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## Structure Reports

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

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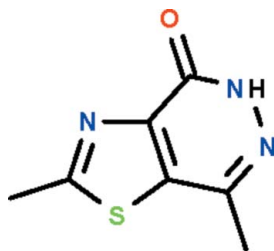
Received 6 August 2011; accepted 20 August 2011

 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  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,  $\text{C}_7\text{H}_7\text{N}_3\text{OS}$ , 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

 $\text{C}_7\text{H}_7\text{N}_3\text{OS}$   
 $M_r = 181.22$ 

 Triclinic,  $P\bar{1}$   
 $a = 6.9262$  (4) Å

 $b = 7.0540$  (4) Å  
 $c = 8.8079$  (6) Å  
 $\alpha = 71.002$  (6)°  
 $\beta = 75.845$  (5)°  
 $\gamma = 85.570$  (5)°  
 $V = 394.54$  (4) Å<sup>3</sup>
 $Z = 2$   
 Cu  $K\alpha$  radiation  
 $\mu = 3.26$  mm<sup>-1</sup>  
 $T = 100$  K  
 $0.30 \times 0.25 \times 0.20$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.012$ 

#### 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  
 $\Delta\rho_{\text{max}} = 0.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O1}^i$	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: *pubCIF* (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).

### References

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## supporting information

*Acta Cryst.* (2011). E67, o2467 [doi:10.1107/S1600536811034192]

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

**Abdulrahman O. Al-Youbi, Abdullah M. Asiri, Hassan M. Faidallah and Seik Weng Ng**

**S1. 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<sub>7</sub>H<sub>7</sub>N<sub>3</sub>OS (Scheme 1) is planar (Fig. 1). The amino group forms a hydrogen bond to the ketonic O atom of a neighboring molecule to form a dimer (Table 1).

**S2. Experimental**

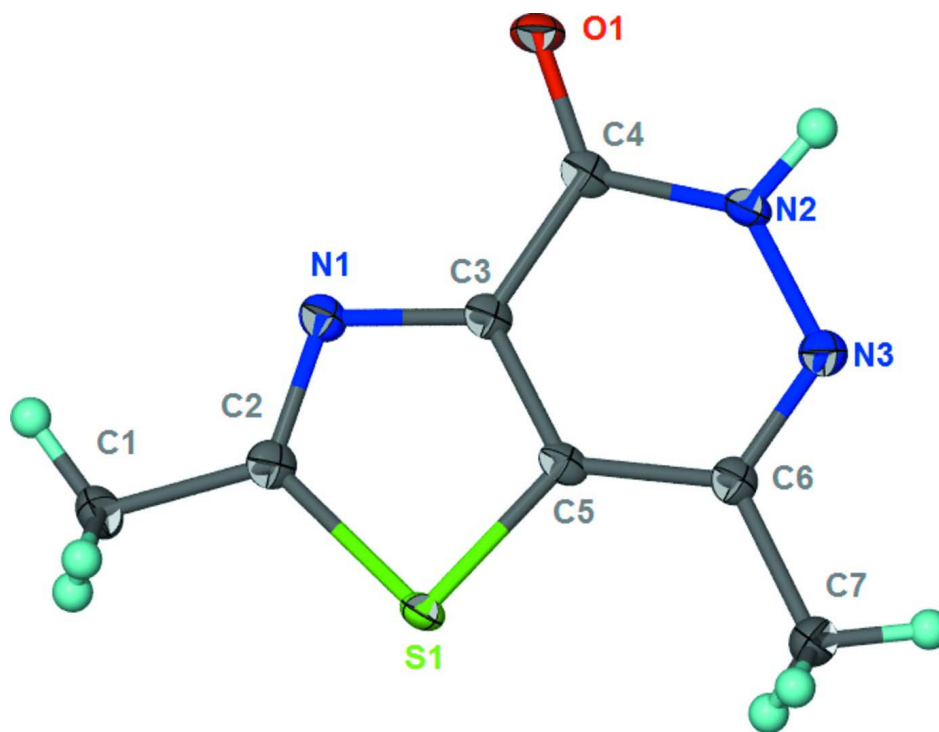
A solution of ethyl 5-acetyl-3-methylisoxazole-4-carboxylate (2.10 g, 10 mmol) in ethanol (25 ml) was refluxed with hydrazine hydrate (0.50 g, 10 mmol) for 2 h. The pyridazine which separated after concentration of the reaction mixture was filtered off, washed with ethanol and recrystallized from the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

**S3. Refinement**

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å,  $U_{\text{iso}}(\text{H})$  1.2 to 1.5 $U_{\text{eq}}(\text{C})$ ] 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).

**Figure 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

$C_7H_7N_3OS$

$M_r = 181.22$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 6.9262$  (4) Å

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$\alpha = 71.002$  (6)°

$\beta = 75.845$  (5)°

$\gamma = 85.570$  (5)°

$V = 394.54$  (4) Å<sup>3</sup>

$Z = 2$

$F(000) = 188$

$D_x = 1.525$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54184$  Å

Cell parameters from 1965 reflections

$\theta = 6.6$ – $74.2$ °

$\mu = 3.26$  mm<sup>-1</sup>

$T = 100$  K

Prism, colorless

$0.30 \times 0.25 \times 0.20$  mm

#### Data collection

Agilent Technologies SuperNova Dual diffractometer with Atlas detector

Radiation source: SuperNova (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.4041 pixels mm<sup>-1</sup>

$\omega$  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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.012$

$\theta_{\max} = 74.4$ °,  $\theta_{\min} = 6.6$ °

$h = -8 \rightarrow 7$

$k = -8 \rightarrow 4$

$l = -10 \rightarrow 10$

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

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

$\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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, °)*

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<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2···O1 <sup>i</sup>	0.88 (2)	1.97 (2)	2.845 (2)	173 (2)

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