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(4*R*,5*R*)-4,5-Bis{2-[3-(2,6-diisopropylphenyl)-2-thioxoimidazolidin-3-yl]ethyl}-2,2-dimethyl-1,3-dioxolane

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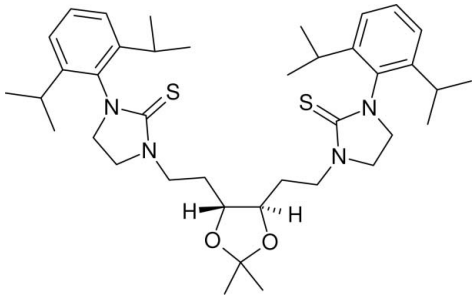
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.058; wR factor = 0.110; data-to-parameter ratio = 21.0.

In the chiral title compound, $C_{39}H_{58}N_4O_2S_2$, the complete molecule is generated by crystallographic twofold symmetry, with one C atom lying on the rotation axis. The packing is established by van der Waals forces.

Related literature

For background, see: Marshall & Harrison (2007); Williamson *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{39}H_{58}N_4O_2S_2$
M_r = 679.02
Orthorhombic, $P2_12_12$
a = 13.5581 (7) Å
b = 19.3022 (9) Å
c = 7.7028 (3) Å
V = 2015.83 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 120 (2) K
0.40 × 0.04 × 0.04 mm

Data collection

Enraf–Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.936, T_{max} = 0.995
16730 measured reflections
4595 independent reflections
2574 reflections with $I > 2\sigma(I)$
R_{int} = 0.171

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.110
S = 0.93
4595 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), with 1958 Friedel pairs
Flack parameter: −0.04 (9)

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK*, *DENZO* (Otwinowski & Minor, 1997) and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2040).

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supplementary materials

Acta Cryst. (2007). E**63**, o4503 [**doi:10.1107/S1600536807050349**]

(4*R*,5*R*)-4,5-Bis{2-[3-(2,6-diisopropylphenyl)-2-thioxoimidazolidin-3-yl]ethyl}-2,2-dimethyl-1,3-dioxolane

C. Marshall and W. T. A. Harrison

Comment

As part of our ongoing investigations of chiral, C_2-symmetric catalysts (Marshall & Harrison, 2007), the title compound, (I), $C_{39}H_{58}N_4O_2S_2$, an intermediate in such materials, has been synthesized and structurally characterized.

The complete molecule of (I) is generated by crystallographic 2-fold symmetry, with C2 lying on the rotation axis (Fig. 1). Thus, of course, both C3 and C3^{i} (i = 1=x, 1 − y, z) must show the same chiralities, where are the expected *R* configurations. The dihedral angle between the C9–C14 and C9^{i}–C14^{i} rings is 67.10 (7)°

The C—N and (nominal) C═S bonds in the 5-membered rings display typical geometrical parameters, which can be correlated with the contribution of resonance structures involving the lone pair electrons of the adjacent N atoms (Williamson *et al.*, 2006). Otherwise, the geometries of the two molecules may be regarded as normal (Allen *et al.*, 1995).

The crystal packing for (I) is established only by van der Waals forces.

Experimental

A mixture of (4*R*,5*R*)-4,5-bis[1-(2,6-diisopropylphenyl)-imidazolidinium-3-ethyl]-2,2- dimethyl-1,3-dioxolane dibromide (0.75 g, 0.963 mmol), sulfur (0.09 g, 2.89 mmol), methanol (10 *cm*3), pyridine (1.5 *cm*3) and 1,8-diazabicyclo[5.4.0]undec-7-ene (0.65 g, 4.29 mmol) was heated at 338 K for 18 h. Once cooled to room temperature the mixture was opened to water (40 ml) and extracted with chloroform (3 × 20 ml). The combined extracts were dried over magnesium sulfate, filtered and concentrated under reduced pressure to leave a brown residue. The crude product was purified by column chromatography (SiO_2, ethyl acetate:petroleum ether *v*/*v* 1:1, loaded as a dichloromethane solution) to give the title compound (0.48 g, 73%) as a colourless solid. Colourless rods and needles of (I) were recrystallized from diethyl ether/acetone (*v*/*v* 1:1). *M*.p 351 K.

Refinement

The H atoms were placed in calculated positions (C—H = 0.95–1.00 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C). The methyl groups were allowed to rotate, but not to tip, to best fit the electron density.

Figures

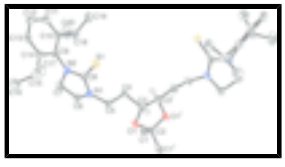


Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids. All the H atoms except H3 (represented as arbitrary spheres) are omitted for clarity. Symmetry code: (i) 1 − x, 1 − y, z.

(4*R*,5*R*)-4,5-Bis{2-[3-(2,6-diisopropylphenyl)-2- thioxoimidazolidin-3-yl]ethyl}-2,2-dimethyl-1,3-dioxolane

Crystal data

$C_{39}H_{58}N_4O_2S_2$	F_{000} = 736
M_r = 679.02	D_x = 1.119 Mg m^{-3}
Orthorhombic, $P2_12_12$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2 2ab	Cell parameters from 9370 reflections
a = 13.5581 (7) Å	θ = 2.9–27.5º
b = 19.3022 (9) Å	μ = 0.17 mm^{-1}
c = 7.7028 (3) Å	T = 120 (2) K
V = 2015.83 (16) Å^3	Rod, colourless
Z = 2	0.40 × 0.04 × 0.04 mm

Data collection

Enraf–Nonius KappaCCD diffractometer	4595 independent reflections
Radiation source: fine-focus sealed tube	2574 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.171
T = 120(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	h = −17→17
T_{min} = 0.936, T_{max} = 0.995	k = −25→22
16730 measured reflections	l = −9→9

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.058	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.110	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
S = 0.93	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
4595 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
219 parameters	Extinction coefficient: 0.0070 (11)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 1958 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.04 (9)
Hydrogen site location: inferred from neighbouring sites	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.5915 (2)	0.50945 (16)	1.2187 (4)	0.0320 (8)
H1A	0.5822	0.5486	1.2982	0.048*
H1B	0.6480	0.5187	1.1426	0.048*
H1C	0.6040	0.4672	1.2859	0.048*
C2	0.5000	0.5000	1.1103 (5)	0.0296 (11)
C3	0.4899 (2)	0.46133 (13)	0.8247 (3)	0.0253 (7)
H3	0.4184	0.4523	0.8028	0.030*
C4	0.5526 (2)	0.41930 (13)	0.7009 (4)	0.0268 (7)
H4A	0.6231	0.4258	0.7301	0.032*
H4B	0.5422	0.4362	0.5810	0.032*
C5	0.5272 (2)	0.34231 (14)	0.7100 (4)	0.0258 (7)
H5A	0.5168	0.3292	0.8329	0.031*
H5B	0.4646	0.3343	0.6472	0.031*
C6	0.6906 (2)	0.28145 (17)	0.7370 (4)	0.0350 (9)
H6A	0.6734	0.2558	0.8441	0.042*
H6B	0.7275	0.3239	0.7684	0.042*
C7	0.7496 (2)	0.23626 (18)	0.6123 (3)	0.0343 (8)
H7A	0.8207	0.2481	0.6149	0.041*
H7B	0.7413	0.1864	0.6389	0.041*
C8	0.6161 (2)	0.28675 (14)	0.4647 (4)	0.0239 (7)
C9	0.7430 (2)	0.22828 (16)	0.2855 (4)	0.0280 (7)
C10	0.80994 (19)	0.27006 (15)	0.1907 (4)	0.0274 (7)
C11	0.8526 (2)	0.24189 (17)	0.0437 (4)	0.0292 (8)
H11	0.8986	0.2686	−0.0208	0.035*
C12	0.8296 (2)	0.17542 (16)	−0.0116 (4)	0.0315 (8)
H12	0.8604	0.1567	−0.1121	0.038*
C13	0.7618 (2)	0.13650 (16)	0.0801 (4)	0.0279 (8)
H13	0.7451	0.0915	0.0397	0.033*
C14	0.7174 (2)	0.16141 (16)	0.2295 (4)	0.0279 (8)
C15	0.6440 (2)	0.11698 (17)	0.3277 (4)	0.0348 (8)
H15	0.6224	0.1438	0.4320	0.042*
C16	0.6897 (3)	0.04963 (19)	0.3921 (5)	0.0575 (11)
H16A	0.7466	0.0601	0.4662	0.086*

H16B	0.7113	0.0219	0.2926	0.086*
H16C	0.6407	0.0236	0.4590	0.086*
C17	0.5526 (2)	0.10291 (17)	0.2180 (5)	0.0484 (10)
H17A	0.5040	0.0776	0.2874	0.073*
H17B	0.5710	0.0752	0.1165	0.073*
H17C	0.5242	0.1470	0.1795	0.073*
C18	0.8353 (2)	0.34351 (17)	0.2495 (4)	0.0352 (9)
H18	0.7933	0.3548	0.3523	0.042*
C19	0.8121 (3)	0.39612 (17)	0.1065 (4)	0.0440 (10)
H19A	0.8264	0.4430	0.1487	0.066*
H19B	0.7423	0.3928	0.0749	0.066*
H19C	0.8529	0.3863	0.0044	0.066*
C20	0.9436 (2)	0.34825 (18)	0.3058 (5)	0.0543 (10)
H20A	0.9570	0.3947	0.3516	0.081*
H20B	0.9864	0.3394	0.2056	0.081*
H20C	0.9567	0.3137	0.3961	0.081*
N1	0.60327 (17)	0.29785 (12)	0.6361 (3)	0.0254 (6)
N2	0.70470 (16)	0.25442 (13)	0.4446 (3)	0.0289 (6)
O1	0.51541 (16)	0.44164 (10)	0.9980 (2)	0.0380 (6)
S1	0.53936 (5)	0.30782 (4)	0.30485 (10)	0.0304 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0428 (18)	0.0205 (18)	0.0326 (17)	−0.0024 (15)	0.0070 (17)	0.0058 (15)
C2	0.052 (3)	0.017 (3)	0.020 (2)	0.004 (2)	0.000	0.000
C3	0.0364 (16)	0.0186 (16)	0.0209 (15)	−0.0012 (14)	−0.0003 (14)	0.0030 (13)
C4	0.0330 (17)	0.0227 (17)	0.0247 (15)	−0.0001 (14)	0.0065 (16)	−0.0004 (15)
C5	0.0296 (16)	0.0216 (16)	0.0263 (15)	0.0010 (14)	0.0069 (16)	−0.0037 (14)
C6	0.0418 (19)	0.037 (2)	0.0257 (17)	0.0109 (16)	0.0008 (15)	−0.0028 (14)
C7	0.0357 (18)	0.044 (2)	0.0236 (15)	0.0088 (17)	−0.0064 (14)	−0.0027 (16)
C8	0.0283 (16)	0.0173 (18)	0.0260 (16)	0.0008 (14)	0.0041 (14)	−0.0005 (14)
C9	0.0278 (16)	0.033 (2)	0.0236 (15)	0.0123 (14)	−0.0023 (15)	−0.0033 (16)
C10	0.0271 (16)	0.0285 (19)	0.0265 (16)	0.0064 (14)	−0.0034 (16)	−0.0002 (16)
C11	0.0265 (16)	0.037 (2)	0.0243 (16)	0.0096 (16)	−0.0035 (14)	0.0014 (16)
C12	0.0340 (18)	0.038 (2)	0.0227 (17)	0.0127 (17)	−0.0051 (15)	−0.0009 (15)
C13	0.0335 (17)	0.025 (2)	0.0252 (16)	0.0037 (15)	−0.0045 (15)	−0.0022 (15)
C14	0.0255 (16)	0.032 (2)	0.0260 (18)	0.0083 (15)	−0.0011 (14)	0.0028 (15)
C15	0.0367 (18)	0.034 (2)	0.0335 (19)	0.0036 (16)	0.0034 (17)	−0.0002 (17)
C16	0.059 (2)	0.049 (3)	0.064 (3)	0.010 (2)	0.014 (2)	0.023 (2)
C17	0.042 (2)	0.048 (2)	0.056 (2)	−0.0065 (18)	0.0016 (19)	−0.006 (2)
C18	0.0380 (19)	0.035 (2)	0.033 (2)	0.0054 (16)	−0.0051 (15)	−0.0059 (16)
C19	0.055 (2)	0.029 (2)	0.047 (2)	0.0102 (18)	−0.0042 (18)	−0.0010 (18)
C20	0.055 (2)	0.041 (2)	0.067 (2)	0.0038 (19)	−0.022 (2)	−0.011 (2)
N1	0.0295 (13)	0.0227 (16)	0.0239 (13)	0.0041 (13)	−0.0001 (11)	−0.0032 (11)
N2	0.0305 (14)	0.0379 (18)	0.0185 (13)	0.0119 (13)	−0.0024 (12)	−0.0016 (12)
O1	0.0749 (16)	0.0188 (12)	0.0203 (10)	0.0094 (12)	−0.0002 (11)	−0.0002 (9)
S1	0.0317 (4)	0.0306 (5)	0.0288 (4)	0.0073 (4)	−0.0040 (4)	−0.0021 (4)

Geometric parameters (Å, °)

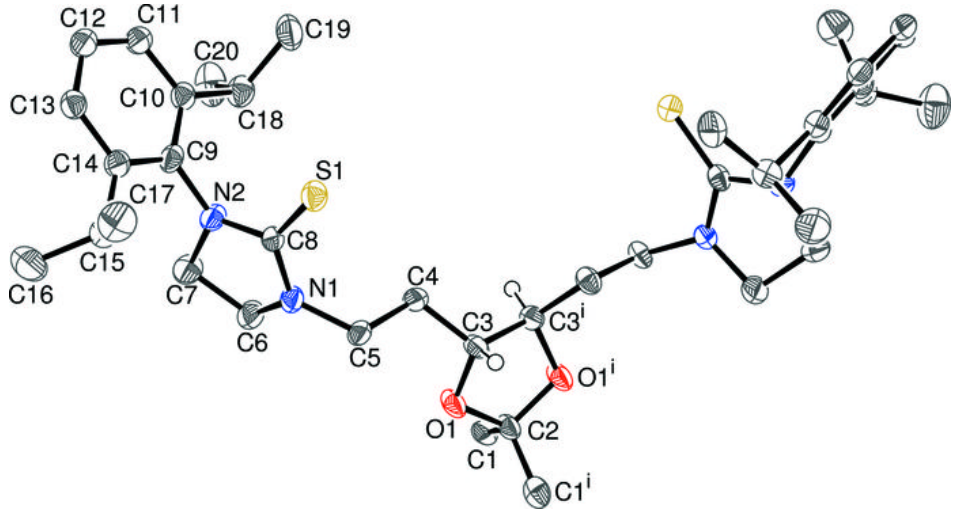
C1—C2	1.507 (3)	C9—N2	1.424 (4)
C1—H1A	0.9800	C10—C11	1.383 (4)
C1—H1B	0.9800	C10—C18	1.527 (4)
C1—H1C	0.9800	C11—C12	1.387 (4)
C2—O1	1.435 (3)	C11—H11	0.9500
C2—O1^{i}	1.435 (3)	C12—C13	1.382 (4)
C2—C1^{i}	1.507 (3)	C12—H12	0.9500
C3—O1	1.430 (3)	C13—C14	1.384 (4)
C3—C4	1.513 (4)	C13—H13	0.9500
C3—C3^{i}	1.518 (5)	C14—C15	1.515 (4)
C3—H3	1.0000	C15—C16	1.523 (4)
C4—C5	1.527 (4)	C15—C17	1.524 (4)
C4—H4A	0.9900	C15—H15	1.0000
C4—H4B	0.9900	C16—H16A	0.9800
C5—N1	1.457 (3)	C16—H16B	0.9800
C5—H5A	0.9900	C16—H16C	0.9800
C5—H5B	0.9900	C17—H17A	0.9800
C6—N1	1.451 (3)	C17—H17B	0.9800
C6—C7	1.524 (4)	C17—H17C	0.9800
C6—H6A	0.9900	C18—C19	1.531 (4)
C6—H6B	0.9900	C18—C20	1.534 (4)
C7—N2	1.470 (3)	C18—H18	1.0000
C7—H7A	0.9900	C19—H19A	0.9800
C7—H7B	0.9900	C19—H19B	0.9800
C8—N1	1.349 (3)	C19—H19C	0.9800
C8—N2	1.362 (3)	C20—H20A	0.9800
C8—S1	1.663 (3)	C20—H20B	0.9800
C9—C14	1.405 (4)	C20—H20C	0.9800
C9—C10	1.416 (4)		
C2—C1—H1A	109.5	C12—C11—H11	119.3
C2—C1—H1B	109.5	C13—C12—C11	119.7 (3)
H1A—C1—H1B	109.5	C13—C12—H12	120.2
C2—C1—H1C	109.5	C11—C12—H12	120.2
H1A—C1—H1C	109.5	C12—C13—C14	121.7 (3)
H1B—C1—H1C	109.5	C12—C13—H13	119.1
O1—C2—O1^{i}	105.9 (3)	C14—C13—H13	119.1
O1—C2—C1^{i}	111.03 (14)	C13—C14—C9	117.8 (3)
O1^{i}—C2—C1^{i}	108.00 (15)	C13—C14—C15	120.2 (3)
O1—C2—C1	108.00 (15)	C9—C14—C15	122.0 (3)
O1^{i}—C2—C1	111.03 (14)	C14—C15—C16	112.3 (3)
C1^{i}—C2—C1	112.7 (3)	C14—C15—C17	110.9 (3)
O1—C3—C4	108.1 (2)	C16—C15—C17	111.0 (3)
O1—C3—C3^{i}	102.59 (16)	C14—C15—H15	107.4
C4—C3—C3^{i}	115.2 (2)	C16—C15—H15	107.4

O1—C3—H3	110.2	C17—C15—H15	107.4
C4—C3—H3	110.2	C15—C16—H16A	109.5
$C3^{i}$—C3—H3	110.2	C15—C16—H16B	109.5
C3—C4—C5	111.5 (2)	H16A—C16—H16B	109.5
C3—C4—H4A	109.3	C15—C16—H16C	109.5
C5—C4—H4A	109.3	H16A—C16—H16C	109.5
C3—C4—H4B	109.3	H16B—C16—H16C	109.5
C5—C4—H4B	109.3	C15—C17—H17A	109.5
H4A—C4—H4B	108.0	C15—C17—H17B	109.5
N1—C5—C4	113.3 (2)	H17A—C17—H17B	109.5
N1—C5—H5A	108.9	C15—C17—H17C	109.5
C4—C5—H5A	108.9	H17A—C17—H17C	109.5
N1—C5—H5B	108.9	H17B—C17—H17C	109.5
C4—C5—H5B	108.9	C10—C18—C19	110.9 (2)
H5A—C5—H5B	107.7	C10—C18—C20	110.8 (3)
N1—C6—C7	102.5 (2)	C19—C18—C20	111.1 (3)
N1—C6—H6A	111.3	C10—C18—H18	108.0
C7—C6—H6A	111.3	C19—C18—H18	108.0
N1—C6—H6B	111.3	C20—C18—H18	108.0
C7—C6—H6B	111.3	C18—C19—H19A	109.5
H6A—C6—H6B	109.2	C18—C19—H19B	109.5
N2—C7—C6	101.5 (2)	H19A—C19—H19B	109.5
N2—C7—H7A	111.5	C18—C19—H19C	109.5
C6—C7—H7A	111.5	H19A—C19—H19C	109.5
N2—C7—H7B	111.5	H19B—C19—H19C	109.5
C6—C7—H7B	111.5	C18—C20—H20A	109.5
H7A—C7—H7B	109.3	C18—C20—H20B	109.5
N1—C8—N2	107.3 (2)	H20A—C20—H20B	109.5
N1—C8—S1	127.2 (2)	C18—C20—H20C	109.5
N2—C8—S1	125.4 (2)	H20A—C20—H20C	109.5
C14—C9—C10	121.6 (3)	H20B—C20—H20C	109.5
C14—C9—N2	120.0 (3)	C8—N1—C6	112.6 (2)
C10—C9—N2	118.4 (3)	C8—N1—C5	124.5 (2)
C11—C10—C9	117.8 (3)	C6—N1—C5	119.8 (2)
C11—C10—C18	120.9 (3)	C8—N2—C9	125.6 (2)
C9—C10—C18	121.3 (3)	C8—N2—C7	112.0 (2)
C10—C11—C12	121.4 (3)	C9—N2—C7	121.4 (2)
C10—C11—H11	119.3	C3—O1—C2	108.6 (2)
O1—C3—C4—C5	66.0 (3)	C9—C10—C18—C20	113.4 (3)
$C3^{i}$—C3—C4—C5	180.0 (2)	N2—C8—N1—C6	8.0 (3)
C3—C4—C5—N1	−162.3 (2)	S1—C8—N1—C6	−172.1 (2)
N1—C6—C7—N2	19.2 (3)	N2—C8—N1—C5	168.0 (2)
C14—C9—C10—C11	−2.4 (4)	S1—C8—N1—C5	−12.2 (4)
N2—C9—C10—C11	175.0 (2)	C7—C6—N1—C8	−17.8 (3)
C14—C9—C10—C18	178.2 (3)	C7—C6—N1—C5	−178.9 (2)
N2—C9—C10—C18	−4.4 (4)	C4—C5—N1—C8	−79.0 (3)
C9—C10—C11—C12	1.1 (4)	C4—C5—N1—C6	79.6 (3)
C18—C10—C11—C12	−179.6 (3)	N1—C8—N2—C9	174.5 (3)

C10—C11—C12—C13	0.9 (4)	S1—C8—N2—C9	−5.3 (5)
C11—C12—C13—C14	−1.7 (4)	N1—C8—N2—C7	6.1 (3)
C12—C13—C14—C9	0.4 (4)	S1—C8—N2—C7	−173.7 (2)
C12—C13—C14—C15	−179.4 (3)	C14—C9—N2—C8	−85.7 (4)
C10—C9—C14—C13	1.7 (4)	C10—C9—N2—C8	96.9 (3)
N2—C9—C14—C13	−175.7 (3)	C14—C9—N2—C7	81.7 (4)
C10—C9—C14—C15	−178.5 (3)	C10—C9—N2—C7	−95.8 (3)
N2—C9—C14—C15	4.1 (4)	C6—C7—N2—C8	−16.5 (3)
C13—C14—C15—C16	60.6 (4)	C6—C7—N2—C9	174.6 (3)
C9—C14—C15—C16	−119.2 (3)	C4—C3—O1—C2	150.36 (19)
C13—C14—C15—C17	−64.3 (4)	C3^{i}—C3—O1—C2	28.2 (3)
C9—C14—C15—C17	115.9 (3)	O1^{i}—C2—O1—C3	−11.50 (14)
C11—C10—C18—C19	57.9 (4)	C1^{i}—C2—O1—C3	105.5 (3)
C9—C10—C18—C19	−122.7 (3)	C1—C2—O1—C3	−130.5 (2)
C11—C10—C18—C20	−65.9 (4)		

Symmetry codes: (i) −*x*+1, −*y*+1, *z*.

Fig. 1


C12
C11
C19
C20
C13
C10
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C14
C9
S1
C17
N2
C8
C15
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C7
N1
C4
C6
C5
C3
C3i
O1i
O1
C2
C1
C1i