—C18—C17	174.4 (3)
O1—C2—C5—C10	−166.9 (3)	C16—C17—C18—C13	0.6 (6)

C1—C2—C5—C10	75.0 (4)	C17—C16—C20—C21	−100.7 (4)
C10—C5—C6—C7	−1.3 (6)	C15—C16—C20—C21	78.6 (5)
C2—C5—C6—C7	179.4 (4)	C16—C20—C21—C22	−169.4 (4)
C5—C6—C7—C8	0.8 (7)	C16—C20—C21—C23	67.2 (5)
C6—C7—C8—C9	−0.6 (7)	O3—C11—N1—C3	−179.6 (3)
C7—C8—C9—C10	1.1 (6)	C12—C11—N1—C3	0.2 (5)
C8—C9—C10—C5	−1.6 (6)	O3—C11—N1—C1	3.3 (5)
C6—C5—C10—C9	1.8 (6)	C12—C11—N1—C1	−176.9 (3)
C2—C5—C10—C9	−179.0 (4)	O2—C3—N1—C11	9.7 (6)
O3—C11—C12—C13	89.6 (4)	O1—C3—N1—C11	−170.3 (3)
N1—C11—C12—C13	−90.2 (4)	O2—C3—N1—C1	−172.9 (4)
O3—C11—C12—C19	−32.5 (4)	O1—C3—N1—C1	7.1 (4)
N1—C11—C12—C19	147.7 (3)	C4—C1—N1—C11	−81.4 (4)
C11—C12—C13—C18	146.6 (4)	C2—C1—N1—C11	155.8 (3)
C19—C12—C13—C18	−92.1 (4)	C4—C1—N1—C3	101.0 (4)
C11—C12—C13—C14	−39.3 (5)	C2—C1—N1—C3	−21.8 (3)
C19—C12—C13—C14	82.0 (4)	O2—C3—O1—C2	−167.4 (4)
C18—C13—C14—C15	−0.9 (6)	N1—C3—O1—C2	12.6 (4)
C12—C13—C14—C15	−175.1 (3)	C5—C2—O1—C3	−151.4 (3)
C13—C14—C15—C16	1.3 (6)	C1—C2—O1—C3	−26.0 (4)