Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

S-2-(Adamant-1-yl)-4-methylphenyl *N*,*N*-dimethylthiocarbamate

Raúl Huerta, Ivan Castillo* and Simón Hernández-Ortega

Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, CU, México, DF 04510, Mexico
Correspondence e-mail: joseivan@servidor.unam.mx

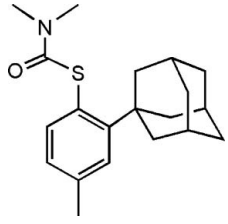
Received 18 October 2007; accepted 12 December 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.120; data-to-parameter ratio = 14.9.

The title compound, $C_{20}H_{27}NOS$, was obtained from the corresponding *O*-thiocarbamate. The structure features a C=O bond distance of 1.209 (2) Å and an sp^3-hybridized S atom [C—S—C = 101.66 (1)°]. The steric bulk of the 1-adamantyl substituent on the 2-position of the aromatic ring is reflected in the S—C—C—C torsion angle [−7.5 (3)°].

Related literature

For related literature, see: Bennett *et al.* (1999); Allen (2002); Bruno *et al.* (2002); Flores-Figueroa *et al.* (2005); Higgs & Carrano (2002); Newman & Karnes (1966).



Experimental

Crystal data

$C_{20}H_{27}NOS$
M_r = 329.49
Triclinic, $P\overline{1}$
a = 6.6161 (7) Å
b = 11.2113 (12) Å
c = 13.2231 (14) Å
α = 101.287 (2)°
β = 103.753 (2)°
γ = 103.025 (2)°
V = 895.40 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 298 (2) K
0.40 × 0.18 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
7346 measured reflections
3147 independent reflections
2231 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.120
S = 0.94
3147 reflections
211 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT-Plus* (Bruker, 1997); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

IC and RH thank DGAPA–UNAM for financial support (PAPIIT IN216806).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2030).

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bennett, S. M. W., Brown, S. M., Conole, G., Dennis, M. R., Fraser, P. K., Radojevic, S., McPartlin, M., Topping, C. M. & Woodward, W. (1999). *J. Chem. Soc. Perkin Trans. 1*, pp. 3127–3132.
Bruker (1997). *SMART* (Version 5.625) and *SAINT-Plus* (Version 7.01A). Bruker AXS Inc., Madison, Wisconsin, USA.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Flores-Figueroa, A., Arista-M, V., Talancón-Sánchez, D. & Castillo, I. (2005). *J. Braz. Chem. Soc.* **16**, 397–403.
Higgs, T. C. & Carrano, C. J. (2002). *Eur. J. Org. Chem.* pp. 3632–3645.
Newman, M. S. & Karnes, H. A. (1966). *J. Org. Chem.* **31**, 3980–3984.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 6.10. University of Göttingen, Germany.

 doi:10.1107/S1600536807066603

supporting information

Acta Cryst. (2008). E**64**, o323 [https://doi.org/10.1107/S1600536807066603]

S-2-(Adamant-1-yl)-4-methylphenyl *N*,*N*-dimethylthiocarbamate

Raúl Huerta, Ivan Castillo and Simón Hernández-Ortega

S1. Comment

Newman–Kwart thermal rearrangement of *O*-thiocarbamates to the corresponding *S*-thiocarbamates is a widely used reaction for the preparation of benzenethiols (Newman & Karnes, 1966). The presence of bulky substituents on the 2-position of phenols represents a synthetic challenge in this methodology, and the experimental difficulties have been attributed by our group to the steric congestion around the thiocarbamate moiety (Flores-Figueroa *et al.*, 2005). We herein report the preparation (see Experimental and Scheme) of the title compound *S*-2-adamant-1-yl-4- methylphenyl *N*,*N*-dimethylthiocarbamate (I).

Compound (I) crystallizes in the triclinic space group P-1 by slow evaporation of a concentrated 2-propanol solution. A search of the Cambridge Crystallographic Database (Version 5.19; Allen, 2002) using *CONQUEST*, Version 1.4; Bruno *et al.*, 2002) revealed that (I) represents one of the very few examples of aromatic *S*-thiocarbamates with sterically demanding substituents adjacent to the S atom. Its structure, which is depicted with atom numbering scheme in Fig. 1, features a C=O bond length of 1.209 (2) Å, and C—S 1.780 (3) Å (Table 1). The bond lengths and angles of the thiocarbamate group of (I) are comparable to those of related compounds (Higgs & Carrano, 2002, Bennett *et al.*, 1999). The steric congestion around the *S*-thiocarbamate group is reflected in the torsion angle of -7.5 (3)° between the S—C(aromatic) and the adjacent C(aromatic)- C(*ortho*subsituent) bond (S—C1—C2—C10).

Molecules of (I) pack in chains on the 100 plane, as shown in Fig. 2. These chains are formed by intermolecular C—H···O interactions between the O atom of one molecule and C8—H8B on an adjacent molecule, with C8···O and H8B···O distances of 3.294 (3) and 2.534 (2) Å, respectively. The C and H atoms are located on one of the NMe_2 groups of a the *S*-thiocarbamate moiety, and the corresponding C—H···O angle is 136.1 (2)°.

S2. Experimental

O-2-adamant-1-yl-4-methylphenyl *N*,*N*-dimethylthiocarbamate (0.26 g, 0.80 mmol) was heated to 593–603 K for 2 h in a round bottom flask equipped with a teflon stopcock. After cooling to room temperature, the material was disolved in dichloromethane, filtered, and evaporated to dryness (30 ml). The solid obtained was disolved in hot 2-propanol, and upon cooling starting material precipitated. After filtering, the mother liquor yielded yellow crystals of (I) by slow evaporation of the solvent. Yield: 0.06 g (23%); m.p. 407–408 K; IR ($CHCl_3$) 3011, 2903, 2852, 1710, 1655, 1598, 1451, 1406, 1365, 1261, 1170, 1100, 1066, 1029, 910 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, TMS internal reference) δ 7.24 (1*H*, d, ArH), 7.13 (1*H*, d, ArH), 6.94 (1*H*, dd, ArH), 3.02 (6*H*, s, NMe), 2.28 (3*H*, s, ArMe), 2.12 (6*H*, s, AdH), 2.02 (3*H*, s, AdH), 1.69 (6*H*, s, AdH); EI mass spectrum: m/*z* 329 (M^+, 18%).

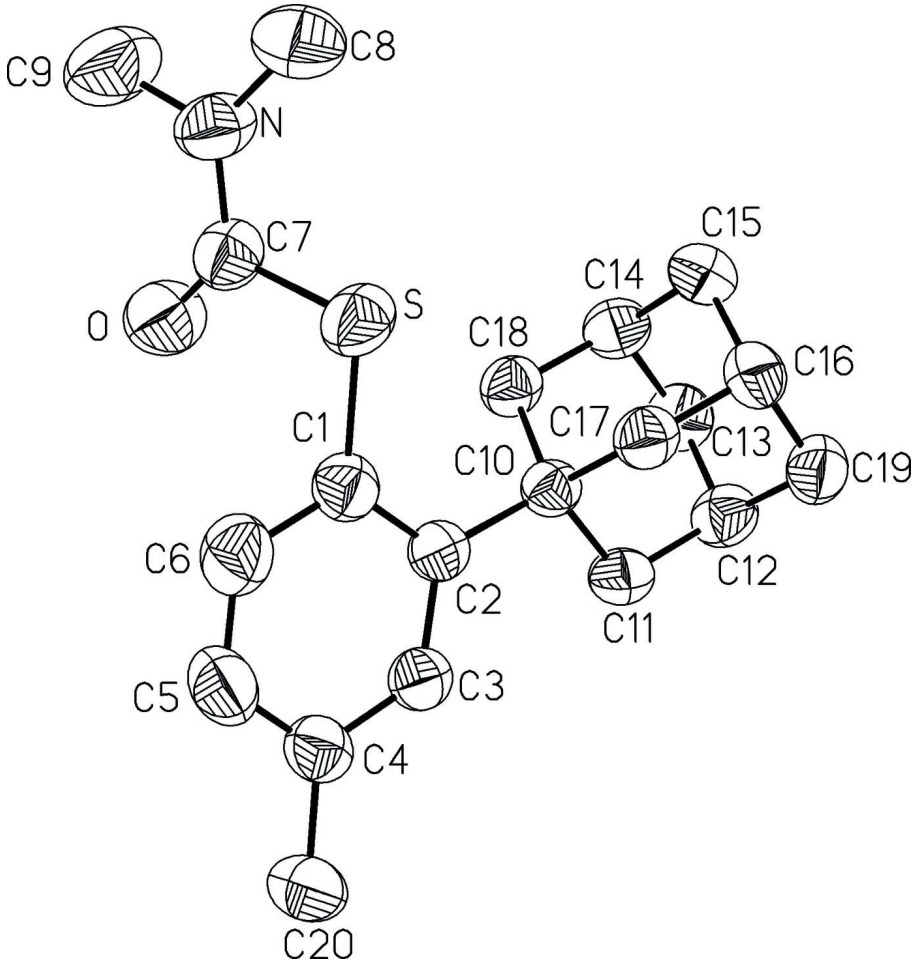


Figure 1

Molecular structure of (I) with atom numbering scheme. Thermal ellipsoids are shown at the 50% probability level.

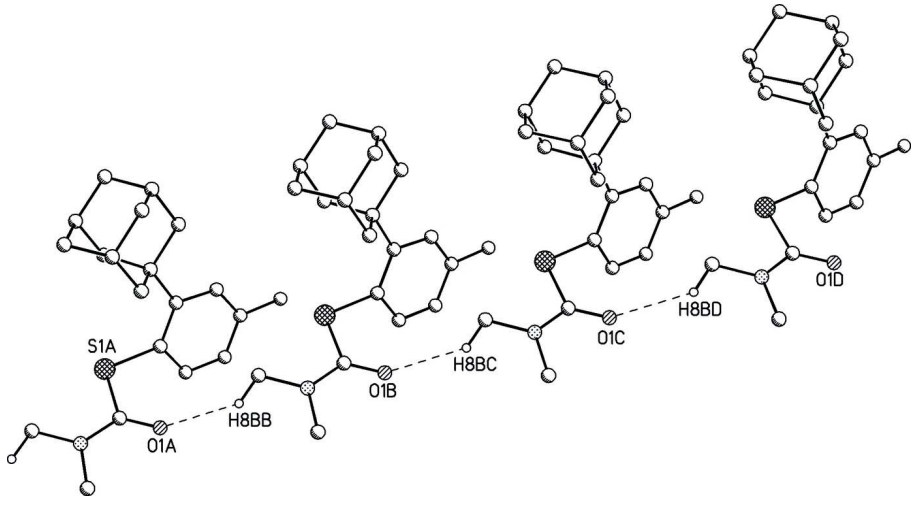


Figure 2

View of the chains of (I) along the 001 axis.

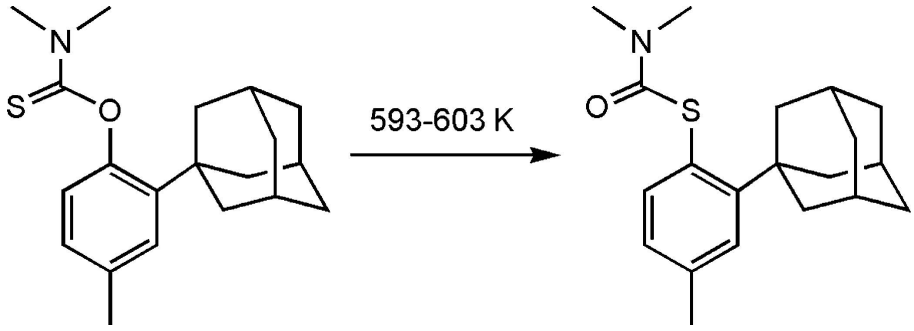


Figure 3

The formation of the title compound.

S-2-(Adamant-1-yl)-4-methylphenyl *N*,*N*-dimethylthiocarbamate

Crystal data

$C_{20}H_{27}NOS$
$M_r = 329.49$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.6161\ (7)$ Å
$b = 11.2113\ (12)$ Å
$c = 13.2231\ (14)$ Å
$\alpha = 101.287\ (2)°$
$\beta = 103.753\ (2)°$
$\gamma = 103.025\ (2)°$
$V = 895.40\ (16)$ Å^3
$Z = 2$
$F(000) = 356$
$D_x = 1.222$ Mg m^{-3}
D_m = No Mg m^{-3}
D_m measured by ?
Melting point = 407–408 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3272 reflections
$\theta = 2.8–25.3°$
$\mu = 0.19$ mm^{-1}
$T = 298$ K
Prism, pale yellow
0.40 × 0.18 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0.83 pixels mm^{-1}
ω scans
7346 measured reflections
3147 independent reflections
2231 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$h = -7\rightarrow7$
$k = -13\rightarrow13$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.120$
$S = 0.94$
3147 reflections
211 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
$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ 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. Hydrogen atoms were placed in idealized positions, and the isotropic thermal parameters were assigned the values U_{iso} = 1.2 times the thermal parameter of the parent atom.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S	1.02047 (9)	0.84253 (6)	0.64328 (4)	0.0637 (2)
O	0.6891 (3)	0.73897 (17)	0.46508 (13)	0.0809 (5)
N	0.9990 (3)	0.68642 (18)	0.46352 (15)	0.0678 (5)
C1	0.8226 (3)	0.91300 (19)	0.67862 (16)	0.0523 (5)
C2	0.7344 (3)	0.89238 (17)	0.76267 (15)	0.0445 (5)
C3	0.6039 (3)	0.96867 (18)	0.78793 (15)	0.0491 (5)
H3	0.5447	0.9581	0.8439	0.059*
C4	0.5563 (3)	1.05877 (19)	0.73570 (17)	0.0558 (5)
C5	0.6397 (4)	1.0725 (2)	0.65162 (19)	0.0686 (6)
H5	0.6055	1.1298	0.6129	0.082*
C6	0.7731 (4)	1.0025 (2)	0.62444 (18)	0.0677 (6)
H6	0.8319	1.0149	0.5687	0.081*
C7	0.8757 (3)	0.7468 (2)	0.50903 (17)	0.0569 (5)
C8	1.2191 (4)	0.6925 (3)	0.5174 (2)	0.0866 (8)
H8A	1.2896	0.7743	0.5677	0.130*
H8B	1.2961	0.6794	0.4650	0.130*
H8C	1.2184	0.6278	0.5554	0.130*
C9	0.9060 (5)	0.6114 (3)	0.3519 (2)	0.0997 (9)
H9A	0.7529	0.6018	0.3295	0.150*
H9B	0.9300	0.5293	0.3457	0.150*
H9C	0.9739	0.6535	0.3068	0.150*
C10	0.7760 (3)	0.79486 (17)	0.82641 (14)	0.0432 (4)
C11	0.6436 (3)	0.78732 (18)	0.90815 (16)	0.0500 (5)
H11A	0.6802	0.8704	0.9578	0.060*
H11B	0.4900	0.7630	0.8697	0.060*
C12	0.6891 (3)	0.69145 (19)	0.97190 (17)	0.0573 (5)
H12	0.6023	0.6892	1.0225	0.069*
C13	0.6294 (4)	0.56006 (19)	0.89568 (18)	0.0620 (6)
H13A	0.4754	0.5325	0.8575	0.074*
H13B	0.6611	0.4999	0.9364	0.074*
C14	0.7607 (3)	0.56505 (19)	0.81512 (16)	0.0577 (6)
H14	0.7225	0.4807	0.7653	0.069*
C15	1.0029 (4)	0.6065 (2)	0.87625 (18)	0.0619 (6)
H15A	1.0364	0.5449	0.9149	0.074*

H15B	1.0871	0.6105	0.8255	0.074*
C16	1.0633 (3)	0.73657 (19)	0.95584 (16)	0.0551 (5)
H16	1.2181	0.7617	0.9956	0.066*
C17	1.0176 (3)	0.83282 (18)	0.89292 (15)	0.0488 (5)
H17A	1.1075	0.8383	0.8448	0.059*
H17B	1.0553	0.9158	0.9429	0.059*
C18	0.7109 (3)	0.65985 (18)	0.75146 (15)	0.0511 (5)
H18A	0.5569	0.6344	0.7136	0.061*
H18B	0.7894	0.6596	0.6981	0.061*
C19	0.9301 (4)	0.7322 (2)	1.03520 (16)	0.0609 (6)
H19A	0.9680	0.8153	1.0851	0.073*
H19B	0.9606	0.6724	1.0765	0.073*
C20	0.4196 (4)	1.1399 (2)	0.7697 (2)	0.0765 (7)
H20A	0.5108	1.2241	0.8080	0.115*
H20B	0.3458	1.1042	0.8159	0.115*
H20C	0.3148	1.1434	0.7070	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0487 (3)	0.0885 (5)	0.0537 (4)	0.0209 (3)	0.0188 (3)	0.0120 (3)
O	0.0518 (10)	0.1095 (14)	0.0698 (10)	0.0296 (9)	0.0059 (8)	0.0049 (9)
N	0.0541 (11)	0.0814 (13)	0.0627 (12)	0.0224 (9)	0.0183 (10)	0.0021 (10)
C1	0.0471 (12)	0.0579 (13)	0.0518 (12)	0.0150 (10)	0.0138 (10)	0.0152 (10)
C2	0.0359 (10)	0.0484 (11)	0.0438 (10)	0.0103 (8)	0.0082 (8)	0.0066 (9)
C3	0.0452 (11)	0.0514 (12)	0.0477 (11)	0.0136 (9)	0.0118 (9)	0.0092 (9)
C4	0.0535 (12)	0.0515 (13)	0.0551 (13)	0.0165 (10)	0.0059 (10)	0.0085 (10)
C5	0.0780 (16)	0.0654 (15)	0.0669 (15)	0.0287 (13)	0.0137 (13)	0.0276 (12)
C6	0.0729 (15)	0.0761 (16)	0.0634 (14)	0.0218 (13)	0.0281 (12)	0.0290 (13)
C7	0.0478 (13)	0.0665 (14)	0.0544 (13)	0.0119 (10)	0.0168 (11)	0.0141 (11)
C8	0.0637 (16)	0.113 (2)	0.097 (2)	0.0411 (15)	0.0336 (15)	0.0275 (17)
C9	0.098 (2)	0.109 (2)	0.0790 (18)	0.0339 (17)	0.0264 (16)	−0.0097 (16)
C10	0.0382 (10)	0.0461 (11)	0.0444 (10)	0.0123 (8)	0.0124 (8)	0.0092 (9)
C11	0.0463 (11)	0.0502 (12)	0.0549 (12)	0.0156 (9)	0.0189 (10)	0.0101 (10)
C12	0.0628 (14)	0.0587 (13)	0.0575 (13)	0.0175 (10)	0.0284 (11)	0.0181 (11)
C13	0.0646 (14)	0.0538 (13)	0.0668 (14)	0.0121 (11)	0.0201 (12)	0.0187 (11)
C14	0.0672 (14)	0.0426 (12)	0.0574 (13)	0.0161 (10)	0.0153 (11)	0.0034 (10)
C15	0.0680 (14)	0.0621 (14)	0.0652 (14)	0.0336 (11)	0.0209 (12)	0.0197 (11)
C16	0.0473 (11)	0.0620 (13)	0.0521 (12)	0.0191 (10)	0.0061 (10)	0.0128 (10)
C17	0.0427 (11)	0.0510 (12)	0.0471 (11)	0.0115 (9)	0.0111 (9)	0.0052 (9)
C18	0.0463 (11)	0.0534 (12)	0.0470 (11)	0.0118 (9)	0.0104 (9)	0.0052 (9)
C19	0.0755 (15)	0.0596 (14)	0.0483 (12)	0.0231 (11)	0.0146 (11)	0.0159 (10)
C20	0.0871 (17)	0.0680 (16)	0.0764 (16)	0.0414 (13)	0.0149 (14)	0.0122 (13)

Geometric parameters (Å, º)

S—C1	1.780 (2)	C11—H11A	0.9700
S—C7	1.790 (2)	C11—H11B	0.9700

O—C7	1.209 (2)	C12—C13	1.520 (3)
N—C7	1.345 (3)	C12—C19	1.530 (3)
N—C8	1.441 (3)	C12—H12	0.9800
N—C9	1.454 (3)	C13—C14	1.527 (3)
C1—C6	1.395 (3)	C13—H13A	0.9700
C1—C2	1.406 (3)	C13—H13B	0.9700
C2—C3	1.395 (3)	C14—C18	1.524 (3)
C2—C10	1.539 (3)	C14—C15	1.529 (3)
C3—C4	1.382 (3)	C14—H14	0.9800
C3—H3	0.9300	C15—C16	1.527 (3)
C4—C5	1.373 (3)	C15—H15A	0.9700
C4—C20	1.500 (3)	C15—H15B	0.9700
C5—C6	1.370 (3)	C16—C19	1.523 (3)
C5—H5	0.9300	C16—C17	1.525 (3)
C6—H6	0.9300	C16—H16	0.9800
C8—H8A	0.9600	C17—H17A	0.9700
C8—H8B	0.9600	C17—H17B	0.9700
C8—H8C	0.9600	C18—H18A	0.9700
C9—H9A	0.9600	C18—H18B	0.9700
C9—H9B	0.9600	C19—H19A	0.9700
C9—H9C	0.9600	C19—H19B	0.9700
C10—C18	1.541 (3)	C20—H20A	0.9600
C10—C17	1.545 (2)	C20—H20B	0.9600
C10—C11	1.548 (2)	C20—H20C	0.9600
C11—C12	1.528 (3)		

C1—S—C7	101.66 (10)	C13—C12—H12	109.2
C7—N—C8	124.42 (19)	C11—C12—H12	109.2
C7—N—C9	118.09 (19)	C19—C12—H12	109.2
C8—N—C9	117.48 (19)	C12—C13—C14	108.95 (17)
C6—C1—C2	120.18 (19)	C12—C13—H13A	109.9
C6—C1—S	115.61 (16)	C14—C13—H13A	109.9
C2—C1—S	123.90 (15)	C12—C13—H13B	109.9
C3—C2—C1	115.62 (18)	C14—C13—H13B	109.9
C3—C2—C10	120.07 (17)	H13A—C13—H13B	108.3
C1—C2—C10	124.31 (16)	C18—C14—C13	109.78 (17)
C4—C3—C2	124.62 (19)	C18—C14—C15	109.31 (17)
C4—C3—H3	117.7	C13—C14—C15	109.31 (17)
C2—C3—H3	117.7	C18—C14—H14	109.5
C5—C4—C3	117.73 (19)	C13—C14—H14	109.5
C5—C4—C20	120.8 (2)	C15—C14—H14	109.5
C3—C4—C20	121.5 (2)	C16—C15—C14	109.94 (16)
C6—C5—C4	120.4 (2)	C16—C15—H15A	109.7
C6—C5—H5	119.8	C14—C15—H15A	109.7
C4—C5—H5	119.8	C16—C15—H15B	109.7
C5—C6—C1	121.3 (2)	C14—C15—H15B	109.7
C5—C6—H6	119.3	H15A—C15—H15B	108.2
C1—C6—H6	119.3	C19—C16—C17	109.52 (17)

O—C7—N	124.6 (2)	C19—C16—C15	110.29 (18)
O—C7—S	123.20 (17)	C17—C16—C15	108.77 (16)
N—C7—S	112.24 (16)	C19—C16—H16	109.4
N—C8—H8A	109.5	C17—C16—H16	109.4
N—C8—H8B	109.5	C15—C16—H16	109.4
H8A—C8—H8B	109.5	C16—C17—C10	111.20 (15)
N—C8—H8C	109.5	C16—C17—H17A	109.4
H8A—C8—H8C	109.5	C10—C17—H17A	109.4
H8B—C8—H8C	109.5	C16—C17—H17B	109.4
N—C9—H9A	109.5	C10—C17—H17B	109.4
N—C9—H9B	109.5	H17A—C17—H17B	108.0
H9A—C9—H9B	109.5	C14—C18—C10	111.19 (16)
N—C9—H9C	109.5	C14—C18—H18A	109.4
H9A—C9—H9C	109.5	C10—C18—H18A	109.4
H9B—C9—H9C	109.5	C14—C18—H18B	109.4
C2—C10—C18	111.72 (15)	C10—C18—H18B	109.4
C2—C10—C17	110.27 (15)	H18A—C18—H18B	108.0
C18—C10—C17	109.83 (14)	C16—C19—C12	108.76 (16)
C2—C10—C11	112.25 (15)	C16—C19—H19A	109.9
C18—C10—C11	106.19 (15)	C12—C19—H19A	109.9
C17—C10—C11	106.37 (15)	C16—C19—H19B	109.9
C12—C11—C10	111.62 (15)	C12—C19—H19B	109.9
C12—C11—H11A	109.3	H19A—C19—H19B	108.3
C10—C11—H11A	109.3	C4—C20—H20A	109.5
C12—C11—H11B	109.3	C4—C20—H20B	109.5
C10—C11—H11B	109.3	H20A—C20—H20B	109.5
H11A—C11—H11B	108.0	C4—C20—H20C	109.5
C13—C12—C11	110.19 (18)	H20A—C20—H20C	109.5
C13—C12—C19	109.73 (17)	H20B—C20—H20C	109.5
C11—C12—C19	109.23 (16)		

C7—S—C1—C6	−69.82 (18)	C2—C10—C11—C12	−179.21 (15)
C7—S—C1—C2	116.52 (17)	C18—C10—C11—C12	58.4 (2)
C6—C1—C2—C3	−1.7 (3)	C17—C10—C11—C12	−58.5 (2)
S—C1—C2—C3	171.68 (14)	C10—C11—C12—C13	−59.9 (2)
C6—C1—C2—C10	179.12 (18)	C10—C11—C12—C19	60.7 (2)
S—C1—C2—C10	−7.5 (3)	C11—C12—C13—C14	58.5 (2)
C1—C2—C3—C4	0.9 (3)	C19—C12—C13—C14	−61.8 (2)
C10—C2—C3—C4	−179.92 (17)	C12—C13—C14—C18	−59.5 (2)
C2—C3—C4—C5	1.3 (3)	C12—C13—C14—C15	60.4 (2)
C2—C3—C4—C20	−178.19 (19)	C18—C14—C15—C16	61.3 (2)
C3—C4—C5—C6	−2.8 (3)	C13—C14—C15—C16	−58.9 (2)
C20—C4—C5—C6	176.8 (2)	C14—C15—C16—C19	58.6 (2)
C4—C5—C6—C1	2.0 (4)	C14—C15—C16—C17	−61.5 (2)
C2—C1—C6—C5	0.4 (3)	C19—C16—C17—C10	−61.6 (2)
S—C1—C6—C5	−173.55 (18)	C15—C16—C17—C10	59.0 (2)
C8—N—C7—O	−177.8 (2)	C2—C10—C17—C16	−179.34 (15)
C9—N—C7—O	3.2 (4)	C18—C10—C17—C16	−55.8 (2)

C8—N—C7—S	2.8 (3)	C11—C10—C17—C16	58.72 (19)
C9—N—C7—S	−176.25 (19)	C13—C14—C18—C10	61.8 (2)
C1—S—C7—O	−1.6 (2)	C15—C14—C18—C10	−58.1 (2)
C1—S—C7—N	177.83 (16)	C2—C10—C18—C14	177.91 (15)
C3—C2—C10—C18	124.16 (18)	C17—C10—C18—C14	55.2 (2)
C1—C2—C10—C18	−56.7 (2)	C11—C10—C18—C14	−59.4 (2)
C3—C2—C10—C17	−113.39 (18)	C17—C16—C19—C12	60.7 (2)
C1—C2—C10—C17	65.7 (2)	C15—C16—C19—C12	−59.0 (2)
C3—C2—C10—C11	5.0 (2)	C13—C12—C19—C16	60.8 (2)
C1—C2—C10—C11	−175.85 (17)	C11—C12—C19—C16	−60.1 (2)