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2,7-Dimethyl-1,3-thiazolo[4,5-*d*]-pyridazin-4(5*H*)-one

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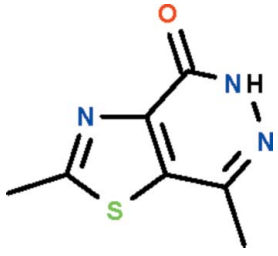
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.080; data-to-parameter ratio = 13.4.

The nine-membered fused-ring system of the title pyridazine derivative, $C_7H_7N_3OS$, is almost planar (r.m.s. deviation 0.012 Å). In the crystal, the amino H atom forms a hydrogen bond to the ketonic O atom of a neighboring molecule to generate a centrosymmetric dimer.

Related literature

For a related structure, see: Abdel-Aziz *et al.* (2010). For the biological activity of the class of pyridazines, see: Faid-Allah *et al.* (2011); Makki & Faid-Allah (1996).



Experimental

Crystal data

$C_7H_7N_3OS$
M_r = 181.22
Triclinic, $P\overline{1}$
a = 6.9262 (4) Å
b = 7.0540 (4) Å
c = 8.8079 (6) Å
α = 71.002 (6)°
β = 75.845 (5)°
γ = 85.570 (5)°
V = 394.54 (4) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 3.26 mm^{-1}
T = 100 K
0.30 × 0.25 × 0.20 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.442, T_{max} = 0.562
2363 measured reflections
1539 independent reflections
1523 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.080
S = 1.05
1539 reflections
115 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.88 (2)	1.97 (2)	2.845 (2)	173 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5288).

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supplementary materials

Acta Cryst. (2011). E**67**, o2467 [**doi:10.1107/S1600536811034192**]

2,7-Dimethyl-1,3-thiazolo[4,5-*d*]pyridazin-4(5*H*)-one

A. O. Al-Youbi, A. M. Asiri, H. M. Faidallah and S. W. Ng

Comment

We have reported the synthesis of some pyridazines, which exhibit biological activity (Faid-Allah *et al.*, 2011; Makki & Faid-Allah, 1996). There are few crystal structure reports of such systems; recently, we reported the crystal structure of 3-methyl-2-(4-methyl)-2*H*-pyrazolo[3,4-*d*]pyridazin-5-ium thiocyanate, a salt (Abdel-Aziz *et al.*, 2010). The nine-membered fused-ring system of $C_7H_7N_3OS$ (Scheme I) is planar (Fig. 1). The amino group forms a hydrogen bond to the ketonic O atom of a neigboring molecule to form a dimer (Table 1).

Experimental

A solution of ethyl 5-acetyl-3-methylisoxazole-4-carboxylate (2.10 g, 10 mmol) in ethanol (25 ml) was refluxed with hydrazine hydrate (0.50 g, 10 mmol) for 2 h. The pyridazine which separated after concentration of the reaction mixture was filtered off, washed with ethanol and recrystallized from the same solvent to give colorless prisms in 90% yield, mp 527 K.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

The amino H-atom was located in a difference Fourier map, and were refined freely.

Omitted were (4 0 4), (1 0 1) and (-7 - 2 1).

Figures

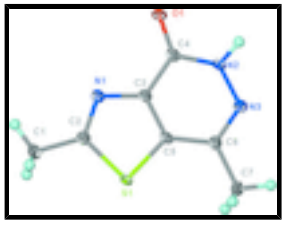

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_7H_7N_3OS$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2,7-Dimethyl-1,3-thiazolo[4,5-*d*]pyridazin-4(5*H*)-one

Crystal data

$C_7H_7N_3OS$	$Z = 2$
$M_r = 181.22$	$F(000) = 188$
Triclinic, $P\overline{1}$	$D_x = 1.525$ Mg m^{-3}

Hall symbol: -P 1
a = 6.9262 (4) Å
b = 7.0540 (4) Å
c = 8.8079 (6) Å
α = 71.002 (6)°
β = 75.845 (5)°
γ = 85.570 (5)°
V = 394.54 (4) Å^3

Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 1965 reflections
θ = 6.6–74.2°
μ = 3.26 mm^{-1}
T = 100 K
Prism, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector
Radiation source: SuperNova (Cu) X-ray Source
Mirror
Detector resolution: 10.4041 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.442, T_{max} = 0.562
2363 measured reflections

1539 independent reflections
1523 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 74.4°, θ_{min} = 6.6°
h = −8→7
k = −8→4
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.080
S = 1.05
1539 reflections
115 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.260P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	1.29210 (5)	0.13257 (5)	0.50269 (4)	0.01037 (14)
O1	0.59921 (15)	0.34439 (15)	0.67118 (13)	0.0136 (2)
N1	0.97795 (18)	0.13725 (17)	0.73210 (15)	0.0114 (3)
N2	0.74300 (18)	0.42456 (18)	0.39677 (15)	0.0112 (3)
H2	0.636 (3)	0.490 (3)	0.371 (3)	0.027 (5)*
N3	0.88967 (18)	0.43408 (18)	0.25907 (15)	0.0121 (3)
C1	1.2623 (2)	−0.0391 (2)	0.84407 (19)	0.0157 (3)
H1A	1.1669	−0.0660	0.9512	0.024*

H1B	1.3732	0.0410	0.8415	0.024*
H1C	1.3131	−0.1663	0.8277	0.024*
C2	1.1611 (2)	0.0736 (2)	0.70979 (18)	0.0118 (3)
C3	0.9338 (2)	0.2388 (2)	0.58191 (17)	0.0103 (3)
C4	0.7459 (2)	0.3356 (2)	0.56003 (18)	0.0107 (3)
C5	1.0839 (2)	0.2502 (2)	0.44375 (18)	0.0101 (3)
C6	1.0596 (2)	0.3495 (2)	0.27985 (18)	0.0111 (3)
C7	1.2245 (2)	0.3608 (2)	0.13145 (18)	0.0167 (3)
H7A	1.1756	0.4244	0.0312	0.025*
H7B	1.2713	0.2252	0.1345	0.025*
H7C	1.3346	0.4401	0.1314	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0081 (2)	0.0092 (2)	0.0123 (2)	0.00189 (13)	−0.00196 (13)	−0.00205 (14)
O1	0.0089 (5)	0.0137 (5)	0.0156 (5)	0.0007 (4)	0.0001 (4)	−0.0034 (4)
N1	0.0113 (6)	0.0082 (6)	0.0136 (6)	−0.0004 (4)	−0.0028 (5)	−0.0019 (5)
N2	0.0081 (6)	0.0104 (6)	0.0140 (6)	0.0020 (5)	−0.0022 (5)	−0.0032 (5)
N3	0.0120 (6)	0.0103 (6)	0.0130 (6)	0.0000 (5)	−0.0018 (5)	−0.0029 (5)
C1	0.0147 (7)	0.0150 (7)	0.0155 (7)	0.0025 (6)	−0.0051 (6)	−0.0015 (6)
C2	0.0124 (7)	0.0076 (6)	0.0142 (7)	−0.0016 (5)	−0.0020 (5)	−0.0021 (5)
C3	0.0103 (7)	0.0057 (6)	0.0137 (7)	−0.0016 (5)	−0.0019 (5)	−0.0016 (5)
C4	0.0103 (7)	0.0057 (6)	0.0157 (7)	−0.0021 (5)	−0.0030 (5)	−0.0025 (5)
C5	0.0095 (6)	0.0060 (6)	0.0151 (7)	0.0002 (5)	−0.0034 (5)	−0.0034 (5)
C6	0.0122 (7)	0.0078 (6)	0.0127 (7)	−0.0011 (5)	−0.0026 (5)	−0.0022 (5)
C7	0.0151 (7)	0.0191 (8)	0.0127 (7)	0.0022 (6)	−0.0017 (6)	−0.0022 (6)

Geometric parameters (Å, °)

S1—C5	1.7141 (14)	C1—H1A	0.9800
S1—C2	1.7546 (15)	C1—H1B	0.9800
O1—C4	1.2404 (18)	C1—H1C	0.9800
N1—C2	1.3025 (19)	C3—C5	1.378 (2)
N1—C3	1.3797 (18)	C3—C4	1.4480 (19)
N2—N3	1.3647 (17)	C5—C6	1.430 (2)
N2—C4	1.3736 (19)	C6—C7	1.4953 (19)
N2—H2	0.88 (2)	C7—H7A	0.9800
N3—C6	1.3037 (19)	C7—H7B	0.9800
C1—C2	1.493 (2)	C7—H7C	0.9800
C5—S1—C2	89.25 (7)	N1—C3—C4	125.15 (13)
C2—N1—C3	110.07 (12)	O1—C4—N2	120.86 (13)
N3—N2—C4	129.17 (12)	O1—C4—C3	126.43 (13)
N3—N2—H2	111.4 (14)	N2—C4—C3	112.70 (12)
C4—N2—H2	119.3 (14)	C3—C5—C6	122.57 (13)
C6—N3—N2	117.76 (12)	C3—C5—S1	109.49 (11)
C2—C1—H1A	109.5	C6—C5—S1	127.94 (11)
C2—C1—H1B	109.5	N3—C6—C5	119.21 (13)

H1A—C1—H1B	109.5	N3—C6—C7	119.01 (13)
C2—C1—H1C	109.5	C5—C6—C7	121.77 (13)
H1A—C1—H1C	109.5	C6—C7—H7A	109.5
H1B—C1—H1C	109.5	C6—C7—H7B	109.5
N1—C2—C1	125.25 (13)	H7A—C7—H7B	109.5
N1—C2—S1	114.91 (11)	C6—C7—H7C	109.5
C1—C2—S1	119.83 (11)	H7A—C7—H7C	109.5
C5—C3—N1	116.28 (12)	H7B—C7—H7C	109.5
C5—C3—C4	118.56 (13)		
C4—N2—N3—C6	−0.4 (2)	N1—C3—C5—C6	179.58 (12)
C3—N1—C2—C1	178.83 (13)	C4—C3—C5—C6	−1.6 (2)
C3—N1—C2—S1	−0.33 (15)	N1—C3—C5—S1	−0.99 (16)
C5—S1—C2—N1	−0.18 (11)	C4—C3—C5—S1	177.81 (10)
C5—S1—C2—C1	−179.39 (12)	C2—S1—C5—C3	0.63 (10)
C2—N1—C3—C5	0.86 (17)	C2—S1—C5—C6	−179.99 (13)
C2—N1—C3—C4	−177.85 (12)	N2—N3—C6—C5	0.55 (19)
N3—N2—C4—O1	178.56 (12)	N2—N3—C6—C7	−178.84 (12)
N3—N2—C4—C3	−0.7 (2)	C3—C5—C6—N3	0.5 (2)
C5—C3—C4—O1	−177.59 (13)	S1—C5—C6—N3	−178.85 (10)
N1—C3—C4—O1	1.1 (2)	C3—C5—C6—C7	179.84 (13)
C5—C3—C4—N2	1.63 (18)	S1—C5—C6—C7	0.5 (2)
N1—C3—C4—N2	−179.69 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.88 (2)	1.97 (2)	2.845 (2)	173 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1