

A new monoclinic polymorph of 3-diethylamino-4-(4-methoxyphenyl)-1,1-dioxo-4H-1λ⁶,2-thiazete-4-carbonitrile

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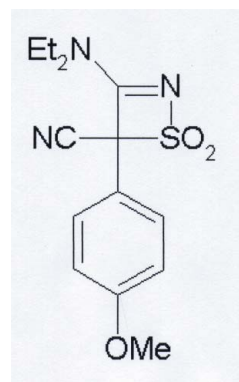
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.037; wR factor = 0.102; data-to-parameter ratio = 10.9.

A new monoclinic form of the title compound, $\text{C}_{14}\text{H}_{17}\text{N}_3\text{O}_3\text{S}$, has been found upon slow crystallization from water. Another monoclinic form of the compound was obtained previously from a mixture of dichloromethane and diethyl ether [Clerici *et al.* (2002). *Tetrahedron*, **58**, 5173–5178]. Both phases crystallize in space group $P2_1/n$ with one molecule in the asymmetric unit. The formally single exocyclic C–N bond that connects the $-\text{NEt}_2$ unit with the thiazete ring is considerably shorter than the adjacent, formally double, endocyclic C=N bond. This is likely to be due to the extended conjugated system between the electron-donor diethylamine fragment and the electron-withdrawing sulfonyl group. In the newly discovered polymorph, the methoxy group is rotated by almost 180° around the phenyl–OCH₃ bond, resulting in a different molecular conformation.

Related literature

For the synthesis of the title compound and the crystal structure of the other polymorph, see: Clerici *et al.* (2002). For a related structure, see: Clerici *et al.* (1996). For the biological activity of β -sultam derivatives, see: Barwick *et al.* (2008) and references therein.



Experimental

Crystal data

$\text{C}_{14}\text{H}_{17}\text{N}_3\text{O}_3\text{S}$	$V = 1533.4$ (5) Å ³
$M_r = 307.37$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.3853$ (17) Å	$\mu = 0.22$ mm ⁻¹
$b = 17.554$ (4) Å	$T = 293$ K
$c = 10.458$ (2) Å	$0.18 \times 0.16 \times 0.16$ mm
$\beta = 95.07$ (3)°	

Data collection

Bruker APEX CCD area-detector diffractometer	16661 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2007)	2814 independent reflections
$T_{\min} = 0.855$, $T_{\max} = 0.947$	1949 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$	258 parameters
$wR(F^2) = 0.102$	All H-atom parameters refined
$S = 1.01$	$\Delta\rho_{\max} = 0.16$ e Å ⁻³
2814 reflections	$\Delta\rho_{\min} = -0.31$ e Å ⁻³

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2005); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); 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: NK2045).

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supporting information

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A new monoclinic polymorph of 3-diethylamino-4-(4-methoxyphenyl)-1,1-dioxo-4*H*-1 λ ⁶,2-thiazete-4-carbonitrile

Ahmed M. Orlando, Leonardo Lo Presti and Raffaella Soave

S1. Comment

The title compound, (I), a thiazete 1,1 dioxo derivative containing a four-membered heterocycle, exhibits a marked similarity with the β -sultamic functionality, which is the key component of promising antibiotic drugs (Barwick *et al.*, 2008). A new monoclinic polymorph of (I) (hereinafter, phase B: Fig. 1, Table 1) was found upon slow recrystallization from water of a little amount of the phase A, originally obtained from a CH₂Cl₂:Et₂O mixture (Clerici *et al.*, 2002). Both polymorphs share the same space group, $P2_1/n$, with one molecule in the asymmetric unit. On average, bond lengths and angles are very similar between the two forms, while the molecular conformations are different. The most important dissimilarity resides in the dihedral angles involving the phenyl-OCH₃ single bond, which is rotated by $\sim 180^\circ$ in the form B with respect to form A (Fig. 2). In both crystal forms the formally single exocyclic C9–N1 bond connecting the –NEt₂ moiety to the thiazete ring is considerably shorter (phase B: 1.307 (3) Å; phase A: 1.318 (3) Å) than the adjacent, formally double, endocyclic C9=N2 bond (phase B: 1.331 (3) Å; phase A: 1.327 (3) Å). A possible explanation resides in the existence of an extended π conjugated system between the electron-donor diethylamine fragment and the electron-withdrawing sulfonyl group. This conjecture is supported by the values of the C–N1–C angles, which in both phases range from $\sim 118^\circ$ to $\sim 122^\circ$ and are compatible with a formally sp^2 tertiary nitrogen atom. Very similar bond distances within the thiazete group have been reported by Clerici *et al.* (1996) for a chemically related derivative of (I). On geometrical grounds, no relevant intermolecular hydrogen bonds have been found in both phases.

S2. Experimental

The compound (I) was synthesized using the procedure reported by Clerici *et al.* (2002). Part of the material obtained from dichloromethane and diethyl ether (phase A) was dissolved in distilled water and crystallized by slow solvent evaporation at room temperature. After roughly 7 days, very small colorless crystals with the same habit (prism) as the most common phase A appeared. Only the X-ray analysis revealed that in fact a new polymorph (phase B) was obtained.

S3. Refinement

All hydrogen atoms have been located by difference Fourier. Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINTE* (Bruker, 2005); data reduction: *SAINTE* (Bruker, 2005); absorption correction: *SADABS* (Bruker, 2007); program used to solve structure: *SHELXS97* (Sheldrick, 2008); program used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphic: *DIAMOND* (Brandenburg, 2010); overlay scheme: Mercury CSD 2.3

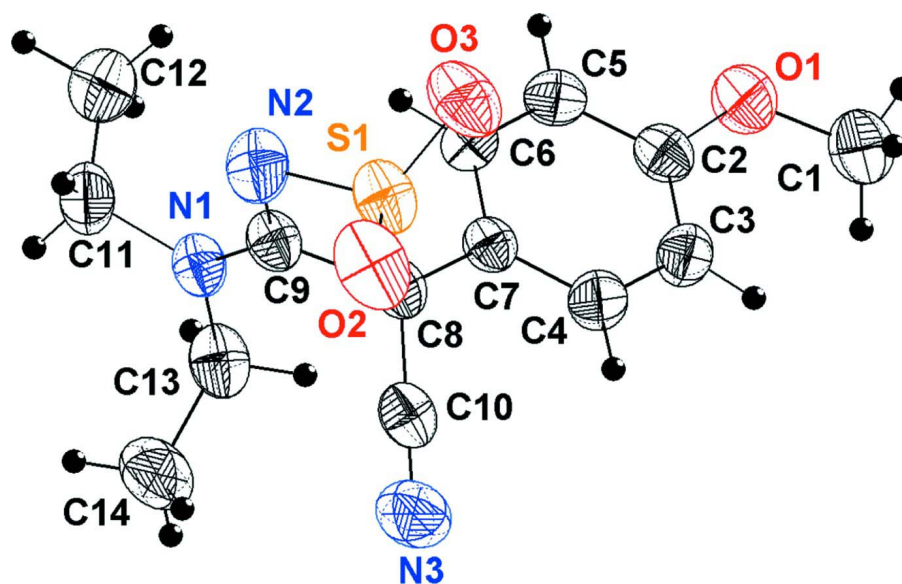


Figure 1

Molecular structure of (I), with the non-H atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

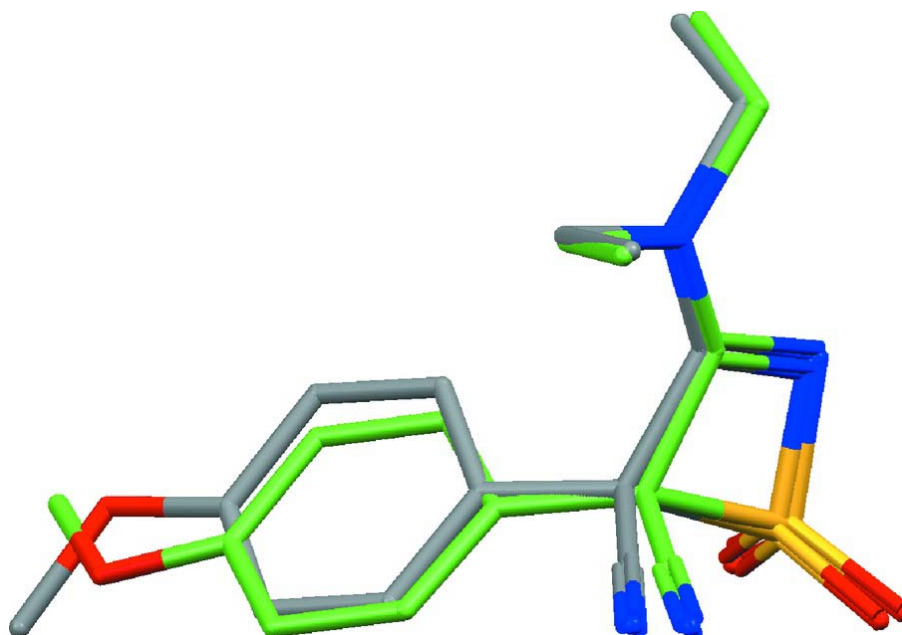


Figure 2

Least-squares overlay scheme of the asymmetric units of (I) within phase B (this work, carbon backbone in gray) and phase A (Clerici *et al.*, 2002; carbon backbone in green). Hydrogen atoms omitted for clarity.

3-diethylamino-4-(4-methoxyphenyl)-1,1-dioxo-4H-1 λ 6,2-thiazete- 4-carbonitrile

Crystal data

$C_{14}H_{17}N_3O_3S$
 $M_r = 307.37$

Monoclinic, $P2_1/n$
Hall symbol: -P 2yn

$a = 8.3853$ (17) Å
 $b = 17.554$ (4) Å
 $c = 10.458$ (2) Å
 $\beta = 95.07$ (3)°
 $V = 1533.4$ (5) Å³
 $Z = 4$
 $F(000) = 648$
 $D_x = 1.331$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 2885 reflections
 $\theta = 2.3$ – 21.6 °
 $\mu = 0.22$ mm⁻¹
 $T = 293$ K
 Prism, colourless
 $0.18 \times 0.16 \times 0.16$ mm

Data collection

Bruker APEX CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2007)
 $T_{\min} = 0.855$, $T_{\max} = 0.947$

16661 measured reflections
 2814 independent reflections
 1949 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$
 $\theta_{\max} = 25.4$ °, $\theta_{\min} = 2.3$ °
 $h = -10 \rightarrow 10$
 $k = -21 \rightarrow 21$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.102$
 $S = 1.01$
 2814 reflections
 258 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: structure-invariant direct methods
 Hydrogen site location: difference Fourier map
 All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0446P)^2 + 0.4078P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³

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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.46791 (6)	0.19850 (4)	0.39836 (6)	0.0569 (2)
O1	0.1824 (2)	0.00687 (9)	-0.10877 (14)	0.0636 (5)
O2	0.57694 (19)	0.19314 (11)	0.51054 (16)	0.0758 (5)
O3	0.53410 (19)	0.20903 (10)	0.27881 (16)	0.0724 (5)
N1	0.0608 (2)	0.20205 (10)	0.44220 (16)	0.0472 (4)
N2	0.3156 (2)	0.25469 (11)	0.41859 (19)	0.0611 (5)
N3	0.3384 (3)	0.02616 (14)	0.5764 (2)	0.0739 (6)
C1	0.2489 (4)	-0.06433 (17)	-0.1428 (3)	0.0698 (8)
C2	0.2106 (2)	0.03021 (12)	0.01541 (19)	0.0458 (5)

C3	0.2867 (3)	-0.01266 (14)	0.1123 (2)	0.0521 (6)
C4	0.3129 (3)	0.01743 (13)	0.2346 (2)	0.0491 (5)
C5	0.1573 (3)	0.10253 (13)	0.0415 (2)	0.0497 (5)
C6	0.1842 (3)	0.13239 (13)	0.1623 (2)	0.0474 (5)
C7	0.2636 (2)	0.09019 (11)	0.26096 (18)	0.0395 (5)
C8	0.3043 (2)	0.12520 (12)	0.39177 (19)	0.0425 (5)
C9	0.2122 (2)	0.19738 (12)	0.42216 (19)	0.0448 (5)
C10	0.3242 (2)	0.06955 (14)	0.4954 (2)	0.0496 (5)
C11	-0.0148 (3)	0.27758 (15)	0.4525 (3)	0.0599 (7)
C12	-0.0724 (4)	0.3089 (2)	0.3236 (3)	0.0769 (8)
C13	-0.0377 (3)	0.13436 (15)	0.4614 (2)	0.0553 (6)
C14	-0.0494 (4)	0.1173 (2)	0.6015 (3)	0.0780 (9)
H1A	0.226 (3)	-0.0650 (17)	-0.234 (3)	0.105 (10)*
H1B	0.201 (3)	-0.1077 (16)	-0.096 (3)	0.085 (9)*
H1C	0.364 (3)	-0.0633 (15)	-0.122 (2)	0.081 (9)*
H3	0.317 (3)	-0.0621 (14)	0.100 (2)	0.066 (7)*
H4	0.367 (2)	-0.0118 (12)	0.299 (2)	0.055 (6)*
H5	0.100 (2)	0.1321 (12)	-0.027 (2)	0.055 (6)*
H6	0.153 (3)	0.1815 (13)	0.176 (2)	0.056 (7)*
H11A	-0.101 (3)	0.2705 (13)	0.502 (2)	0.068 (7)*
H11B	0.064 (3)	0.3094 (15)	0.495 (2)	0.078 (9)*
H12A	-0.122 (3)	0.3602 (18)	0.334 (3)	0.095 (9)*
H12B	-0.152 (4)	0.2716 (19)	0.279 (3)	0.114 (12)*
H12C	0.016 (4)	0.3143 (15)	0.271 (3)	0.088 (9)*
H13A	-0.139 (3)	0.1458 (12)	0.4177 (19)	0.053 (6)*
H13B	0.008 (2)	0.0906 (13)	0.4177 (19)	0.052 (6)*
H14A	-0.113 (4)	0.073 (2)	0.613 (3)	0.126 (12)*
H14B	-0.094 (3)	0.1583 (18)	0.642 (3)	0.095 (10)*
H14C	0.062 (4)	0.1065 (18)	0.653 (3)	0.116 (12)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0428 (3)	0.0691 (4)	0.0599 (4)	-0.0149 (3)	0.0108 (3)	-0.0137 (3)
O1	0.0840 (12)	0.0642 (11)	0.0414 (9)	0.0047 (9)	-0.0024 (8)	-0.0079 (8)
O2	0.0492 (9)	0.1081 (15)	0.0690 (11)	-0.0171 (9)	-0.0014 (8)	-0.0233 (10)
O3	0.0624 (10)	0.0883 (13)	0.0705 (11)	-0.0220 (9)	0.0270 (9)	-0.0068 (10)
N1	0.0434 (10)	0.0506 (11)	0.0489 (10)	-0.0011 (8)	0.0116 (8)	-0.0073 (8)
N2	0.0559 (12)	0.0537 (12)	0.0755 (14)	-0.0126 (9)	0.0162 (10)	-0.0154 (10)
N3	0.0798 (15)	0.0884 (17)	0.0534 (13)	0.0113 (13)	0.0047 (11)	0.0129 (12)
C1	0.092 (2)	0.0672 (19)	0.0505 (17)	-0.0020 (17)	0.0059 (15)	-0.0149 (14)
C2	0.0466 (12)	0.0514 (13)	0.0392 (12)	-0.0049 (10)	0.0033 (9)	-0.0013 (10)
C3	0.0619 (14)	0.0448 (14)	0.0492 (13)	0.0077 (11)	0.0032 (10)	-0.0051 (11)
C4	0.0510 (13)	0.0524 (14)	0.0428 (13)	0.0089 (11)	-0.0011 (10)	0.0024 (11)
C5	0.0563 (13)	0.0506 (14)	0.0417 (12)	0.0046 (11)	0.0010 (10)	0.0066 (11)
C6	0.0517 (13)	0.0415 (13)	0.0495 (14)	0.0046 (10)	0.0072 (10)	0.0021 (11)
C7	0.0355 (10)	0.0430 (12)	0.0405 (11)	-0.0034 (9)	0.0066 (8)	-0.0013 (9)
C8	0.0371 (11)	0.0492 (13)	0.0415 (12)	-0.0022 (9)	0.0054 (9)	-0.0042 (10)

C9	0.0437 (11)	0.0491 (13)	0.0422 (12)	-0.0050 (10)	0.0064 (9)	-0.0074 (10)
C10	0.0447 (12)	0.0619 (15)	0.0421 (13)	0.0007 (11)	0.0040 (10)	-0.0062 (12)
C11	0.0602 (16)	0.0581 (16)	0.0635 (17)	0.0092 (13)	0.0169 (13)	-0.0099 (13)
C12	0.083 (2)	0.073 (2)	0.077 (2)	0.0205 (18)	0.0162 (17)	0.0058 (17)
C13	0.0408 (13)	0.0619 (16)	0.0640 (16)	-0.0094 (11)	0.0095 (11)	-0.0148 (13)
C14	0.085 (2)	0.078 (2)	0.077 (2)	-0.0188 (19)	0.0353 (18)	-0.0019 (17)

Geometric parameters (Å, °)

S1—O3	1.4241 (17)	C5—C6	1.369 (3)
S1—O2	1.4252 (18)	C5—H5	0.98 (2)
S1—N2	1.642 (2)	C6—C7	1.391 (3)
S1—C8	1.878 (2)	C6—H6	0.92 (2)
O1—C2	1.362 (2)	C7—C8	1.511 (3)
O1—C1	1.426 (3)	C8—C10	1.457 (3)
N1—C9	1.307 (3)	C8—C9	1.532 (3)
N1—C13	1.471 (3)	C11—C12	1.496 (4)
N1—C11	1.478 (3)	C11—H11A	0.94 (2)
N2—C9	1.331 (3)	C11—H11B	0.95 (3)
N3—C10	1.138 (3)	C12—H12A	1.00 (3)
C1—H1A	0.96 (3)	C12—H12B	1.02 (3)
C1—H1B	1.01 (3)	C12—H12C	0.97 (3)
C1—H1C	0.97 (3)	C13—C14	1.508 (4)
C2—C3	1.373 (3)	C13—H13A	0.95 (2)
C2—C5	1.381 (3)	C13—H13B	0.99 (2)
C3—C4	1.384 (3)	C14—H14A	0.95 (4)
C3—H3	0.92 (2)	C14—H14B	0.93 (3)
C4—C7	1.377 (3)	C14—H14C	1.06 (3)
C4—H4	0.94 (2)		
O3—S1—O2	117.38 (11)	C10—C8—C7	113.72 (18)
O3—S1—N2	113.77 (11)	C10—C8—C9	115.25 (17)
O2—S1—N2	112.54 (11)	C7—C8—C9	116.52 (17)
O3—S1—C8	113.38 (10)	C10—C8—S1	113.39 (14)
O2—S1—C8	113.47 (10)	C7—C8—S1	114.70 (13)
N2—S1—C8	80.92 (9)	C9—C8—S1	78.81 (12)
C2—O1—C1	117.5 (2)	N1—C9—N2	127.0 (2)
C9—N1—C13	122.43 (19)	N1—C9—C8	126.87 (18)
C9—N1—C11	119.8 (2)	N2—C9—C8	106.11 (17)
C13—N1—C11	117.72 (19)	N3—C10—C8	179.4 (2)
C9—N2—S1	93.77 (15)	N1—C11—C12	111.7 (2)
O1—C1—H1A	102.2 (18)	N1—C11—H11A	106.2 (15)
O1—C1—H1B	111.1 (15)	C12—C11—H11A	110.1 (15)
H1A—C1—H1B	115 (2)	N1—C11—H11B	106.1 (16)
O1—C1—H1C	109.3 (16)	C12—C11—H11B	111.2 (16)
H1A—C1—H1C	109 (2)	H11A—C11—H11B	111 (2)
H1B—C1—H1C	110 (2)	C11—C12—H12A	109.8 (16)
O1—C2—C3	124.6 (2)	C11—C12—H12B	108.9 (18)

O1—C2—C5	115.63 (19)	H12A—C12—H12B	111 (2)
C3—C2—C5	119.7 (2)	C11—C12—H12C	110.2 (17)
C2—C3—C4	119.9 (2)	H12A—C12—H12C	109 (2)
C2—C3—H3	122.2 (15)	H12B—C12—H12C	108 (2)
C4—C3—H3	117.9 (15)	N1—C13—C14	112.2 (2)
C7—C4—C3	120.9 (2)	N1—C13—H13A	104.7 (13)
C7—C4—H4	120.0 (13)	C14—C13—H13A	112.1 (13)
C3—C4—H4	119.1 (13)	N1—C13—H13B	108.5 (12)
C6—C5—C2	120.3 (2)	C14—C13—H13B	110.8 (12)
C6—C5—H5	120.4 (12)	H13A—C13—H13B	108.2 (17)
C2—C5—H5	119.3 (12)	C13—C14—H14A	111 (2)
C5—C6—C7	120.7 (2)	C13—C14—H14B	110.7 (19)
C5—C6—H6	118.4 (14)	H14A—C14—H14B	109 (3)
C7—C6—H6	120.8 (14)	C13—C14—H14C	113.6 (17)
C4—C7—C6	118.55 (19)	H14A—C14—H14C	106 (3)
C4—C7—C8	120.69 (18)	H14B—C14—H14C	106 (3)
C6—C7—C8	120.64 (19)		
O3—S1—N2—C9	116.10 (15)	N2—S1—C8—C10	-116.78 (16)
O2—S1—N2—C9	-107.28 (15)	O3—S1—C8—C7	-1.80 (19)
C8—S1—N2—C9	4.46 (13)	O2—S1—C8—C7	-139.02 (15)
C1—O1—C2—C3	-5.7 (3)	N2—S1—C8—C7	110.27 (16)
C1—O1—C2—C5	174.0 (2)	O3—S1—C8—C9	-116.00 (13)
O1—C2—C3—C4	178.3 (2)	O2—S1—C8—C9	106.78 (13)
C5—C2—C3—C4	-1.5 (3)	N2—S1—C8—C9	-3.94 (12)
C2—C3—C4—C7	-0.1 (3)	C13—N1—C9—N2	-171.6 (2)
O1—C2—C5—C6	-177.87 (19)	C11—N1—C9—N2	5.4 (3)
C3—C2—C5—C6	1.9 (3)	C13—N1—C9—C8	11.5 (3)
C2—C5—C6—C7	-0.8 (3)	C11—N1—C9—C8	-171.5 (2)
C3—C4—C7—C6	1.2 (3)	S1—N2—C9—N1	176.98 (19)
C3—C4—C7—C8	-174.95 (19)	S1—N2—C9—C8	-5.62 (17)
C5—C6—C7—C4	-0.7 (3)	C10—C8—C9—N1	-66.9 (3)
C5—C6—C7—C8	175.38 (19)	C7—C8—C9—N1	70.2 (3)
C4—C7—C8—C10	-28.1 (3)	S1—C8—C9—N1	-177.6 (2)
C6—C7—C8—C10	155.89 (18)	C10—C8—C9—N2	115.7 (2)
C4—C7—C8—C9	-165.80 (18)	C7—C8—C9—N2	-107.2 (2)
C6—C7—C8—C9	18.2 (3)	S1—C8—C9—N2	5.00 (15)
C4—C7—C8—S1	104.7 (2)	C9—N1—C11—C12	85.4 (3)
C6—C7—C8—S1	-71.3 (2)	C13—N1—C11—C12	-97.4 (3)
O3—S1—C8—C10	131.15 (16)	C9—N1—C13—C14	96.4 (3)
O2—S1—C8—C10	-6.06 (19)	C11—N1—C13—C14	-80.6 (3)
