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2-[[5-(Adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfanyl]-N,N-dimethylethanamine

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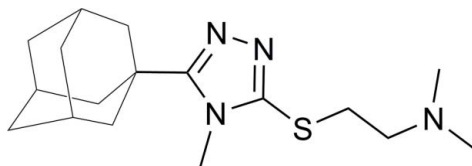
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.064; wR factor = 0.184; data-to-parameter ratio = 16.1.

In the title compound, $\text{C}_{17}\text{H}_{28}\text{N}_4\text{S}$, the 1,2,4-triazole ring is nearly planar [maximum deviation = 0.005 (2) Å]. There are no significant hydrogen bonds observed in the crystal structure. The crystal studied was a non-merohedral twin, the refined ratio of twin components being 0.281 (3):0.719 (3).

Related literature

For the biological activity of adamantyl derivatives see: Al-Omar *et al.* (2010); Al-Deeb *et al.* (2006); El-Emam *et al.* (2004); Kadi *et al.* (2007, 2010); Vernier *et al.* (1969). For the structures of related adamantyl-1,2,4-triazoles, see: Almutairi *et al.* (2012); Al-Tamimi *et al.* (2010); Al-Abdullah *et al.* (2012). For the structures of substituted sulfanyl-1,2,4-triazoles, see: Fun *et al.* (2011); Wang *et al.* (2011). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{28}\text{N}_4\text{S}$
 $M_r = 320.49$
Monoclinic, $P2_1/c$
 $a = 12.5133$ (7) Å

$b = 10.3779$ (5) Å
 $c = 14.3044$ (8) Å
 $\beta = 106.766$ (3)°
 $V = 1778.63$ (16) Å³

$Z = 4$
Cu $K\alpha$ radiation
 $\mu = 1.62$ mm⁻¹

$T = 296$ K
 $0.64 \times 0.59 \times 0.05$ mm

Data collection

Bruker SMART APEXII CCD
area-detector diffractometer
Absorption correction: multi-scan
(SADABS; Bruker, 2009)
 $T_{\min} = 0.204$, $T_{\max} = 0.923$

3267 measured reflections
3267 independent reflections
2846 reflections with $I > 2\sigma(I)$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$
 $wR(F^2) = 0.184$
 $S = 1.13$
3267 reflections

203 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.32$ e Å⁻³
 $\Delta\rho_{\min} = -0.37$ e Å⁻³

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2734).

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supporting information

Acta Cryst. (2012). E68, o1356 [doi:10.1107/S160053681201464X]

2-[[5-(Adamantan-1-yl)-4-methyl-4*H*-1,2,4-triazol-3-yl]sulfanyl]-*N,N*-dimethylethanamine

Ali A. El-Emam, Siham Lahsasni, Hanadi H. Asiri, Ching Kheng Quah and Hoong-Kun Fun

S1. Comment

Considerable attention has been devoted to adamantane derivatives which have long been known for their diverse biological properties as antiviral against the influenza (Vernier *et al.*, 1969) and HIV viruses (El-Emam, Al-Deeb, Al-Omar & Lehmann, 2004). Moreover, adamantane derivatives were recently reported to exhibit marked antibacterial activity (Kadi *et al.*, 2007, 2010). In continuation of our interest in the chemical and pharmacological properties of adamantane derivatives, we synthesized the title compound as a potential chemotherapeutic agent.

In the title molecule, Fig. 1, the 1,2,4-triazole ring (N1-N3/C11/C12) is nearly planar with a maximum deviation of 0.005 (2) Å at atom N2. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to those reported for related structures (Almutairi *et al.*, 2012; Al-Tamimi *et al.*, 2010; Al-Abdullah *et al.*, 2012; Fun *et al.*, 2011; Wang *et al.*, 2011). The crystal studied was a non-merohedral twin, the refined ratio of twin components being 0.281 (3):0.719 (3). There are no significant hydrogen bonds observed in this compound.

S2. Experimental

A mixture of 3-(adamantan-1-yl)-4-methyl-4*H*-1,2,4-triazole-5-thiol (2.49 g, 0.01 mol), potassium hydroxide (1.12 g, 0.02 mol) and 2-dimethylaminoethyl chloride hydrochloride (1.44 g, 0.01 mol) in ethanol (15 ml) was heated under reflux with stirring for 3 h and the solvent was distilled off *in vacuo*. The obtained residue was washed with water and purified by column chromatography on silica gel column using CHCl₃:MeOH (9:1 v/v) as eluent to yield 2.02 g (63%) of the title compound as colorless powder. M.p. 133–135°C. Single crystals suitable for X-ray diffraction were obtained by crystallization from aqueous ethanol. ¹H NMR (CDCl₃, 500.13 MHz): δ 1.69–1.75 (m, 6H, adamantane-H), 2.04–2.85 (m, 9H, adamantane-H), 2.21 (s, 6H, 2xCH₃), 2.62 (t, 2H, CH₂N, *J* = 6.5 Hz), 3.28 (t, 2H, SCH₂, *J* = 6.5 Hz), 3.59 (s, 3H, CH₃). ¹³C NMR (CDCl₃, 125.76 MHz): δ 28.07, 34.98, 36.50, 49.56 (adamantane-C), 31.05 (CH₃), 32.33 (SCH₂), 45.21 (2xCH₃), 58.24 (CH₂N), 152.16, 161.21 (triazole C).

S3. Refinement

All hydrogen atoms were positioned geometrically [C–H = 0.96–0.98 Å] and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C})$. A rotating group model was applied to the methyl groups. The crystal studied was a non-merohedral twin, the refined ratio of twin components being 0.281 (3):0.719 (3).

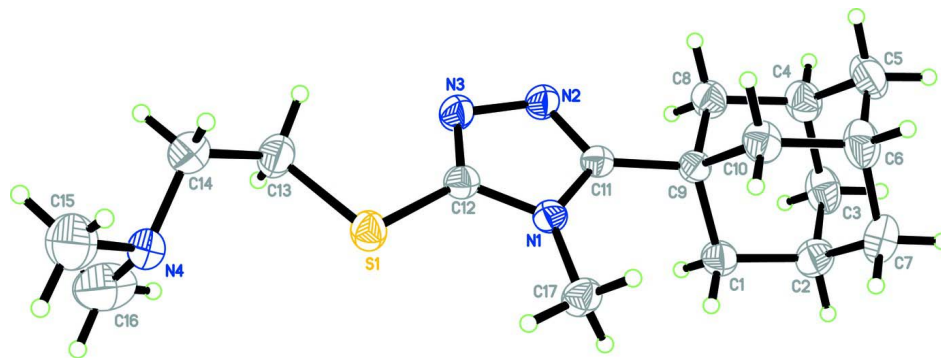


Figure 1

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms.

2-[[5-(Adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfonyl]-*N,N*-dimethylethanamine

Crystal data

$C_{17}H_{28}N_4S$

$M_r = 320.49$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.5133$ (7) Å

$b = 10.3779$ (5) Å

$c = 14.3044$ (8) Å

$\beta = 106.766$ (3)°

$V = 1778.63$ (16) Å³

$Z = 4$

$F(000) = 696$

$D_x = 1.197$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 3932 reflections

$\theta = 7.7$ – 69.2 °

$\mu = 1.62$ mm⁻¹

$T = 296$ K

Plate, colourless

$0.64 \times 0.59 \times 0.05$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)

$T_{\min} = 0.204$, $T_{\max} = 0.923$

3267 measured reflections

3267 independent reflections

2846 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$

$\theta_{\max} = 69.8$ °, $\theta_{\min} = 7.7$ °

$h = -15$ → 14

$k = -12$ → 12

$l = 0$ → 16

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.064$

$wR(F^2) = 0.184$

$S = 1.13$

3267 reflections

203 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.P)^2 + 1.1111P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.32$ e Å⁻³

$\Delta\rho_{\min} = -0.37$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.59451 (7)	0.30472 (8)	0.05471 (7)	0.0589 (3)
N1	0.4306 (2)	0.2967 (2)	0.14471 (19)	0.0478 (6)
N4	0.7649 (3)	0.2967 (3)	-0.0644 (2)	0.0630 (7)
C9	0.2838 (2)	0.2248 (3)	0.2293 (2)	0.0476 (7)
C10	0.3344 (3)	0.2856 (4)	0.3307 (3)	0.0672 (9)
H10A	0.3944	0.2315	0.3689	0.081*
H10B	0.3653	0.3694	0.3234	0.081*
C6	0.2449 (4)	0.3001 (5)	0.3838 (3)	0.0814 (12)
H6A	0.2779	0.3402	0.4477	0.098*
C5	0.1995 (4)	0.1692 (5)	0.3976 (3)	0.0893 (14)
H5A	0.1441	0.1778	0.4328	0.107*
H5B	0.2594	0.1149	0.4359	0.107*
C4	0.1465 (4)	0.1071 (4)	0.2985 (3)	0.0765 (11)
H4A	0.1169	0.0222	0.3077	0.092*
C3	0.0526 (3)	0.1919 (5)	0.2391 (3)	0.0817 (13)
H3A	0.0183	0.1524	0.1761	0.098*
H3B	-0.0041	0.2011	0.2728	0.098*
C13	0.6508 (4)	0.1620 (4)	0.0134 (4)	0.0803 (12)
H13A	0.6560	0.0927	0.0600	0.096*
H13B	0.6015	0.1344	-0.0490	0.096*
C2	0.0985 (3)	0.3229 (4)	0.2249 (3)	0.0757 (11)
H2A	0.0375	0.3775	0.1869	0.091*
C7	0.1513 (4)	0.3853 (5)	0.3230 (4)	0.0861 (13)
H7A	0.0954	0.3977	0.3571	0.103*
H7B	0.1810	0.4691	0.3136	0.103*
C1	0.1858 (3)	0.3084 (4)	0.1699 (3)	0.0653 (9)
H1A	0.2132	0.3927	0.1586	0.078*
H1B	0.1520	0.2684	0.1069	0.078*
C8	0.2350 (3)	0.0923 (3)	0.2444 (3)	0.0666 (9)
H8A	0.2018	0.0521	0.1814	0.080*
H8B	0.2944	0.0367	0.2817	0.080*
C11	0.3702 (2)	0.2040 (3)	0.1772 (2)	0.0477 (7)
N2	0.4021 (2)	0.0897 (2)	0.1572 (2)	0.0577 (7)
N3	0.4859 (3)	0.1046 (3)	0.1120 (2)	0.0599 (7)
C12	0.5001 (3)	0.2289 (3)	0.1054 (2)	0.0516 (7)

C14	0.7641 (4)	0.1909 (5)	0.0031 (4)	0.0874 (14)
H14A	0.8139	0.2124	0.0669	0.105*
H14B	0.7930	0.1140	-0.0196	0.105*
C16	0.7117 (7)	0.2636 (6)	-0.1633 (5)	0.126 (2)
H16A	0.7180	0.3341	-0.2048	0.189*
H16B	0.6342	0.2457	-0.1713	0.189*
H16C	0.7468	0.1886	-0.1805	0.189*
C17	0.4269 (3)	0.4366 (3)	0.1495 (3)	0.0633 (9)
H17A	0.4899	0.4723	0.1330	0.095*
H17B	0.4292	0.4626	0.2145	0.095*
H17C	0.3593	0.4674	0.1043	0.095*
C15	0.8793 (5)	0.3349 (7)	-0.0500 (6)	0.120 (2)
H15A	0.8822	0.4023	-0.0951	0.181*
H15B	0.9217	0.2623	-0.0608	0.181*
H15C	0.9101	0.3655	0.0156	0.181*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0605 (5)	0.0553 (5)	0.0668 (6)	-0.0051 (3)	0.0278 (4)	-0.0023 (4)
N1	0.0524 (14)	0.0418 (13)	0.0497 (15)	0.0000 (10)	0.0156 (11)	0.0003 (10)
N4	0.0598 (17)	0.0665 (18)	0.0661 (19)	0.0050 (13)	0.0236 (14)	0.0030 (14)
C9	0.0478 (15)	0.0505 (16)	0.0430 (16)	0.0012 (12)	0.0105 (13)	-0.0010 (12)
C10	0.060 (2)	0.084 (2)	0.051 (2)	-0.0009 (18)	0.0042 (16)	-0.0097 (17)
C6	0.076 (3)	0.113 (4)	0.054 (2)	-0.003 (2)	0.0162 (19)	-0.021 (2)
C5	0.082 (3)	0.133 (4)	0.059 (3)	0.012 (3)	0.031 (2)	0.017 (2)
C4	0.079 (3)	0.078 (3)	0.083 (3)	-0.011 (2)	0.039 (2)	0.003 (2)
C3	0.056 (2)	0.123 (4)	0.070 (3)	-0.011 (2)	0.0232 (19)	-0.009 (2)
C13	0.081 (3)	0.064 (2)	0.114 (4)	0.0078 (19)	0.056 (3)	0.006 (2)
C2	0.057 (2)	0.095 (3)	0.073 (3)	0.0195 (19)	0.0154 (18)	0.007 (2)
C7	0.085 (3)	0.092 (3)	0.091 (3)	0.009 (2)	0.042 (3)	-0.018 (2)
C1	0.059 (2)	0.080 (2)	0.055 (2)	0.0125 (16)	0.0139 (16)	0.0096 (17)
C8	0.070 (2)	0.063 (2)	0.072 (2)	-0.0051 (16)	0.0289 (18)	0.0026 (17)
C11	0.0505 (16)	0.0440 (15)	0.0476 (17)	0.0002 (12)	0.0126 (13)	0.0023 (12)
N2	0.0657 (16)	0.0454 (14)	0.0686 (18)	0.0029 (12)	0.0299 (14)	0.0032 (12)
N3	0.0682 (17)	0.0466 (15)	0.0727 (19)	0.0041 (12)	0.0327 (15)	0.0027 (12)
C12	0.0531 (17)	0.0499 (17)	0.0499 (18)	0.0020 (13)	0.0118 (14)	0.0008 (13)
C14	0.080 (3)	0.094 (3)	0.096 (3)	0.024 (2)	0.038 (3)	0.024 (3)
C16	0.181 (6)	0.097 (4)	0.082 (4)	0.030 (4)	0.008 (4)	-0.013 (3)
C17	0.069 (2)	0.0442 (17)	0.080 (2)	-0.0017 (15)	0.0273 (18)	-0.0028 (15)
C15	0.082 (3)	0.137 (5)	0.151 (6)	0.003 (3)	0.047 (4)	0.032 (4)

Geometric parameters (Å, °)

S1—C12	1.742 (3)	C13—C14	1.498 (6)
S1—C13	1.811 (4)	C13—H13A	0.9700
N1—C12	1.361 (4)	C13—H13B	0.9700
N1—C11	1.384 (4)	C2—C7	1.513 (7)

N1—C17	1.455 (4)	C2—C1	1.527 (5)
N4—C16	1.421 (7)	C2—H2A	0.9800
N4—C15	1.441 (6)	C7—H7A	0.9700
N4—C14	1.464 (5)	C7—H7B	0.9700
C9—C11	1.495 (4)	C1—H1A	0.9700
C9—C10	1.539 (5)	C1—H1B	0.9700
C9—C1	1.542 (4)	C8—H8A	0.9700
C9—C8	1.546 (5)	C8—H8B	0.9700
C10—C6	1.531 (6)	C11—N2	1.310 (4)
C10—H10A	0.9700	N2—N3	1.390 (4)
C10—H10B	0.9700	N3—C12	1.309 (4)
C6—C5	1.508 (7)	C14—H14A	0.9700
C6—C7	1.524 (7)	C14—H14B	0.9700
C6—H6A	0.9800	C16—H16A	0.9600
C5—C4	1.524 (7)	C16—H16B	0.9600
C5—H5A	0.9700	C16—H16C	0.9600
C5—H5B	0.9700	C17—H17A	0.9600
C4—C3	1.517 (7)	C17—H17B	0.9600
C4—C8	1.531 (5)	C17—H17C	0.9600
C4—H4A	0.9800	C15—H15A	0.9600
C3—C2	1.513 (7)	C15—H15B	0.9600
C3—H3A	0.9700	C15—H15C	0.9600
C3—H3B	0.9700		
C12—S1—C13	98.05 (17)	C7—C2—H2A	109.2
C12—N1—C11	104.8 (2)	C1—C2—H2A	109.2
C12—N1—C17	124.6 (3)	C2—C7—C6	109.8 (4)
C11—N1—C17	130.5 (3)	C2—C7—H7A	109.7
C16—N4—C15	111.7 (5)	C6—C7—H7A	109.7
C16—N4—C14	112.6 (4)	C2—C7—H7B	109.7
C15—N4—C14	107.9 (4)	C6—C7—H7B	109.7
C11—C9—C10	111.7 (3)	H7A—C7—H7B	108.2
C11—C9—C1	112.4 (3)	C2—C1—C9	110.2 (3)
C10—C9—C1	109.5 (3)	C2—C1—H1A	109.6
C11—C9—C8	108.2 (3)	C9—C1—H1A	109.6
C10—C9—C8	107.7 (3)	C2—C1—H1B	109.6
C1—C9—C8	107.1 (3)	C9—C1—H1B	109.6
C6—C10—C9	110.3 (3)	H1A—C1—H1B	108.1
C6—C10—H10A	109.6	C4—C8—C9	110.7 (3)
C9—C10—H10A	109.6	C4—C8—H8A	109.5
C6—C10—H10B	109.6	C9—C8—H8A	109.5
C9—C10—H10B	109.6	C4—C8—H8B	109.5
H10A—C10—H10B	108.1	C9—C8—H8B	109.5
C5—C6—C7	109.9 (4)	H8A—C8—H8B	108.1
C5—C6—C10	109.5 (4)	N2—C11—N1	109.0 (3)
C7—C6—C10	109.0 (4)	N2—C11—C9	123.3 (3)
C5—C6—H6A	109.5	N1—C11—C9	127.6 (3)
C7—C6—H6A	109.5	C11—N2—N3	108.6 (3)

C10—C6—H6A	109.5	C12—N3—N2	106.3 (3)
C6—C5—C4	109.8 (3)	N3—C12—N1	111.2 (3)
C6—C5—H5A	109.7	N3—C12—S1	126.8 (3)
C4—C5—H5A	109.7	N1—C12—S1	122.0 (2)
C6—C5—H5B	109.7	N4—C14—C13	113.7 (4)
C4—C5—H5B	109.7	N4—C14—H14A	108.8
H5A—C5—H5B	108.2	C13—C14—H14A	108.8
C3—C4—C5	109.5 (4)	N4—C14—H14B	108.8
C3—C4—C8	109.4 (4)	C13—C14—H14B	108.8
C5—C4—C8	109.2 (4)	H14A—C14—H14B	107.7
C3—C4—H4A	109.6	N4—C16—H16A	109.5
C5—C4—H4A	109.6	N4—C16—H16B	109.5
C8—C4—H4A	109.6	H16A—C16—H16B	109.5
C2—C3—C4	109.5 (3)	N4—C16—H16C	109.5
C2—C3—H3A	109.8	H16A—C16—H16C	109.5
C4—C3—H3A	109.8	H16B—C16—H16C	109.5
C2—C3—H3B	109.8	N1—C17—H17A	109.5
C4—C3—H3B	109.8	N1—C17—H17B	109.5
H3A—C3—H3B	108.2	H17A—C17—H17B	109.5
C14—C13—S1	109.7 (3)	N1—C17—H17C	109.5
C14—C13—H13A	109.7	H17A—C17—H17C	109.5
S1—C13—H13A	109.7	H17B—C17—H17C	109.5
C14—C13—H13B	109.7	N4—C15—H15A	109.5
S1—C13—H13B	109.7	N4—C15—H15B	109.5
H13A—C13—H13B	108.2	H15A—C15—H15B	109.5
C3—C2—C7	110.0 (4)	N4—C15—H15C	109.5
C3—C2—C1	109.7 (4)	H15A—C15—H15C	109.5
C7—C2—C1	109.6 (3)	H15B—C15—H15C	109.5
C3—C2—H2A	109.2		
C11—C9—C10—C6	-177.5 (3)	C10—C9—C8—C4	58.6 (4)
C1—C9—C10—C6	57.3 (4)	C1—C9—C8—C4	-59.2 (4)
C8—C9—C10—C6	-58.8 (4)	C12—N1—C11—N2	-0.5 (4)
C9—C10—C6—C5	60.9 (4)	C17—N1—C11—N2	-179.8 (3)
C9—C10—C6—C7	-59.3 (5)	C12—N1—C11—C9	178.0 (3)
C7—C6—C5—C4	58.9 (5)	C17—N1—C11—C9	-1.3 (5)
C10—C6—C5—C4	-60.8 (5)	C10—C9—C11—N2	113.2 (4)
C6—C5—C4—C3	-59.6 (5)	C1—C9—C11—N2	-123.3 (4)
C6—C5—C4—C8	60.2 (5)	C8—C9—C11—N2	-5.3 (4)
C5—C4—C3—C2	59.8 (5)	C10—C9—C11—N1	-65.1 (4)
C8—C4—C3—C2	-59.8 (5)	C1—C9—C11—N1	58.4 (4)
C12—S1—C13—C14	-157.1 (3)	C8—C9—C11—N1	176.4 (3)
C4—C3—C2—C7	-59.9 (5)	N1—C11—N2—N3	0.8 (4)
C4—C3—C2—C1	60.7 (4)	C9—C11—N2—N3	-177.8 (3)
C3—C2—C7—C6	59.1 (5)	C11—N2—N3—C12	-0.8 (4)
C1—C2—C7—C6	-61.6 (5)	N2—N3—C12—N1	0.5 (4)
C5—C6—C7—C2	-58.6 (5)	N2—N3—C12—S1	-179.9 (3)
C10—C6—C7—C2	61.3 (5)	C11—N1—C12—N3	-0.1 (4)

C3—C2—C1—C9	-61.4 (4)	C17—N1—C12—N3	179.3 (3)
C7—C2—C1—C9	59.4 (5)	C11—N1—C12—S1	-179.7 (2)
C11—C9—C1—C2	178.2 (3)	C17—N1—C12—S1	-0.3 (5)
C10—C9—C1—C2	-57.1 (4)	C13—S1—C12—N3	3.1 (4)
C8—C9—C1—C2	59.5 (4)	C13—S1—C12—N1	-177.3 (3)
C3—C4—C8—C9	60.2 (5)	C16—N4—C14—C13	-69.9 (6)
C5—C4—C8—C9	-59.7 (5)	C15—N4—C14—C13	166.4 (5)
C11—C9—C8—C4	179.4 (3)	S1—C13—C14—N4	-58.1 (5)
