Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Methylthiosemicarbazide

Thomas M. Klapötke* and Stefan M. Sproll

Department of Chemistry and Biochemistry, Ludwig-Maximilian University, Butenandtstrasse 5-13 (Haus D), D-81377 Munich, Germany
Correspondence e-mail: tmk@cup.uni-muenchen.de

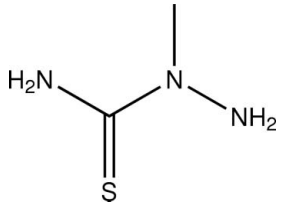
Received 4 September 2007; accepted 2 October 2007

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(N–C) = 0.003 Å; R factor = 0.034; wR factor = 0.079; data-to-parameter ratio = 11.0.

The crystal structure of the title compound, $C_2H_7N_3S$, displays N—H···S and N—H···N hydrogen bonding.

Related literature

The title compound was synthesized according to the method of Stefanic *et al.* (1990).



Experimental

Crystal data

$C_2H_7N_3S$
M_r = 105.17
Monoclinic, $P2_1/n$
a = 8.6071 (9) Å
b = 5.9337 (6) Å
c = 9.7415 (10) Å
β = 98.508 (9)°
V = 492.04 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.50 mm^{-1}
T = 200 (2) K
0.4 × 0.4 × 0.1 mm

Data collection

Oxford Diffraction Xcalibur3 CCD diffractometer
Absorption correction: none
4506 measured reflections
913 independent reflections
900 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.079
S = 1.13
913 reflections
83 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···S1^{i}	0.83 (2)	2.84 (2)	3.4150 (18)	127.6 (17)
N1—H1A···N3	0.83 (2)	2.25 (2)	2.584 (3)	104.5 (17)
N1—H1B···S1^{ii}	0.82 (2)	2.64 (3)	3.4573 (19)	170 (2)
N3—H3A···S1^{iii}	0.85 (3)	2.77 (3)	3.598 (2)	163 (2)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *PLATON* (Spek, 2003), *SHELXL97* and *publCIF* (Westrip, 2007).

The authors thank Dipl.-Chem. Michael Göbel for his valuable advice. Financial support of this work by the University of Munich (LMU), the Fonds der Chemischen Industrie (FCI), the European Research Office (ERO) of the US Army Research Laboratory (ARL) under contract Nos. 62558-05-C-0027 and 9939-AN-01, and the Bundeswehr Research Institute for Materials, Explosives, Fuels and Lubricants (WIWEB) under contract Nos. E/E210/4D004/X5143 and E/E210/7D002/4 F088, is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BV2072).

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  doi:10.1107/S1600536807048398

supplementary materials

Acta Cryst. (2007). E**63**, o4270 [**doi:10.1107/S1600536807048398**]

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Comment

The stucture of the title compound, (I), is shown below. Dimensions are available in the archived CIF.

For related literature, see [type here to add references to related literature].

Refinement

The hydrogen atoms were directly located in the crystallographic study using difference Fourier maps and were refined isotropically.

Figures

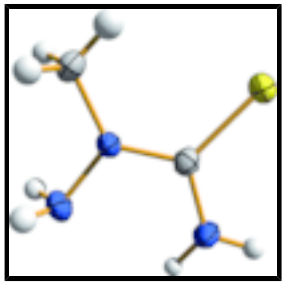

Fig. 1. *DIAMOND* representation of the assymetric unit of 2-methylthiosemicarbazide. The thermal ellipsoids are shown at the 50% probability level.

2-methylthiosemicarbazide

Crystal data

$C_2H_7N_3S$	F_{000} = 224
M_r = 105.17	D_x = 1.420 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 173 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.6071 (9) Å	Cell parameters from 913 reflections
b = 5.9337 (6) Å	μ = 0.50 mm^{-1}
c = 9.7415 (10) Å	T = 200 (2) K
β = 98.508 (9)°	Block, colorless
V = 492.04 (9) Å^3	0.4 × 0.4 × 0.1 mm
Z = 4	

Data collection

Oxford Xcalibur 3CCD diffractometer	900 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.038$
Monochromator: graphite	$\theta_{max} = 25.5°$
$T = 200(2)$ K	$\theta_{min} = 4.5°$
ω scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = -7 \rightarrow 7$
4506 measured reflections	$l = -11 \rightarrow 11$
913 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 0.3245P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} < 0.001$
913 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
83 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
H3B	0.776 (3)	0.157 (4)	1.033 (3)	0.049 (7)*
H1B	0.366 (3)	0.151 (4)	0.798 (2)	0.033 (6)*
H1A	0.504 (2)	0.043 (4)	0.862 (2)	0.025 (5)*
H2B	0.809 (3)	0.572 (4)	1.027 (3)	0.046 (7)*
H2A	0.875 (3)	0.546 (4)	0.885 (2)	0.040 (6)*

H2C	0.732 (3)	0.688 (5)	0.891 (3)	0.057 (8)*
H3A	0.837 (3)	0.130 (4)	0.911 (3)	0.041 (7)*
S1	0.44036 (5)	0.59448 (8)	0.76678 (5)	0.02764 (19)
C1	0.5343 (2)	0.3573 (3)	0.83652 (18)	0.0213 (4)
N2	0.68539 (17)	0.3589 (2)	0.89476 (16)	0.0228 (4)
N3	0.7511 (2)	0.1490 (3)	0.9432 (2)	0.0300 (4)
N1	0.4598 (2)	0.1604 (3)	0.83089 (19)	0.0292 (4)
C2	0.7809 (2)	0.5601 (4)	0.9259 (2)	0.0291 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0213 (3)	0.0227 (3)	0.0375 (3)	0.00257 (18)	−0.00012 (19)	0.00346 (19)
C1	0.0196 (9)	0.0221 (9)	0.0225 (9)	0.0003 (7)	0.0044 (7)	−0.0016 (7)
N2	0.0191 (8)	0.0189 (8)	0.0293 (8)	0.0015 (6)	−0.0005 (6)	0.0016 (6)
N3	0.0254 (9)	0.0276 (9)	0.0359 (10)	0.0059 (7)	0.0012 (7)	0.0062 (7)
N1	0.0204 (9)	0.0208 (9)	0.0452 (10)	−0.0025 (7)	0.0003 (7)	0.0010 (7)
C2	0.0217 (10)	0.0277 (11)	0.0363 (11)	−0.0046 (8)	−0.0004 (8)	0.0009 (9)

Geometric parameters (Å, °)

S1—C1	1.7128 (18)	N3—H3A	0.85 (3)
C1—N1	1.330 (2)	N1—H1B	0.82 (2)
C1—N2	1.340 (2)	N1—H1A	0.83 (2)
N2—N3	1.420 (2)	C2—H2B	0.98 (3)
N2—C2	1.456 (2)	C2—H2A	0.95 (2)
N3—H3B	0.87 (3)	C2—H2C	0.91 (3)
N1—C1—N2	117.09 (16)	C1—N1—H1B	120.8 (16)
N1—C1—S1	120.63 (14)	C1—N1—H1A	122.2 (15)
N2—C1—S1	122.25 (13)	H1B—N1—H1A	117 (2)
C1—N2—N3	116.65 (15)	N2—C2—H2B	108.5 (14)
C1—N2—C2	125.24 (15)	N2—C2—H2A	109.2 (15)
N3—N2—C2	117.73 (14)	H2B—C2—H2A	109 (2)
N2—N3—H3B	108.3 (17)	N2—C2—H2C	112.9 (17)
N2—N3—H3A	108.5 (16)	H2B—C2—H2C	110 (2)
H3B—N3—H3A	106 (2)	H2A—C2—H2C	107 (2)
N1—C1—N2—N3	0.7 (2)	N1—C1—N2—C2	−172.04 (18)
S1—C1—N2—N3	−177.29 (13)	S1—C1—N2—C2	10.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···S1^{i}	0.83 (2)	2.84 (2)	3.4150 (18)	127.6 (17)
N1—H1A···N3	0.83 (2)	2.25 (2)	2.584 (3)	104.5 (17)
N1—H1B···S1^{ii}	0.82 (2)	2.64 (3)	3.4573 (19)	170 (2)
N3—H3A···S1^{iii}	0.85 (3)	2.77 (3)	3.598 (2)	163 (2)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1/2, *y*−1/2, −*z*+3/2; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2.

Fig. 1