organic compounds

rac-3-{4-[(Furan-2-ylmethylidene)-amino]-3-methyl-5-sulfanylidene-4,5-dihydro-1H-1,2,4-triazol-1-yl}-1,3-diphenylpropan-1-one

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In the title molecule, $C_{23}H_{20}N_4O_2S$, the triazole ring forms dihedral angles of 150.3 (2), 77.3 (2) and 77.6 (2)°, respectively, with the furan ring and the phenyl rings. The furan ring is almost perpendicular to the central phenyl ring, making a dihedral angle of 86.0 (3)°.

Related literature

For the crystal structures of related 1,2,4-triazole-5(4H)-thione derivatives, see: Al-Tamimi *et al.* (2010); Fun *et al.* (2009); Gao *et al.* (2011); Tan *et al.* (2010); Wang *et al.* (2011); Zhao *et al.* (2010).
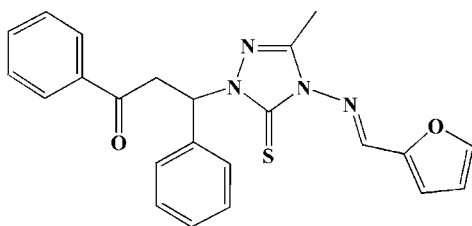
Experimental

Crystal data

$C_{23}H_{20}N_4O_2S$
$M_r = 416.50$
Monoclinic, $P2_1/c$
$a = 8.154$ (3) Å
$b = 21.194$ (6) Å
$c = 12.878$ (4) Å
$\beta = 107.965$ (5)°

$V = 2117.0$ (12) Å³
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.18$ mm^{-1}
$T = 113$ K
$0.24 \times 0.20 \times 0.12$ mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.958$, $T_{max} = 0.979$

26979 measured reflections
5030 independent reflections
4229 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.106$
$S = 1.07$
5030 reflections

272 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2141).

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supporting information

rac-3-{4-[(Furan-2-ylmethylidene)amino]-3-methyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-yl}-1,3-diphenylpropan-1-one

Wei Wang, Yan Gao, Wen-peng Wu, Chao Xu and Qing-lei Liu

S1. Comment

In a continuation of structural studies by our group (Wang *et al.*, 2011) of Mannich base derivatives synthesized by reactions of amino heterocycles and aromatic aldehydes, we present here the crystal structure of the title compound, $C_{23}H_{20}N_4O_2S$.

The bond lengths and angles in this compound are found to have values comparable with those reported in related 1,2,4-triazole- 5(4*H*)-thione derivatives (Al-Tamimi *et al.*, 2010; Fun *et al.* (2009); Tan *et al.* (2010); Wang *et al.*, 2011;). The C1 and C2 atoms in the 1,2,4-triazole ring show distorted C_{sp}^2 hybridization states with bond angles of 102.03 (10)° (N1—C1—N3), 131.01 (9)° (N3—C1—S1), 110.81 (11)° (N2—C2—N3) and 125.29 (12) ° (N2—C2—C23), which are similar to those in other reported triazole derivatives (Zhao *et al.*, 2010; Gao *et al.*, 2011). The 1,2,4-triazole ring forms dihedral angles of 150.3 (2), 77.3 (2) and 77.6 (2)° with the furan ring and the phenyl rings, respectively. The furan ring is almost perpendicular to the C12—C17 phenyl ring, with a dihedral angle of 94.0 (3)°.

S2. Experimental

The title compound was synthesized in the reaction of 2-furfural (2.0 mmol) with 3-(4-amino-3-methyl-5-thioxo-4,5- dihydro-1*H*-1,2,4-triazol-1-yl)-1,3-diphenylpropan-1-one (2.0 mmol), by refluxing in ethanol. The reaction progress was monitored *via* TLC. The resulting precipitate was filtered off, washed with cold ethanol, dried and purified to give the target product as a colorless solid in 75% yield. Crystals suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform–ethanol (1:1).

S3. Refinement

Hydrogen atoms were positioned geometrically and refined as riding (C—H = 0.95–1.00 Å) and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.
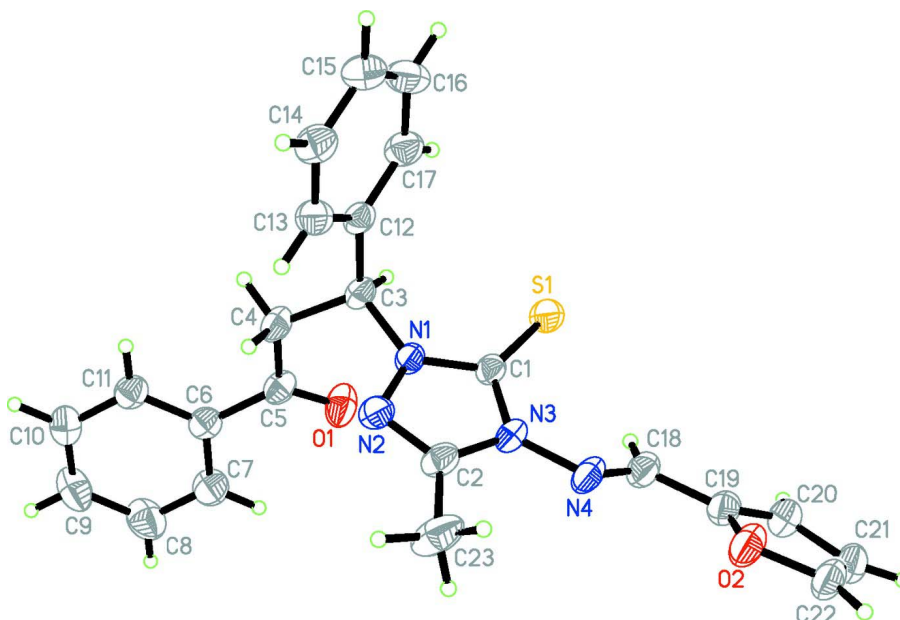
Figure 1

A view of the molecule of the title compound showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 60% probability level.

rac-3-{4-[(Furan-2-ylmethylidene)amino]-3-methyl-5-sulfanylidene- 4,5-dihydro-1*H*-1,2,4-triazol-1-yl}-1,3-diphenylpropan-1-one

Crystal data

$C_{23}H_{20}N_4O_2S$	$F(000) = 872$
$M_r = 416.50$	$D_x = 1.307$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 7435 reflections
$a = 8.154$ (3) Å	$\theta = 1.7$–27.9°
$b = 21.194$ (6) Å	$\mu = 0.18$ mm^{-1}
$c = 12.878$ (4) Å	$T = 113$ K
$\beta = 107.965$ (5)°	Prism, colorless
$V = 2117.0$ (12) Å^3	$0.24 \times 0.20 \times 0.12$ mm
$Z = 4$	

Data collection

Rigaku Saturn CCD area-detector diffractometer	26979 measured reflections
	5030 independent reflections
Radiation source: rotating anode	4229 reflections with $I > 2\sigma(I)$
Multilayer monochromator	$R_{int} = 0.043$
Detector resolution: 14.63 pixels mm^{-1}	$\theta_{max} = 27.9°$, $\theta_{min} = 1.9°$
φ and ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan	$k = -27 \rightarrow 27$
(*CrystalClear*; Rigaku/MSC, 2005)	$l = -16 \rightarrow 16$
$T_{min} = 0.958$, $T_{max} = 0.979$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.040$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.106$	
$S = 1.07$	H-atom parameters constrained
5030 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.0507P]$
272 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.33$ e Å^{-3}
	$\Delta\rho_{min} = -0.18$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	1.09278 (4)	0.678722 (17)	0.64588 (3)	0.03095 (11)
O1	0.74128 (14)	0.76825 (5)	0.75402 (7)	0.0366 (2)
O2	0.80256 (13)	0.49556 (5)	0.33988 (7)	0.0370 (2)
N1	0.89702 (13)	0.64352 (5)	0.77200 (8)	0.0210 (2)
N2	0.76948 (13)	0.60222 (5)	0.77821 (8)	0.0258 (2)
N3	0.82733 (13)	0.59160 (5)	0.62302 (8)	0.0231 (2)
N4	0.81208 (14)	0.55961 (5)	0.52572 (8)	0.0287 (3)
C1	0.93901 (15)	0.63862 (6)	0.67870 (9)	0.0215 (3)
C2	0.73025 (17)	0.57115 (6)	0.68692 (10)	0.0265 (3)
C3	0.98664 (16)	0.68280 (6)	0.86642 (9)	0.0231 (3)
H3	1.0421	0.7187	0.8396	0.028*
C4	0.85808 (17)	0.71013 (6)	0.91857 (10)	0.0272 (3)
H4A	0.7942	0.6751	0.9394	0.033*
H4B	0.9219	0.7329	0.9861	0.033*
C5	0.73023 (17)	0.75493 (6)	0.84367 (10)	0.0265 (3)
C6	0.59252 (16)	0.78340 (6)	0.88329 (10)	0.0254 (3)
C7	0.45618 (19)	0.81411 (6)	0.80761 (12)	0.0339 (3)
H7	0.4509	0.8154	0.7329	0.041*
C8	0.3287 (2)	0.84270 (7)	0.84094 (13)	0.0431 (4)
H8	0.2349	0.8630	0.7889	0.052*
C9	0.3374 (2)	0.84195 (7)	0.95004 (13)	0.0414 (4)
H9	0.2509	0.8625	0.9729	0.050*
C10	0.47170 (19)	0.81126 (6)	1.02590 (12)	0.0327 (3)
H10	0.4766	0.8104	1.1005	0.039*
C11	0.59897 (17)	0.78178 (6)	0.99299 (10)	0.0275 (3)

H11	0.6907	0.7605	1.0450	0.033*
C12	1.12820 (16)	0.64429 (6)	0.94503 (9)	0.0234 (3)
C13	1.08906 (17)	0.59523 (6)	1.00540 (10)	0.0288 (3)
H13	0.9722	0.5870	1.0001	0.035*
C14	1.21854 (18)	0.55835 (7)	1.07314 (11)	0.0325 (3)
H14	1.1904	0.5249	1.1137	0.039*
C15	1.38920 (18)	0.57036 (7)	1.08172 (11)	0.0373 (3)
H15	1.4783	0.5452	1.1281	0.045*
C16	1.42945 (18)	0.61911 (7)	1.02258 (12)	0.0401 (4)
H16	1.5466	0.6274	1.0287	0.048*
C17	1.30023 (17)	0.65601 (7)	0.95437 (11)	0.0314 (3)
H17	1.3291	0.6894	0.9139	0.038*
C18	0.86294 (17)	0.58860 (7)	0.45364 (10)	0.0296 (3)
H18	0.9078	0.6302	0.4672	0.036*
C19	0.85153 (17)	0.55772 (7)	0.35217 (10)	0.0309 (3)
C20	0.87864 (18)	0.57953 (8)	0.26002 (11)	0.0385 (3)
H20	0.9137	0.6209	0.2477	0.046*
C21	0.84408 (19)	0.52813 (8)	0.18528 (12)	0.0420 (4)
H21	0.8514	0.5284	0.1131	0.050*
C22	0.79925 (19)	0.47929 (8)	0.23657 (11)	0.0410 (4)
H22	0.7691	0.4387	0.2053	0.049*
C23	0.5960 (2)	0.52161 (7)	0.65264 (11)	0.0430 (4)
H23A	0.5505	0.5122	0.7130	0.064*
H23B	0.6465	0.4833	0.6326	0.064*
H23C	0.5023	0.5366	0.5896	0.064*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02698 (19)	0.0442 (2)	0.02233 (18)	−0.00676 (14)	0.00865 (14)	0.00319 (14)
O1	0.0485 (6)	0.0389 (5)	0.0253 (5)	0.0118 (5)	0.0157 (5)	0.0049 (4)
O2	0.0429 (6)	0.0387 (5)	0.0242 (5)	0.0133 (5)	0.0029 (4)	−0.0078 (4)
N1	0.0226 (5)	0.0225 (5)	0.0178 (5)	−0.0028 (4)	0.0064 (4)	−0.0018 (4)
N2	0.0259 (6)	0.0297 (6)	0.0211 (5)	−0.0072 (4)	0.0063 (4)	0.0013 (4)
N3	0.0281 (6)	0.0235 (5)	0.0160 (5)	−0.0001 (4)	0.0043 (4)	−0.0017 (4)
N4	0.0341 (6)	0.0309 (6)	0.0172 (5)	0.0061 (5)	0.0023 (4)	−0.0055 (4)
C1	0.0229 (6)	0.0241 (6)	0.0166 (6)	0.0029 (5)	0.0046 (5)	0.0011 (5)
C2	0.0301 (7)	0.0274 (6)	0.0192 (6)	−0.0050 (5)	0.0035 (5)	0.0027 (5)
C3	0.0271 (7)	0.0229 (6)	0.0183 (6)	−0.0037 (5)	0.0055 (5)	−0.0036 (5)
C4	0.0339 (7)	0.0273 (7)	0.0195 (6)	0.0040 (6)	0.0069 (5)	−0.0033 (5)
C5	0.0323 (7)	0.0236 (6)	0.0222 (6)	−0.0004 (5)	0.0063 (5)	−0.0041 (5)
C6	0.0275 (7)	0.0218 (6)	0.0263 (6)	−0.0025 (5)	0.0074 (5)	−0.0016 (5)
C7	0.0347 (8)	0.0358 (7)	0.0308 (7)	0.0035 (6)	0.0097 (6)	0.0065 (6)
C8	0.0360 (8)	0.0490 (9)	0.0460 (9)	0.0126 (7)	0.0153 (7)	0.0151 (7)
C9	0.0392 (9)	0.0420 (8)	0.0509 (9)	0.0085 (7)	0.0255 (8)	0.0075 (7)
C10	0.0379 (8)	0.0320 (7)	0.0327 (7)	−0.0012 (6)	0.0175 (6)	−0.0010 (6)
C11	0.0304 (7)	0.0251 (6)	0.0263 (6)	−0.0038 (5)	0.0078 (5)	−0.0023 (5)
C12	0.0257 (6)	0.0235 (6)	0.0197 (6)	−0.0018 (5)	0.0051 (5)	−0.0053 (5)

C13	0.0259 (7)	0.0316 (7)	0.0276 (7)	−0.0014 (5)	0.0064 (5)	0.0006 (5)
C14	0.0349 (8)	0.0333 (7)	0.0270 (7)	0.0004 (6)	0.0059 (6)	0.0043 (6)
C15	0.0300 (7)	0.0457 (8)	0.0307 (7)	0.0070 (6)	0.0013 (6)	0.0049 (6)
C16	0.0231 (7)	0.0558 (10)	0.0374 (8)	−0.0030 (7)	0.0035 (6)	0.0030 (7)
C17	0.0293 (7)	0.0355 (7)	0.0268 (7)	−0.0071 (6)	0.0052 (6)	−0.0001 (6)
C18	0.0312 (7)	0.0346 (7)	0.0203 (6)	0.0082 (6)	0.0038 (5)	−0.0023 (5)
C19	0.0271 (7)	0.0390 (7)	0.0233 (6)	0.0104 (6)	0.0026 (5)	−0.0044 (6)
C20	0.0343 (8)	0.0556 (9)	0.0252 (7)	0.0017 (7)	0.0086 (6)	−0.0073 (6)
C21	0.0342 (8)	0.0678 (11)	0.0231 (7)	0.0116 (8)	0.0073 (6)	−0.0102 (7)
C22	0.0372 (8)	0.0515 (9)	0.0266 (7)	0.0192 (7)	−0.0012 (6)	−0.0157 (7)
C23	0.0523 (10)	0.0433 (9)	0.0259 (7)	−0.0241 (7)	0.0012 (7)	0.0018 (6)

Geometric parameters (Å, º)

S1—C1	1.6734 (13)	C9—H9	0.9500
O1—C5	1.2185 (15)	C10—C11	1.3851 (19)
O2—C22	1.3666 (16)	C10—H10	0.9500
O2—C19	1.3715 (18)	C11—H11	0.9500
N1—C1	1.3511 (15)	C12—C17	1.3927 (18)
N1—N2	1.3803 (14)	C12—C13	1.3930 (18)
N1—C3	1.4688 (15)	C13—C14	1.3852 (19)
N2—C2	1.2984 (16)	C13—H13	0.9500
N3—C2	1.3760 (16)	C14—C15	1.385 (2)
N3—C1	1.3906 (15)	C14—H14	0.9500
N3—N4	1.3961 (14)	C15—C16	1.382 (2)
N4—C18	1.2840 (17)	C15—H15	0.9500
C2—C23	1.4823 (18)	C16—C17	1.387 (2)
C3—C12	1.5174 (17)	C16—H16	0.9500
C3—C4	1.5232 (17)	C17—H17	0.9500
C3—H3	1.0000	C18—C19	1.4386 (18)
C4—C5	1.5160 (18)	C18—H18	0.9500
C4—H4A	0.9900	C19—C20	1.354 (2)
C4—H4B	0.9900	C20—C21	1.423 (2)
C5—C6	1.4961 (18)	C20—H20	0.9500
C6—C7	1.3932 (19)	C21—C22	1.338 (2)
C6—C11	1.3978 (17)	C21—H21	0.9500
C7—C8	1.381 (2)	C22—H22	0.9500
C7—H7	0.9500	C23—H23A	0.9800
C8—C9	1.385 (2)	C23—H23B	0.9800
C8—H8	0.9500	C23—H23C	0.9800
C9—C10	1.385 (2)		
C22—O2—C19	105.81 (11)	C11—C10—H10	120.0
C1—N1—N2	113.88 (10)	C10—C11—C6	120.00 (13)
C1—N1—C3	125.58 (10)	C10—C11—H11	120.0
N2—N1—C3	120.19 (9)	C6—C11—H11	120.0
C2—N2—N1	104.40 (10)	C17—C12—C13	118.88 (12)
C2—N3—C1	108.86 (10)	C17—C12—C3	120.02 (11)

C2—N3—N4	118.39 (10)	C13—C12—C3	121.05 (11)
C1—N3—N4	132.36 (10)	C14—C13—C12	120.76 (13)
C18—N4—N3	117.20 (11)	C14—C13—H13	119.6
N1—C1—N3	102.03 (10)	C12—C13—H13	119.6
N1—C1—S1	126.93 (9)	C15—C14—C13	119.89 (13)
N3—C1—S1	131.01 (9)	C15—C14—H14	120.1
N2—C2—N3	110.81 (11)	C13—C14—H14	120.1
N2—C2—C23	125.59 (12)	C16—C15—C14	119.81 (13)
N3—C2—C23	123.58 (11)	C16—C15—H15	120.1
N1—C3—C12	109.22 (9)	C14—C15—H15	120.1
N1—C3—C4	110.25 (10)	C15—C16—C17	120.51 (13)
C12—C3—C4	113.31 (10)	C15—C16—H16	119.7
N1—C3—H3	108.0	C17—C16—H16	119.7
C12—C3—H3	108.0	C16—C17—C12	120.16 (13)
C4—C3—H3	108.0	C16—C17—H17	119.9
C5—C4—C3	112.91 (10)	C12—C17—H17	119.9
C5—C4—H4A	109.0	N4—C18—C19	119.61 (13)
C3—C4—H4A	109.0	N4—C18—H18	120.2
C5—C4—H4B	109.0	C19—C18—H18	120.2
C3—C4—H4B	109.0	C20—C19—O2	110.32 (12)
H4A—C4—H4B	107.8	C20—C19—C18	131.19 (14)
O1—C5—C6	120.81 (12)	O2—C19—C18	118.48 (12)
O1—C5—C4	120.71 (12)	C19—C20—C21	106.23 (14)
C6—C5—C4	118.47 (11)	C19—C20—H20	126.9
C7—C6—C11	119.45 (12)	C21—C20—H20	126.9
C7—C6—C5	118.08 (11)	C22—C21—C20	106.60 (13)
C11—C6—C5	122.44 (12)	C22—C21—H21	126.7
C8—C7—C6	120.15 (13)	C20—C21—H21	126.7
C8—C7—H7	119.9	C21—C22—O2	111.03 (13)
C6—C7—H7	119.9	C21—C22—H22	124.5
C7—C8—C9	120.18 (14)	O2—C22—H22	124.5
C7—C8—H8	119.9	C2—C23—H23A	109.5
C9—C8—H8	119.9	C2—C23—H23B	109.5
C10—C9—C8	120.17 (13)	H23A—C23—H23B	109.5
C10—C9—H9	119.9	C2—C23—H23C	109.5
C8—C9—H9	119.9	H23A—C23—H23C	109.5
C9—C10—C11	120.03 (13)	H23B—C23—H23C	109.5
C9—C10—H10	120.0		
C1—N1—N2—C2	−0.35 (13)	C11—C6—C7—C8	0.0 (2)
C3—N1—N2—C2	−173.97 (11)	C5—C6—C7—C8	−178.09 (13)
C2—N3—N4—C18	160.90 (12)	C6—C7—C8—C9	1.1 (2)
C1—N3—N4—C18	−27.24 (19)	C7—C8—C9—C10	−1.5 (2)
N2—N1—C1—N3	0.93 (13)	C8—C9—C10—C11	0.7 (2)
C3—N1—C1—N3	174.15 (10)	C9—C10—C11—C6	0.5 (2)
N2—N1—C1—S1	−177.18 (9)	C7—C6—C11—C10	−0.84 (19)
C3—N1—C1—S1	−3.96 (17)	C5—C6—C11—C10	177.21 (12)
C2—N3—C1—N1	−1.14 (13)	N1—C3—C12—C17	106.97 (13)

N4—N3—C1—N1	−173.59 (11)	C4—C3—C12—C17	−129.70 (12)
C2—N3—C1—S1	176.86 (10)	N1—C3—C12—C13	−70.35 (14)
N4—N3—C1—S1	4.4 (2)	C4—C3—C12—C13	52.98 (15)
N1—N2—C2—N3	−0.43 (14)	C17—C12—C13—C14	−0.41 (18)
N1—N2—C2—C23	−178.64 (13)	C3—C12—C13—C14	176.94 (11)
C1—N3—C2—N2	1.04 (15)	C12—C13—C14—C15	0.3 (2)
N4—N3—C2—N2	174.70 (10)	C13—C14—C15—C16	0.0 (2)
C1—N3—C2—C23	179.29 (12)	C14—C15—C16—C17	−0.2 (2)
N4—N3—C2—C23	−7.05 (18)	C15—C16—C17—C12	0.1 (2)
C1—N1—C3—C12	−90.83 (13)	C13—C12—C17—C16	0.19 (19)
N2—N1—C3—C12	81.99 (13)	C3—C12—C17—C16	−177.19 (12)
C1—N1—C3—C4	144.04 (11)	N3—N4—C18—C19	179.51 (11)
N2—N1—C3—C4	−43.14 (14)	C22—O2—C19—C20	−0.25 (15)
N1—C3—C4—C5	−64.25 (13)	C22—O2—C19—C18	178.72 (11)
C12—C3—C4—C5	172.98 (10)	N4—C18—C19—C20	172.22 (14)
C3—C4—C5—O1	−3.40 (17)	N4—C18—C19—O2	−6.51 (19)
C3—C4—C5—C6	177.83 (11)	O2—C19—C20—C21	0.22 (16)
O1—C5—C6—C7	13.79 (19)	C18—C19—C20—C21	−178.59 (14)
C4—C5—C6—C7	−167.44 (12)	C19—C20—C21—C22	−0.10 (16)
O1—C5—C6—C11	−164.29 (12)	C20—C21—C22—O2	−0.06 (17)
C4—C5—C6—C11	14.49 (18)	C19—O2—C22—C21	0.19 (15)