organic compounds

2-[(1R,3S)-6,7-Dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinolin-3-yl]-4-phenyl-1,3-thiazole

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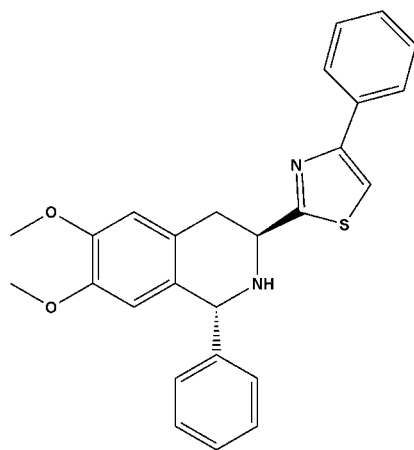Correspondence e-mail: maguireg@ukzn.ac.za

In the title compound, $C_{26}H_{24}N_2O_2S$, the dihedral angle between the thiazole ring and the adjacent phenyl ring is 3.02 (15)°. The N-containing six-membered ring of the tetrahydroisoquinoline unit adopts a half-chair conformation. The dihedral angle between the least-squares plane of the tetrahydroisoquinoline ring system and its nearest phenyl ring is 76.90 (13)°. No classical hydrogen bonds nor π–π interactions were found in the crystal structure.

Related literature

For reactions associated with TIQ ligands, see: Chakka *et al.* (2010); Naicker *et al.* (2010). For related structures, see: Naicker *et al.* (2011*a*,*b*).

Experimental

Crystal data

$C_{26}H_{24}N_2O_2S$	V = 2248.95 (18) Å^3
M_r = 428.53	Z = 4
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
a = 5.9178 (2) Å	μ = 0.17 mm^{-1}
b = 16.6269 (9) Å	T = 293 K
c = 22.8564 (11) Å	$0.32 \times 0.16 \times 0.13$ mm

Data collection

Nonius KappaCCD diffractometer	92668 measured reflections
Absorption correction: multi-scan	4948 independent reflections
(*SADABS*; Sheldrick, 1996)	3141 reflections with $I > 2\sigma(I)$
T_{min} = 0.886, T_{max} = 0.978	R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075	H atoms treated by a mixture of
$wR(F^2)$ = 0.109	independent and constrained
S = 1.21	refinement
4948 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
285 parameters	$\Delta\rho_{min}$ = −0.13 e Å^{-3}
1 restraint	Absolute structure: Flack (1983),
	2094 Friedel pairs
	Flack parameter: 0.01 (10)

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *SHELXL97*.

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supporting information

2-[(1*R*,3*S*)-6,7-Dimethoxy-1-phenyl-1,2,3,4-tetrahydroisoquinolin-3-yl]-4-phenyl-1,3-thiazole

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S1. Comment

As a part of our studies on the synthesis and application of new tetrahydroisoquinoline compounds for catalysis of asymmetric hydogenation reactions (Chakka *et al.*, 2010) and the Diels-Alder reaction (Naicker *et al.*, 2010), the title compound, a novel ligand containing a TIQ backbone with thiazole moiety, and its′ analogues are currently being tested in our laboratory for the asymmetric Henry reaction.

  The absolute stereochemistry was confirmed to be *R* and *S* at C1 and C9 positions, respectively, by two-dimensional NMR studies. From the crystal structure it is evident that the *N*-containing six-membered ring assumes a half chair conformation [Q = 0.446 (4) Å, θ = 54.0 (5)° and φ = 315.6 (6)°]. The torsion angle for C1—N1—C9—C10 is 57.9 (4)°. The maximum displacements from the C1/C2/C7–C9/N1 plane are 0.256 Å for N1 and 0.314 Å for C9 (Fig. 1). This is similar to our previously reported structures which also assume half chair conformations (Naicker *et al.*, 2011*a*, *b*). There are no hydrogen bonding interactions nor π–π interactions in the crystal structure.

S2. Experimental

A solution of Cbz protected thiazole compound (0.100 g, 0.177 mmol, 1 eq.) in dry DCM (4 ml) under argon atmosphere was treated with dipropylsulfide (0.788 ml, 5.338 mmol, 30 eq.), boron trifluoride diethyl etherate (0.230 ml, 10 eq.) and stirred at room temperature for 1.5 h, then dipropylsulfide (0.499 ml, 2.336 mmol, 20 eq.) was added, the reaction was allowed to proceed for another 2 h. The reaction was monitored by TLC using EtOAc/Hexane (20:80, R_f = 1/2). The mixture was then poured into water (5 ml) and 10% aqueous NH_4OH (10 ml) was added and extracted with ethylacetate (30 ml) followed by washing with water (2 × 10 ml). The organic layer was separated and dried over anhydrous $MgSO_4$ and the solvent evaporated under reduced pressure to afford crude thiazole, which was purified by column chromatography using silica gel (deactivated with 5% Et_3N) using 95:5 hexane/Et_3N - 10:90:5% EtOAc /hexane/Et_3N as the eluent to yield approximately 0.05 g (65%) of pure thiazole compound. *M*.p. = 388–390 K

  Crystals suitable for X-ray analysis were grown at room temperature from a solution of EtOAc/hexane.

S3. Refinement

All H atoms, except atom H1N, were placed in idealized positions (C—H = 0.93–0.97 Å) and refined using a riding model, with U_{iso}(H) set at 1.2 or 1.5 times those of their parent atoms. The H1N was refined freely [N1—H1N = 0.927 (17) Å].

Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. Hydrogen atoms have been omitted for clarity.

2-[(1*R*,3*S*)-6,7-Dimethoxy-1-phenyl-1,2,3,4- tetrahydroisoquinolin-3-yl]-4-phenyl-1,3-thiazole

Crystal data

$C_{26}H_{24}N_2O_2S$	$F(000) = 904$
$M_r = 428.53$	$D_x = 1.266$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 92668 reflections
$a = 5.9178 (2)$ Å	$\theta = 3.0–27.1°$
$b = 16.6269 (9)$ Å	$\mu = 0.17$ mm^{-1}
$c = 22.8564 (11)$ Å	$T = 293$ K
$V = 2248.95 (18)$ Å^3	Block, colourless
$Z = 4$	$0.32 \times 0.16 \times 0.13$ mm

Data collection

Nonius KappaCCD diffractometer	1.2° φ scans and ω scans
Radiation source: fine-focus sealed tube	Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
Graphite monochromator	$T_{min} = 0.886$, $T_{max} = 0.978$

92668 measured reflections
4948 independent reflections
3141 reflections with $I > 2\sigma(I)$
$R_{int} = 0.093$

$\theta_{max} = 27.1°$, $\theta_{min} = 3.0°$
$h = -7 \rightarrow 7$
$k = -21 \rightarrow 21$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.075$
$wR(F^2) = 0.109$
$S = 1.21$
4948 reflections
285 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 0.4897P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.0072 (9)
Absolute structure: Flack (1983), 2094 Friedel pairs
Absolute structure parameter: 0.01 (10)

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 $F^2 > \sigma(F^2)$ 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}
S1	0.31297 (13)	0.27081 (5)	0.16545 (4)	0.0756 (3)
O1	1.3723 (4)	0.11255 (15)	0.43058 (11)	0.0981 (8)
O2	1.4727 (4)	0.02633 (14)	0.34014 (11)	0.0864 (7)
N1	0.5823 (4)	0.23535 (15)	0.27440 (10)	0.0623 (6)
H1N	0.490 (4)	0.1910 (13)	0.2803 (11)	0.069 (9)*
N2	0.6162 (4)	0.18000 (14)	0.12153 (10)	0.0564 (6)
C1	0.7220 (5)	0.23931 (17)	0.32849 (12)	0.0620 (7)
H1	0.6242	0.2210	0.3604	0.074*
C2	0.9256 (5)	0.18372 (17)	0.32871 (13)	0.0595 (7)
C3	1.0545 (6)	0.17525 (19)	0.37999 (13)	0.0708 (9)
H3	1.0166	0.2054	0.4129	0.085*
C4	1.2354 (6)	0.1235 (2)	0.38266 (14)	0.0717 (9)
C5	1.2916 (5)	0.07670 (17)	0.33380 (15)	0.0663 (8)
C6	1.1660 (5)	0.08514 (16)	0.28383 (14)	0.0643 (8)
H6	1.2022	0.0542	0.2512	0.077*
C7	0.9852 (5)	0.13892 (16)	0.28054 (12)	0.0590 (7)
C8	0.8571 (5)	0.14618 (16)	0.22391 (13)	0.0651 (8)

H8A	0.7586	0.1000	0.2195	0.078*
H8B	0.9632	0.1461	0.1916	0.078*
C9	0.7172 (4)	0.22227 (16)	0.22165 (11)	0.0552 (7)
H9	0.8209	0.2679	0.2175	0.066*
C10	0.5672 (4)	0.22039 (16)	0.16855 (12)	0.0542 (7)
C11	0.2745 (5)	0.23434 (18)	0.09645 (12)	0.0668 (8)
H11	0.1493	0.2455	0.0732	0.080*
C12	0.4483 (5)	0.18743 (16)	0.07989 (12)	0.0543 (7)
C13	0.4750 (5)	0.14401 (16)	0.02377 (12)	0.0556 (7)
C14	0.6676 (6)	0.09961 (18)	0.01269 (14)	0.0673 (8)
H14	0.7819	0.0980	0.0406	0.081*
C15	0.6937 (7)	0.0574 (2)	−0.03919 (15)	0.0804 (10)
H15	0.8243	0.0277	−0.0460	0.096*
C16	0.5244 (8)	0.0598 (2)	−0.08076 (16)	0.0882 (11)
H16	0.5400	0.0315	−0.1156	0.106*
C17	0.3339 (7)	0.1041 (2)	−0.07042 (17)	0.0935 (11)
H17	0.2209	0.1064	−0.0987	0.112*
C18	0.3074 (6)	0.1455 (2)	−0.01871 (14)	0.0746 (9)
H18	0.1758	0.1748	−0.0122	0.089*
C19	0.7776 (5)	0.32691 (17)	0.34164 (12)	0.0592 (7)
C20	0.6135 (6)	0.3740 (2)	0.36789 (14)	0.0801 (10)
H20	0.4733	0.3518	0.3767	0.096*
C21	0.6556 (7)	0.4538 (2)	0.38112 (16)	0.0941 (12)
H21	0.5430	0.4849	0.3983	0.113*
C22	0.8609 (7)	0.4872 (2)	0.36917 (15)	0.0852 (11)
H22	0.8902	0.5405	0.3791	0.102*
C23	1.0220 (6)	0.44213 (19)	0.34258 (16)	0.0833 (10)
H23	1.1607	0.4652	0.3333	0.100*
C24	0.9825 (5)	0.36207 (18)	0.32905 (13)	0.0707 (8)
H24	1.0956	0.3318	0.3113	0.085*
C25	1.3075 (9)	0.1475 (3)	0.48294 (17)	0.153 (2)
H25A	1.4160	0.1346	0.5127	0.230*
H25B	1.1618	0.1274	0.4942	0.230*
H25C	1.2998	0.2048	0.4782	0.230*
C26	1.5162 (7)	−0.0274 (2)	0.29331 (17)	0.1042 (12)
H26A	1.6461	−0.0596	0.3024	0.156*
H26B	1.5445	0.0028	0.2582	0.156*
H26C	1.3876	−0.0616	0.2875	0.156*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0669 (5)	0.0765 (5)	0.0833 (6)	0.0138 (4)	−0.0023 (5)	−0.0113 (5)
O1	0.108 (2)	0.1159 (19)	0.0704 (16)	−0.0031 (16)	−0.0193 (15)	0.0182 (14)
O2	0.0864 (16)	0.0804 (15)	0.0922 (17)	0.0051 (14)	−0.0139 (14)	0.0272 (14)
N1	0.0589 (14)	0.0688 (16)	0.0591 (15)	−0.0141 (13)	0.0045 (13)	−0.0059 (13)
N2	0.0537 (14)	0.0571 (14)	0.0586 (15)	−0.0013 (12)	−0.0042 (12)	0.0025 (12)
C1	0.0660 (17)	0.0680 (18)	0.0521 (17)	−0.0134 (16)	0.0078 (15)	0.0001 (15)

C2	0.0680 (18)	0.0550 (16)	0.0553 (19)	−0.0132 (15)	−0.0013 (16)	0.0076 (15)
C3	0.088 (2)	0.067 (2)	0.0572 (19)	−0.015 (2)	−0.0008 (19)	0.0066 (16)
C4	0.083 (2)	0.075 (2)	0.058 (2)	−0.0156 (19)	−0.0130 (18)	0.0236 (18)
C5	0.072 (2)	0.0569 (18)	0.070 (2)	−0.0090 (17)	−0.004 (2)	0.0211 (17)
C6	0.073 (2)	0.0554 (17)	0.065 (2)	−0.0027 (17)	−0.0031 (18)	0.0074 (15)
C7	0.0682 (19)	0.0512 (16)	0.0577 (18)	−0.0083 (16)	−0.0037 (16)	0.0059 (15)
C8	0.073 (2)	0.0579 (17)	0.0642 (18)	0.0008 (16)	−0.0060 (16)	−0.0030 (15)
C9	0.0561 (16)	0.0525 (16)	0.0569 (17)	−0.0083 (14)	0.0004 (14)	0.0011 (14)
C10	0.0524 (15)	0.0470 (15)	0.0632 (18)	−0.0039 (13)	0.0024 (15)	0.0046 (16)
C11	0.0632 (19)	0.0667 (18)	0.071 (2)	0.0064 (17)	−0.0118 (16)	0.0021 (16)
C12	0.0542 (17)	0.0480 (16)	0.0608 (19)	−0.0026 (14)	−0.0030 (15)	0.0087 (14)
C13	0.0574 (18)	0.0494 (16)	0.0601 (18)	−0.0087 (15)	−0.0013 (15)	0.0080 (14)
C14	0.070 (2)	0.0705 (19)	0.062 (2)	−0.0012 (18)	0.0015 (17)	−0.0013 (16)
C15	0.085 (2)	0.071 (2)	0.085 (3)	−0.004 (2)	0.011 (2)	−0.0061 (19)
C16	0.100 (3)	0.089 (3)	0.076 (3)	−0.035 (2)	0.007 (2)	−0.019 (2)
C17	0.091 (3)	0.113 (3)	0.077 (3)	−0.029 (3)	−0.017 (2)	−0.011 (2)
C18	0.0670 (19)	0.084 (2)	0.073 (2)	−0.0108 (19)	−0.0110 (19)	0.0016 (18)
C19	0.0670 (19)	0.0643 (18)	0.0465 (16)	−0.0024 (16)	−0.0002 (15)	−0.0030 (14)
C20	0.070 (2)	0.091 (3)	0.079 (2)	−0.002 (2)	0.0061 (17)	−0.017 (2)
C21	0.102 (3)	0.085 (3)	0.095 (3)	0.016 (2)	0.004 (2)	−0.029 (2)
C22	0.108 (3)	0.063 (2)	0.084 (3)	−0.002 (2)	−0.015 (2)	−0.0087 (18)
C23	0.082 (2)	0.065 (2)	0.103 (3)	−0.0104 (19)	−0.002 (2)	0.008 (2)
C24	0.069 (2)	0.0606 (19)	0.082 (2)	−0.0033 (17)	0.0095 (18)	0.0037 (17)
C25	0.166 (4)	0.223 (6)	0.071 (3)	0.033 (5)	−0.032 (3)	−0.015 (3)
C26	0.108 (3)	0.080 (2)	0.125 (3)	0.022 (2)	−0.005 (3)	0.017 (2)

Geometric parameters (Å, º)

S1—C11	1.705 (3)	C12—C13	1.480 (4)
S1—C10	1.724 (3)	C13—C14	1.381 (4)
O1—C4	1.374 (4)	C13—C18	1.388 (4)
O1—C25	1.385 (4)	C14—C15	1.386 (4)
O2—C5	1.368 (4)	C14—H14	0.9300
O2—C26	1.417 (4)	C15—C16	1.381 (5)
N1—C9	1.462 (3)	C15—H15	0.9300
N1—C1	1.489 (3)	C16—C17	1.368 (5)
N1—H1N	0.927 (17)	C16—H16	0.9300
N2—C10	1.300 (3)	C17—C18	1.376 (5)
N2—C12	1.381 (3)	C17—H17	0.9300
C1—C2	1.519 (4)	C18—H18	0.9300
C1—C19	1.523 (4)	C19—C24	1.377 (4)
C1—H1	0.9800	C19—C20	1.385 (4)
C2—C7	1.375 (4)	C20—C21	1.382 (5)
C2—C3	1.406 (4)	C20—H20	0.9300
C3—C4	1.376 (4)	C21—C22	1.364 (5)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.401 (4)	C22—C23	1.357 (5)
C5—C6	1.370 (4)	C22—H22	0.9300

C6—C7	1.397 (4)	C23—C24	1.386 (4)
C6—H6	0.9300	C23—H23	0.9300
C7—C8	1.505 (4)	C24—H24	0.9300
C8—C9	1.513 (4)	C25—H25A	0.9600
C8—H8A	0.9700	C25—H25B	0.9600
C8—H8B	0.9700	C25—H25C	0.9600
C9—C10	1.504 (4)	C26—H26A	0.9600
C9—H9	0.9800	C26—H26B	0.9600
C11—C12	1.345 (4)	C26—H26C	0.9600
C11—H11	0.9300		
C11—S1—C10	88.95 (14)	C11—C12—C13	127.4 (3)
C4—O1—C25	118.1 (3)	N2—C12—C13	118.5 (2)
C5—O2—C26	116.6 (3)	C14—C13—C18	118.1 (3)
C9—N1—C1	112.8 (2)	C14—C13—C12	120.5 (3)
C9—N1—H1N	108.9 (17)	C18—C13—C12	121.4 (3)
C1—N1—H1N	103.9 (17)	C13—C14—C15	121.3 (3)
C10—N2—C12	111.3 (2)	C13—C14—H14	119.4
N1—C1—C2	114.6 (2)	C15—C14—H14	119.4
N1—C1—C19	109.0 (2)	C16—C15—C14	119.5 (4)
C2—C1—C19	114.2 (2)	C16—C15—H15	120.2
N1—C1—H1	106.1	C14—C15—H15	120.2
C2—C1—H1	106.1	C17—C16—C15	119.7 (3)
C19—C1—H1	106.1	C17—C16—H16	120.2
C7—C2—C3	118.3 (3)	C15—C16—H16	120.2
C7—C2—C1	122.0 (3)	C16—C17—C18	120.8 (4)
C3—C2—C1	119.6 (3)	C16—C17—H17	119.6
C4—C3—C2	121.5 (3)	C18—C17—H17	119.6
C4—C3—H3	119.3	C17—C18—C13	120.7 (3)
C2—C3—H3	119.3	C17—C18—H18	119.7
O1—C4—C3	125.2 (3)	C13—C18—H18	119.7
O1—C4—C5	115.0 (3)	C24—C19—C20	117.9 (3)
C3—C4—C5	119.8 (3)	C24—C19—C1	123.7 (3)
O2—C5—C6	125.2 (3)	C20—C19—C1	118.4 (3)
O2—C5—C4	116.2 (3)	C21—C20—C19	120.7 (3)
C6—C5—C4	118.6 (3)	C21—C20—H20	119.6
C5—C6—C7	121.7 (3)	C19—C20—H20	119.6
C5—C6—H6	119.1	C22—C21—C20	120.5 (4)
C7—C6—H6	119.1	C22—C21—H21	119.7
C2—C7—C6	120.0 (3)	C20—C21—H21	119.7
C2—C7—C8	121.1 (3)	C23—C22—C21	119.3 (3)
C6—C7—C8	118.9 (3)	C23—C22—H22	120.3
C7—C8—C9	111.8 (2)	C21—C22—H22	120.3
C7—C8—H8A	109.2	C22—C23—C24	120.8 (3)
C9—C8—H8A	109.2	C22—C23—H23	119.6
C7—C8—H8B	109.2	C24—C23—H23	119.6
C9—C8—H8B	109.2	C19—C24—C23	120.6 (3)
H8A—C8—H8B	107.9	C19—C24—H24	119.7

N1—C9—C10	110.3 (2)	C23—C24—H24	119.7
N1—C9—C8	113.3 (2)	O1—C25—H25A	109.5
C10—C9—C8	109.5 (2)	O1—C25—H25B	109.5
N1—C9—H9	107.9	H25A—C25—H25B	109.5
C10—C9—H9	107.9	O1—C25—H25C	109.5
C8—C9—H9	107.9	H25A—C25—H25C	109.5
N2—C10—C9	123.1 (2)	H25B—C25—H25C	109.5
N2—C10—S1	114.3 (2)	O2—C26—H26A	109.5
C9—C10—S1	122.6 (2)	O2—C26—H26B	109.5
C12—C11—S1	111.4 (2)	H26A—C26—H26B	109.5
C12—C11—H11	124.3	O2—C26—H26C	109.5
S1—C11—H11	124.3	H26A—C26—H26C	109.5
C11—C12—N2	114.1 (2)	H26B—C26—H26C	109.5
C9—N1—C1—C2	−35.5 (3)	C8—C9—C10—N2	−26.3 (3)
C9—N1—C1—C19	94.0 (3)	N1—C9—C10—S1	27.5 (3)
N1—C1—C2—C7	5.4 (3)	C8—C9—C10—S1	152.8 (2)
C19—C1—C2—C7	−121.4 (3)	C11—S1—C10—N2	0.0 (2)
N1—C1—C2—C3	−172.5 (2)	C11—S1—C10—C9	−179.2 (2)
C19—C1—C2—C3	60.6 (3)	C10—S1—C11—C12	0.3 (2)
C7—C2—C3—C4	−0.3 (4)	S1—C11—C12—N2	−0.4 (3)
C1—C2—C3—C4	177.7 (2)	S1—C11—C12—C13	178.9 (2)
C25—O1—C4—C3	9.3 (5)	C10—N2—C12—C11	0.4 (3)
C25—O1—C4—C5	−170.6 (4)	C10—N2—C12—C13	−179.0 (2)
C2—C3—C4—O1	178.9 (3)	C11—C12—C13—C14	178.3 (3)
C2—C3—C4—C5	−1.2 (4)	N2—C12—C13—C14	−2.4 (4)
C26—O2—C5—C6	−7.4 (4)	C11—C12—C13—C18	−2.7 (4)
C26—O2—C5—C4	173.5 (3)	N2—C12—C13—C18	176.6 (3)
O1—C4—C5—O2	0.4 (4)	C18—C13—C14—C15	−0.2 (4)
C3—C4—C5—O2	−179.6 (2)	C12—C13—C14—C15	178.9 (3)
O1—C4—C5—C6	−178.8 (2)	C13—C14—C15—C16	0.1 (5)
C3—C4—C5—C6	1.3 (4)	C14—C15—C16—C17	0.4 (5)
O2—C5—C6—C7	−179.0 (2)	C15—C16—C17—C18	−0.9 (6)
C4—C5—C6—C7	0.1 (4)	C16—C17—C18—C13	0.9 (5)
C3—C2—C7—C6	1.7 (4)	C14—C13—C18—C17	−0.3 (5)
C1—C2—C7—C6	−176.3 (2)	C12—C13—C18—C17	−179.3 (3)
C3—C2—C7—C8	−178.9 (2)	N1—C1—C19—C24	−101.3 (3)
C1—C2—C7—C8	3.2 (4)	C2—C1—C19—C24	28.4 (4)
C5—C6—C7—C2	−1.6 (4)	N1—C1—C19—C20	78.9 (3)
C5—C6—C7—C8	178.9 (3)	C2—C1—C19—C20	−151.4 (3)
C2—C7—C8—C9	17.6 (4)	C24—C19—C20—C21	−0.2 (5)
C6—C7—C8—C9	−162.9 (2)	C1—C19—C20—C21	179.6 (3)
C1—N1—C9—C10	−179.0 (2)	C19—C20—C21—C22	−0.8 (5)
C1—N1—C9—C8	58.0 (3)	C20—C21—C22—C23	1.9 (6)
C7—C8—C9—N1	−48.1 (3)	C21—C22—C23—C24	−1.9 (5)
C7—C8—C9—C10	−171.6 (2)	C20—C19—C24—C23	0.2 (4)
C12—N2—C10—C9	178.9 (2)	C1—C19—C24—C23	−179.6 (3)
C12—N2—C10—S1	−0.2 (3)	C22—C23—C24—C19	0.9 (5)

N1—C9—C10—N2   −151.6 (2)