Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(−)-(1*S*,4*S*,6*R*,8*R*)-[11,11-Dimethyl-5-(4-tolylsulfonyl)-3-oxa-5-azatricyclo-[6.2.1.0^{1,6}]undec-4-yl](phenyl)-methanone

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Received 27 October 2007; accepted 7 November 2007

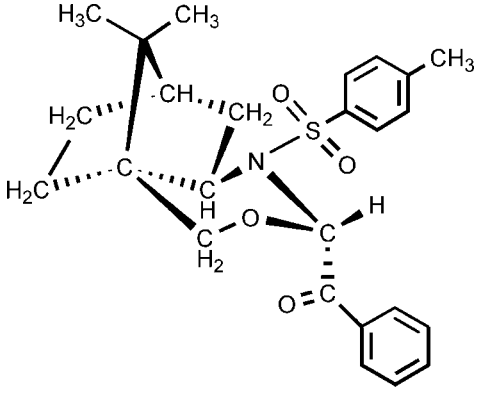
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.091; data-to-parameter ratio = 18.6.

The absolute configuration of the title compound, $C_{25}H_{29}NO_4S$, has been determined unambiguously. The benzoyl group lies in an axial position and the oxazine ring adopts a chair conformation. One of the interesting features of this structure is that the carbonyl group is nearly perpendicular to the α-C—O bond.

Related literature

A similar *N*-tosyl-1,3-oxazine ring derived from pulegone has been reported to possess a boat conformation (Rochon & Breau, 1999).

For related literature, see: Juaristi *et al.* (1986); Ko & Park (1997).



Experimental

Crystal data

$C_{25}H_{29}NO_4S$
M_r = 439.55
Orthorhombic, $P2_12_12_1$
a = 6.60966 (14) Å
b = 17.0902 (4) Å
c = 20.1206 (5) Å
V = 2272.83 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.17 mm^{-1}
T = 295 (2) K
0.48 × 0.29 × 0.27 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: numerical (*NUMABS*; Higashi, 2000)
T_{min} = 0.92, T_{max} = 0.95
22149 measured reflections
5215 independent reflections
4683 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.07
5215 reflections
281 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), 2231 Friedel pairs
Flack parameter: −0.02 (5)

Data collection: *RAPID-AUTO* (Rigaku, 2005); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: locally modified version of *ORTEP* (Johnson, 1965); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This research was supported by the Korean Research Foundation (grant No. KRF-2006-521-C00088). The authors are grateful to Ajou University for use of the X-ray facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2042).

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  doi:10.1107/S1600536807056917

supplementary materials

Acta Cryst. (2007). E**63**, o4712 [**doi:10.1107/S1600536807056917**]

(-)-(1*S*,4*S*,6*R*,8*R*)-[11,11-Dimethyl-5-(4-tolylsulfonyl)-3-oxa-5-azatricyclo[6.2.1.0^{1,6}]undec-4-yl](phenyl)methanone

K.-Y. Ko and H. Yun

Comment

As part of a project on the diastereoselective reaction employing 2-acyl-1,3-oxazines, we prepared (1*R*)-(+)-camphor-based 2-benzoyl-1,3-oxazines as a 4.0:1 mixture from the condensation of *N*-(toluene-4-sulfonyl)amino alcohol and phenylglyoxal. Based on our previous experience, we anticipated that equatorial conformer would be the major product (Ko & Park, 1997). However, ^{1}H-NMR spectrum of the mixture suggested the formation of axial conformer, *viz.* the title compound as the major product; H4 of the major product resonated at lower field, implying the equatorial position of H4. To confirm the axial nature of the benzoyl group, the crystal structure determination of the title compound was performed.

As shown in Fig. 1, the title compound clearly has the benzoyl group in an axial position. According to a low-temperature study on conformational equilibria of 2-benzoyl-1,3-dithianes (Juaristi *et al.*, 1986), axial conformer is more stable than equatorial one by 4.85 kJ/mol due to the so called anomeric effect. In the present case of 1,3-oxazine ring, the axial conformer seems to be more stable by 3.4 kJ/mol.

In contrast to the boat conformation of the similar *N*-tosyl-1,3-oxazine ring (Rochon & Breau, 1999), the oxazine ring has a chair conformation with torsion angles: C4—O3—C2—C1 = −59.2 (2)° and C4—N5—C6—C1 = 39.6 (2)°. The environment around atom N5 is pseudopyramidal wherein atom N5 is located 0.281 (1) Å from the plane composed of atoms S22, C4, and C6.

The orientation of carbonyl group relative to three α-groups is quite interesting. Carbonyl group, situated inside the oxazine ring has 92.0 (2)° of dihedral angle [O3—C4—C14—O21], meaning that the carbonyl group is nearly perpendicular to α-C—O bond. The relative orientation of C=O group is important in the context of stereoselection that carbonyl group reveals during nucleophilic additions.

Experimental

The title compound was prepared from the reaction of (2-*N*-tosylamino-7,7-dimethyl-bicyclo[2.2.1]hept-1-yl)-methanol with phenylglyoxal in the presence of catalytic amount of *p*-toluenesulfonic acid at 355 K in benzene. The crude product (90%) consisting of axial and equatorial isomer in a ratio of 4:1 was recrystallized from ethanol to give colorless crystals of pure axial isomer (60%), mp 454–455 K. $[\alpha]_D^{20}$ −65.1 (c = 0.98, $CHCl_3$). Analysis found: C 68.16, H 6.68, N 3.16, S 6.91%; calculated for $C_{25}H_{29}NO_4S$: C 68.23, H 6.66, N 3.19, S 7.29%.

Refinement

The H atoms were introduced at calculated positions (tertiary C—H, 0.98 Å; secondary CH_2, 0.97 Å; –CH_3, 0.96 Å; aromatic C—H, 0.93 Å) and treated as riding. Their displacement parameters were fixed to be equivalent to 1.2U_{eq} (tertiary C—H,

secondary CH_2, aromatic C—H) or $1.5U_{eq}$ ($-CH_3$) of the parent C atoms. The Flack paratemeter (x=1.00 (6)) for the inverted enantiomeric form indicated that the current absolute structure is correct. The highest residual electron density (0.16 e/Å^3) is 0.81 Å from the C23 site. The deepest hole (−0.22 e/Å^3) is 0.68 Å from the S22 site.

Figures

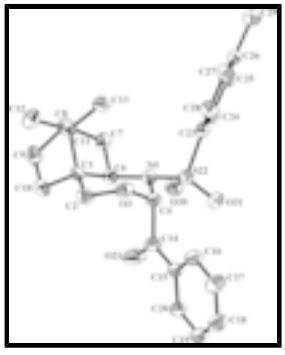


Fig. 1. Molecular structure of the title compound; displacement ellipsoides are drawn at the 30% probability level and H atoms are omitted for clarity.

(-)-(1*S*,4*S*,6*R*,8*R*)-[11,11-Dimethyl-5-(4-\ tolylsulfonyl)-3-oxa-5-azatricyclo[6.2.1.0^{1,6}]undec-4-yl](phenyl)methanone

Crystal data

$C_{25}H_{29}NO_4S$	F_{000} = 936
M_r = 439.55	D_x = 1.285 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 19715 reflections
a = 6.60966 (14) Å	θ = 3.0–27.5º
b = 17.0902 (4) Å	μ = 0.17 mm^{-1}
c = 20.1206 (5) Å	T = 295 (2) K
V = 2272.83 (9) Å^3	Block, colourless
Z = 4	0.48 × 0.29 × 0.27 mm

Data collection

Rigaku R-axis RAPID diffractometer	4683 reflections with $I > 2\sigma(I)$
T = 295(2) K	R_{int} = 0.019
ω scans	θ_{max} = 27.5º
Absorption correction: numerical (NUMABS; Higashi, 2000)	θ_{min} = 3.1º
T_{min} = 0.92, T_{max} = 0.95	h = −8→8
22149 measured reflections	k = −22→22
5215 independent reflections	l = −26→26

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.1501P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	$(\Delta/\sigma)_{max} = 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.032$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$wR(F^2) = 0.091$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
$S = 1.07$	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
5215 reflections	Extinction coefficient: 0.0102 (12)
281 parameters	Absolute structure: Flack (1983), 2231 Friedel pairs
H-atom parameters constrained	Flack parameter: −0.02 (5)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3134 (2)	0.13409 (7)	0.58801 (7)	0.0450 (3)
C2	0.1345 (3)	0.16292 (9)	0.54875 (8)	0.0560 (4)
H2A	0.0518	0.1962	0.5768	0.067*
H2B	0.1820	0.1941	0.5116	0.067*
O3	0.01302 (16)	0.09940 (7)	0.52405 (5)	0.0558 (3)
C4	0.1182 (2)	0.04754 (9)	0.48239 (7)	0.0504 (3)
H4	0.0258	0.0050	0.4703	0.061*
N5	0.29237 (18)	0.01282 (7)	0.51794 (6)	0.0479 (3)
C6	0.4313 (2)	0.06731 (8)	0.55322 (7)	0.0450 (3)
H6	0.5270	0.0898	0.5213	0.054*
C7	0.5506 (2)	0.02914 (9)	0.61142 (7)	0.0527 (3)
H7A	0.5003	−0.0230	0.6210	0.063*
H7B	0.6939	0.0262	0.6014	0.063*
C8	0.5103 (2)	0.08473 (9)	0.66919 (7)	0.0516 (3)
H8	0.5457	0.0634	0.7129	0.062*
C9	0.6132 (3)	0.16320 (10)	0.65297 (10)	0.0651 (4)
H9A	0.7499	0.1552	0.6367	0.078*
H9B	0.6176	0.1969	0.6917	0.078*
C10	0.4763 (3)	0.19802 (9)	0.59837 (9)	0.0605 (4)
H10A	0.5519	0.2072	0.5578	0.073*
H10B	0.4157	0.2468	0.6129	0.073*
C11	0.2829 (2)	0.10415 (9)	0.66079 (7)	0.0486 (3)
C12	0.2079 (3)	0.16776 (12)	0.70935 (9)	0.0714 (5)
H12A	0.2919	0.2133	0.7054	0.107*

H12B	0.2145	0.1482	0.7540	0.107*
H12C	0.0706	0.1813	0.6988	0.107*
C13	0.1443 (3)	0.03318 (10)	0.66924 (8)	0.0582 (4)
H13A	0.1869	−0.0078	0.6397	0.087*
H13B	0.0076	0.0478	0.6590	0.087*
H13C	0.1514	0.0149	0.7143	0.087*
C14	0.1826 (2)	0.09002 (9)	0.41743 (7)	0.0545 (4)
C15	0.0379 (3)	0.09349 (8)	0.36117 (7)	0.0489 (3)
C16	−0.1601 (3)	0.06745 (11)	0.36551 (8)	0.0592 (4)
H16	−0.2083	0.0472	0.4054	0.071*
C17	−0.2870 (3)	0.07141 (13)	0.31061 (9)	0.0725 (5)
H17	−0.4197	0.0538	0.3137	0.087*
C18	−0.2153 (4)	0.10165 (12)	0.25144 (9)	0.0755 (6)
H18	−0.3003	0.1042	0.2147	0.091*
C19	−0.0204 (4)	0.12783 (11)	0.24656 (8)	0.0701 (5)
H19	0.0263	0.1483	0.2066	0.084*
C20	0.1077 (3)	0.12409 (9)	0.30086 (7)	0.0581 (4)
H20	0.2402	0.1419	0.2973	0.070*
O21	0.3472 (2)	0.12121 (10)	0.41429 (7)	0.0874 (5)
S22	0.39491 (7)	−0.06417 (2)	0.482955 (18)	0.05435 (11)
C23	0.3513 (2)	−0.14272 (8)	0.53849 (7)	0.0521 (3)
C24	0.5074 (3)	−0.19357 (10)	0.55215 (8)	0.0642 (4)
H24	0.6358	−0.1845	0.5349	0.077*
C25	0.4719 (3)	−0.25846 (10)	0.59190 (9)	0.0695 (5)
H25	0.5774	−0.2929	0.6009	0.083*
C26	0.2833 (4)	−0.27289 (9)	0.61827 (8)	0.0643 (5)
C27	0.1281 (3)	−0.22108 (11)	0.60438 (9)	0.0673 (4)
H27	0.0001	−0.2299	0.6221	0.081*
C28	0.1608 (3)	−0.15594 (10)	0.56425 (9)	0.0627 (4)
H28	0.0553	−0.1217	0.5549	0.075*
C29	0.2471 (5)	−0.34462 (12)	0.66090 (10)	0.0911 (7)
H29A	0.3207	−0.3882	0.6429	0.137*
H29B	0.1053	−0.3566	0.6614	0.137*
H29C	0.2926	−0.3345	0.7054	0.137*
O30	0.6094 (2)	−0.05411 (7)	0.47826 (6)	0.0680 (3)
O31	0.2807 (2)	−0.07975 (7)	0.42374 (6)	0.0760 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0484 (7)	0.0391 (6)	0.0475 (7)	−0.0035 (6)	−0.0016 (6)	0.0052 (5)
C2	0.0596 (8)	0.0528 (7)	0.0557 (8)	0.0078 (7)	−0.0034 (7)	0.0089 (6)
O3	0.0467 (5)	0.0721 (6)	0.0486 (5)	0.0003 (5)	−0.0029 (5)	0.0074 (5)
C4	0.0527 (7)	0.0590 (8)	0.0397 (6)	−0.0107 (6)	−0.0062 (6)	0.0091 (6)
N5	0.0543 (6)	0.0445 (5)	0.0447 (6)	−0.0056 (5)	−0.0056 (5)	0.0019 (5)
C6	0.0463 (7)	0.0436 (6)	0.0452 (7)	−0.0051 (6)	−0.0008 (5)	0.0026 (6)
C7	0.0500 (8)	0.0510 (7)	0.0572 (8)	0.0025 (6)	−0.0089 (6)	−0.0008 (6)
C8	0.0512 (7)	0.0539 (8)	0.0496 (7)	−0.0037 (7)	−0.0111 (7)	0.0014 (6)

C9	0.0574 (8)	0.0599 (9)	0.0780 (11)	−0.0131 (8)	−0.0095 (9)	−0.0080 (8)
C10	0.0675 (9)	0.0446 (7)	0.0694 (9)	−0.0134 (7)	0.0001 (8)	0.0030 (7)
C11	0.0512 (8)	0.0508 (7)	0.0436 (7)	−0.0032 (6)	−0.0026 (6)	0.0015 (6)
C12	0.0711 (11)	0.0823 (12)	0.0608 (10)	0.0077 (10)	0.0020 (9)	−0.0163 (9)
C13	0.0557 (8)	0.0673 (9)	0.0515 (8)	−0.0116 (7)	−0.0019 (7)	0.0137 (7)
C14	0.0589 (8)	0.0602 (8)	0.0442 (7)	−0.0082 (7)	0.0003 (6)	0.0102 (6)
C15	0.0652 (9)	0.0437 (6)	0.0379 (6)	0.0062 (6)	0.0011 (6)	0.0023 (5)
C16	0.0640 (9)	0.0671 (9)	0.0464 (7)	−0.0005 (8)	−0.0025 (7)	0.0066 (7)
C17	0.0685 (11)	0.0861 (12)	0.0630 (10)	0.0053 (10)	−0.0140 (8)	0.0023 (10)
C18	0.1007 (16)	0.0759 (12)	0.0500 (9)	0.0165 (11)	−0.0219 (9)	−0.0017 (8)
C19	0.1109 (16)	0.0602 (9)	0.0391 (7)	0.0084 (11)	−0.0009 (8)	0.0056 (7)
C20	0.0801 (11)	0.0506 (8)	0.0436 (7)	0.0040 (8)	0.0074 (8)	0.0051 (6)
O21	0.0723 (8)	0.1270 (12)	0.0628 (7)	−0.0363 (8)	−0.0072 (6)	0.0344 (8)
S22	0.0704 (2)	0.04833 (17)	0.04433 (18)	−0.00821 (17)	0.00749 (17)	−0.00204 (15)
C23	0.0670 (9)	0.0429 (6)	0.0464 (7)	−0.0056 (6)	0.0046 (7)	−0.0045 (5)
C24	0.0772 (11)	0.0564 (8)	0.0590 (9)	0.0054 (9)	0.0101 (9)	−0.0068 (7)
C25	0.0982 (14)	0.0540 (8)	0.0564 (9)	0.0145 (9)	0.0005 (10)	−0.0045 (7)
C26	0.1053 (14)	0.0471 (7)	0.0405 (7)	−0.0112 (9)	−0.0074 (9)	−0.0039 (6)
C27	0.0756 (11)	0.0637 (9)	0.0627 (10)	−0.0199 (9)	0.0037 (9)	0.0042 (8)
C28	0.0663 (10)	0.0546 (8)	0.0672 (10)	−0.0070 (8)	0.0019 (8)	0.0035 (7)
C29	0.149 (2)	0.0685 (11)	0.0560 (10)	−0.0235 (13)	−0.0137 (13)	0.0144 (9)
O30	0.0715 (7)	0.0602 (6)	0.0722 (7)	−0.0050 (6)	0.0271 (6)	−0.0032 (6)
O31	0.1147 (11)	0.0689 (7)	0.0443 (6)	−0.0149 (7)	−0.0044 (6)	−0.0066 (5)

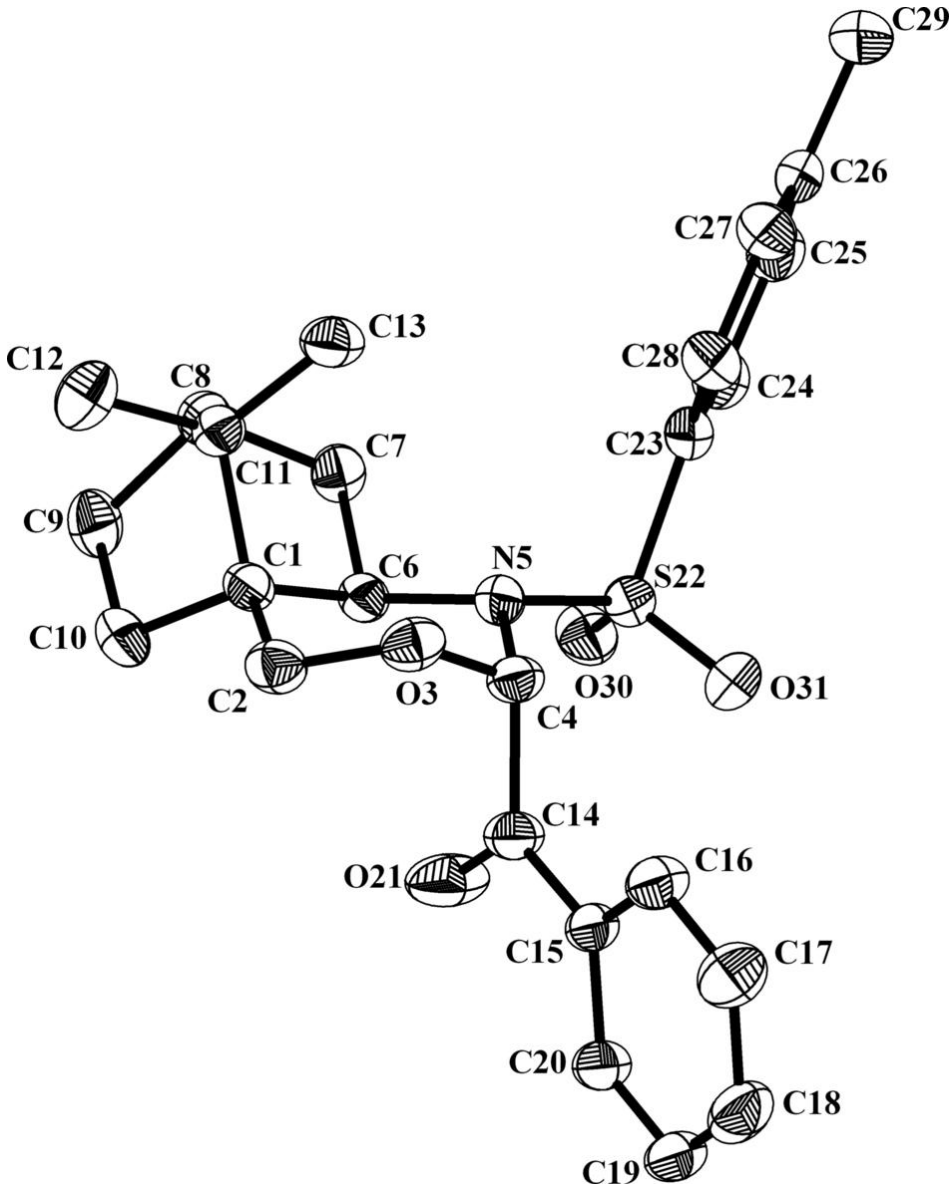
Geometric parameters (Å, °)

C1—C2	1.505 (2)	C13—H13B	0.9600
C1—C10	1.548 (2)	C13—H13C	0.9600
C1—C6	1.549 (2)	C14—O21	1.213 (2)
C1—C11	1.5641 (19)	C14—C15	1.483 (2)
C2—O3	1.439 (2)	C15—C16	1.385 (2)
C2—H2A	0.9700	C15—C20	1.400 (2)
C2—H2B	0.9700	C16—C17	1.389 (2)
O3—C4	1.4042 (19)	C16—H16	0.9300
C4—N5	1.4794 (19)	C17—C18	1.381 (3)
C4—C14	1.5545 (19)	C17—H17	0.9300
C4—H4	0.9800	C18—C19	1.367 (3)
N5—C6	1.4882 (17)	C18—H18	0.9300
N5—S22	1.6389 (13)	C19—C20	1.384 (3)
C6—C7	1.5549 (19)	C19—H19	0.9300
C6—H6	0.9800	C20—H20	0.9300
C7—C8	1.525 (2)	S22—O30	1.4310 (13)
C7—H7A	0.9700	S22—O31	1.4352 (13)
C7—H7B	0.9700	S22—C23	1.7703 (15)
C8—C9	1.539 (2)	C23—C24	1.377 (3)
C8—C11	1.549 (2)	C23—C28	1.380 (2)
C8—H8	0.9800	C24—C25	1.387 (3)
C9—C10	1.543 (3)	C24—H24	0.9300
C9—H9A	0.9700	C25—C26	1.377 (3)

C9—H9B	0.9700	C25—H25	0.9300
C10—H10A	0.9700	C26—C27	1.384 (3)
C10—H10B	0.9700	C26—C29	1.515 (2)
C11—C13	1.529 (2)	C27—C28	1.392 (2)
C11—C12	1.543 (2)	C27—H27	0.9300
C12—H12A	0.9600	C28—H28	0.9300
C12—H12B	0.9600	C29—H29A	0.9600
C12—H12C	0.9600	C29—H29B	0.9600
C13—H13A	0.9600	C29—H29C	0.9600
C2—C1—C10	112.72 (12)	C11—C12—H12C	109.5
C2—C1—C6	113.53 (12)	H12A—C12—H12C	109.5
C10—C1—C6	103.33 (12)	H12B—C12—H12C	109.5
C2—C1—C11	119.81 (13)	C11—C13—H13A	109.5
C10—C1—C11	101.22 (12)	C11—C13—H13B	109.5
C6—C1—C11	104.29 (11)	H13A—C13—H13B	109.5
O3—C2—C1	111.89 (12)	C11—C13—H13C	109.5
O3—C2—H2A	109.2	H13A—C13—H13C	109.5
C1—C2—H2A	109.2	H13B—C13—H13C	109.5
O3—C2—H2B	109.2	O21—C14—C15	121.40 (14)
C1—C2—H2B	109.2	O21—C14—C4	119.64 (14)
H2A—C2—H2B	107.9	C15—C14—C4	118.94 (13)
C4—O3—C2	113.96 (12)	C16—C15—C20	119.11 (15)
O3—C4—N5	110.48 (11)	C16—C15—C14	123.25 (13)
O3—C4—C14	110.04 (12)	C20—C15—C14	117.63 (15)
N5—C4—C14	112.39 (12)	C15—C16—C17	120.31 (16)
O3—C4—H4	107.9	C15—C16—H16	119.8
N5—C4—H4	107.9	C17—C16—H16	119.8
C14—C4—H4	107.9	C18—C17—C16	119.8 (2)
C4—N5—C6	117.38 (11)	C18—C17—H17	120.1
C4—N5—S22	115.86 (10)	C16—C17—H17	120.1
C6—N5—S22	116.87 (10)	C19—C18—C17	120.49 (18)
N5—C6—C1	111.46 (11)	C19—C18—H18	119.8
N5—C6—C7	114.18 (11)	C17—C18—H18	119.8
C1—C6—C7	102.94 (11)	C18—C19—C20	120.31 (17)
N5—C6—H6	109.3	C18—C19—H19	119.8
C1—C6—H6	109.3	C20—C19—H19	119.8
C7—C6—H6	109.3	C19—C20—C15	119.99 (18)
C8—C7—C6	102.95 (12)	C19—C20—H20	120.0
C8—C7—H7A	111.2	C15—C20—H20	120.0
C6—C7—H7A	111.2	O30—S22—O31	119.23 (9)
C8—C7—H7B	111.2	O30—S22—N5	109.97 (7)
C6—C7—H7B	111.2	O31—S22—N5	106.74 (8)
H7A—C7—H7B	109.1	O30—S22—C23	107.11 (8)
C7—C8—C9	107.70 (14)	O31—S22—C23	107.31 (7)
C7—C8—C11	102.69 (12)	N5—S22—C23	105.68 (7)
C9—C8—C11	102.68 (13)	C24—C23—C28	120.36 (15)
C7—C8—H8	114.2	C24—C23—S22	118.84 (13)
C9—C8—H8	114.2	C28—C23—S22	120.66 (13)
C11—C8—H8	114.2	C23—C24—C25	119.52 (18)

C8—C9—C10	103.16 (13)	C23—C24—H24	120.2
C8—C9—H9A	111.1	C25—C24—H24	120.2
C10—C9—H9A	111.1	C26—C25—C24	121.23 (18)
C8—C9—H9B	111.1	C26—C25—H25	119.4
C10—C9—H9B	111.1	C24—C25—H25	119.4
H9A—C9—H9B	109.1	C25—C26—C27	118.60 (16)
C9—C10—C1	103.40 (12)	C25—C26—C29	120.4 (2)
C9—C10—H10A	111.1	C27—C26—C29	121.0 (2)
C1—C10—H10A	111.1	C26—C27—C28	120.90 (18)
C9—C10—H10B	111.1	C26—C27—H27	119.6
C1—C10—H10B	111.1	C28—C27—H27	119.6
H10A—C10—H10B	109.0	C23—C28—C27	119.39 (17)
C13—C11—C12	107.21 (14)	C23—C28—H28	120.3
C13—C11—C8	113.53 (13)	C27—C28—H28	120.3
C12—C11—C8	113.17 (13)	C26—C29—H29A	109.5
C13—C11—C1	116.15 (12)	C26—C29—H29B	109.5
C12—C11—C1	113.80 (13)	H29A—C29—H29B	109.5
C8—C11—C1	92.70 (11)	C26—C29—H29C	109.5
C11—C12—H12A	109.5	H29A—C29—H29C	109.5
C11—C12—H12B	109.5	H29B—C29—H29C	109.5
H12A—C12—H12B	109.5		
C4—O3—C2—C1	−59.24 (16)	O3—C4—C14—O21	92.0 (2)
C4—N5—C6—C1	39.60 (16)		

Fig. 1


C29
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