Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4,6-Dimethoxy-2-(methylsulfanyl)-pyrimidine

**Kasthuri Balasubramani and Hoong-Kun Fun*‡**

X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia
Correspondence e-mail: hkfun@usm.my

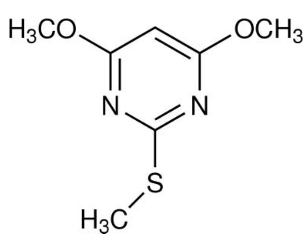
Received 10 July 2009; accepted 11 July 2009

Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.056; $wR$ factor = 0.133; data-to-parameter ratio = 14.5.

The title compound, $C_7H_{10}N_2O_2S$, is essentially planar [maximum deviation 0.018 (4) Å]. In the crystal, molecules are linked into chains by C—H···N hydrogen bonds and the chains are arranged in layers parallel to the *ab* plane.

## Related literature

For general background to substituted pyrimidines, see: Salas *et al.* (1995); Holy *et al.* (1974); Hunt *et al.* (1980); Baker & Santi, (1965) For bond-length data, see: Allen *et al.* (1987). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).




## Experimental

*Crystal data*

$C_7H_{10}N_2O_2S$
$M_r$ = 186.23
Orthorhombic, $P2_12_12_1$
$a$ = 3.9537 (2) Å
$b$ = 7.1822 (4) Å
$c$ = 30.5723 (15) Å
$V$ = 868.14 (8) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.33 mm$^{-1}$
$T$ = 100 K
0.55 × 0.31 × 0.05 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005) $T_{min}$ = 0.838, $T_{max}$ = 0.985
4467 measured reflections
1620 independent reflections
1555 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.133
$S$ = 1.28
1620 reflections
112 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$
Absolute structure: Flack (1983), 584 Friedel pairs
Flack parameter: 0.2 (2)

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C7—H7$A$···N1$^{i}$ | 0.96 | 2.62 | 3.573 (6) | 171 |

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

KBS and HKF thank the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312. KBS thanks Universiti Sains Malaysia for a post–doctoral research fellowship. HKF also thanks Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2850).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Baker, B. R. & Santi, D. V. (1965). *J. Pharm. Sci.* **54**, 1252–1257.
Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Holy, A., Votruba, I. & Jost, K. (1974). *Collect. Czech. Chem. Commun.* **39**, 634–646.
Hunt, W. E., Schwalbe, C. H., Bird, K. & Mallinson, P. D. (1980). *Biochem. J.* **187**, 533–536.
Salas, J. M., Romero, M. A. & Faure, R. (1995). *Acta Cryst.* C**51**, 2532–2534.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

‡ Thomson Reuters ResearcherID: A-3561-2009.

# supplementary materials

*Acta Cryst.* (2009). E**65**, o1895 [ **doi:10.1107/S1600536809027263** ]

# 4,6-Dimethoxy-2-(methylsulfanyl)pyrimidine

**K. Balasubramani** and **H.-K. Fun**

## Comment

Purine and pyrimidine derivatives are the constituents of nucleic acids and play important roles in many biological systems (Salas *et al.*, 1995). 2-Thiopyrimidine shows a strong bacteriostatic activity *in vitro* on *E. coli* (Holy *et al.*, 1974). Some aminopyrimidine derivatives are used as antifolate drugs (Hunt *et al.*, 1980; Baker & Santi, 1965). The crystal structure of the title compound is presented here.

The molecule (Fig.1) is essentially planar, with atom N1 deviating a maximum of 0.018 (4) Å. The bond lengths (Allen *et al.*, 1987) and angles are normal.

The molecules are linked into chains by C—H···N hydrogen bonds (Table 1). The chains are arranged in layers parallel to the *ab* plane (Fig.2).

## Experimental

Hot methanol solution (20 ml) of 4,6-dimethoxy-2-methylthiopyrimidine (46 mg, Aldrich) was warmed over a heating magnetic stirrer for 5 minutes. The resulting solution was allowed to cool slowly at room temperature. Crystals of the title compound appeared from the mother liquor after a few days.

## Refinement

H atoms were positioned geometrically [C–H = 0.93–0.96 Å] and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C) and 1.5$U_{eq}$(methyl C). A rotating–group model was used for the methyl groups.

## Figures

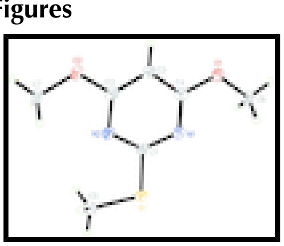


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

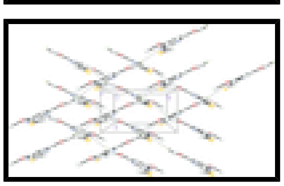


Fig. 2. The crystal packing of the title compound, viewed along the *c* axis. H atoms not involved in hydrogen bonding (dashed line) have been omitted for clarity.

## 4,6-Dimethoxy-2-(methylsulfanyl)pyrimidine

### *Crystal data*

| | |
|---|---|
| $C_7H_{10}N_2O_2S$ | $F_{000} = 392$ |
| $M_r = 186.23$ | $D_x = 1.425$ Mg m$^{-3}$ |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2ac 2ab | Cell parameters from 3133 reflections |
| $a = 3.9537$ (2) Å | $\theta = 2.7–30.7°$ |
| $b = 7.1822$ (4) Å | $\mu = 0.33$ mm$^{-1}$ |
| $c = 30.5723$ (15) Å | $T = 100$ K |
| $V = 868.14$ (8) Å$^3$ | Plate, yellow |
| $Z = 4$ | 0.55 × 0.31 × 0.05 mm |

### *Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD area-detector diffractometer | 1620 independent reflections |
| Radiation source: fine-focus sealed tube | 1555 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.033$ |
| $T = 100$ K | $\theta_{max} = 26.0°$ |
| φ and ω scans | $\theta_{min} = 1.3°$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2005) | $h = -4 \rightarrow 4$ |
| $T_{min} = 0.838$, $T_{max} = 0.985$ | $k = -6 \rightarrow 8$ |
| 4467 measured reflections | $l = -37 \rightarrow 37$ |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)] = 0.056$ | $w = 1/[\sigma^2(F_o^2) + 2.7239P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.133$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $S = 1.28$ | $\Delta\rho_{max} = 0.42$ e Å$^{-3}$ |
| 1620 reflections | $\Delta\rho_{min} = -0.47$ e Å$^{-3}$ |
| 112 parameters | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 584 Friedel pairs |
| Secondary atom site location: difference Fourier map | Flack parameter: 0.2 (2) |

### *Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cyrosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 | 0.6163 (3) | 0.16537 (16) | 0.05410 (4) | 0.0194 (3) |
| O1 | 0.7269 (9) | 0.2088 (4) | 0.21365 (10) | 0.0207 (8) |
| O2 | 1.1384 (9) | −0.3287 (4) | 0.14636 (9) | 0.0200 (7) |
| N1 | 0.6864 (9) | 0.1795 (5) | 0.13848 (11) | 0.0140 (8) |
| N2 | 0.8979 (11) | −0.0980 (5) | 0.10377 (11) | 0.0177 (8) |
| C1 | 0.7499 (12) | 0.0691 (6) | 0.10392 (14) | 0.0163 (9) |
| C2 | 0.9874 (12) | −0.1607 (7) | 0.14346 (14) | 0.0190 (10) |
| C3 | 0.9362 (12) | −0.0645 (6) | 0.18210 (14) | 0.0184 (10) |
| H3A | 0.9998 | −0.1113 | 0.2092 | 0.022* |
| C4 | 0.7818 (11) | 0.1081 (7) | 0.17698 (13) | 0.0159 (9) |
| C5 | 0.7262 (13) | −0.0160 (7) | 0.01606 (14) | 0.0206 (10) |
| H5A | 0.6651 | 0.0217 | −0.0130 | 0.031* |
| H5B | 0.6069 | −0.1279 | 0.0236 | 0.031* |
| H5C | 0.9653 | −0.0385 | 0.0173 | 0.031* |
| C6 | 0.5624 (13) | 0.3873 (6) | 0.20817 (14) | 0.0200 (10) |
| H6A | 0.5276 | 0.4436 | 0.2363 | 0.030* |
| H6B | 0.3481 | 0.3699 | 0.1940 | 0.030* |
| H6C | 0.7023 | 0.4670 | 0.1906 | 0.030* |
| C7 | 1.1937 (13) | −0.4273 (7) | 0.10586 (14) | 0.0210 (11) |
| H7A | 1.3211 | −0.5385 | 0.1115 | 0.032* |
| H7B | 1.3170 | −0.3492 | 0.0860 | 0.032* |
| H7C | 0.9797 | −0.4598 | 0.0931 | 0.032* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0226 (6) | 0.0161 (5) | 0.0194 (5) | 0.0009 (6) | −0.0013 (5) | 0.0026 (5) |
| O1 | 0.0265 (19) | 0.0147 (16) | 0.0207 (15) | 0.0071 (14) | 0.0014 (14) | −0.0017 (12) |
| O2 | 0.0249 (17) | 0.0127 (14) | 0.0225 (14) | 0.0059 (18) | 0.0005 (14) | 0.0001 (13) |
| N1 | 0.0059 (18) | 0.0141 (17) | 0.0221 (17) | −0.0036 (16) | 0.0012 (13) | 0.0001 (15) |
| N2 | 0.019 (2) | 0.0143 (17) | 0.0200 (17) | 0.0012 (19) | −0.0030 (17) | 0.0004 (14) |
| C1 | 0.019 (2) | 0.012 (2) | 0.019 (2) | −0.006 (2) | −0.0011 (19) | 0.0031 (16) |
| C2 | 0.018 (2) | 0.016 (2) | 0.023 (2) | 0.000 (2) | 0.0023 (17) | 0.005 (2) |
| C3 | 0.020 (3) | 0.016 (2) | 0.019 (2) | 0.001 (2) | 0.0027 (19) | 0.0040 (18) |
| C4 | 0.010 (2) | 0.019 (2) | 0.018 (2) | −0.0014 (19) | 0.0056 (17) | 0.0014 (17) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.017 (3) | 0.024 (2) | 0.021 (2) | 0.001 (2) | −0.0007 (19) | 0.0000 (19) |
| C6 | 0.022 (3) | 0.012 (2) | 0.026 (2) | 0.010 (2) | 0.003 (2) | −0.0018 (18) |
| C7 | 0.021 (3) | 0.017 (2) | 0.026 (2) | 0.007 (2) | −0.0007 (19) | −0.0013 (18) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.754 (4) | C3—C4 | 1.390 (7) |
| S1—C5 | 1.799 (5) | C3—H3A | 0.93 |
| O1—C4 | 1.352 (5) | C5—H5A | 0.96 |
| O1—C6 | 1.448 (5) | C5—H5B | 0.96 |
| O2—C2 | 1.349 (6) | C5—H5C | 0.96 |
| O2—C7 | 1.443 (5) | C6—H6A | 0.96 |
| N1—C4 | 1.338 (5) | C6—H6B | 0.96 |
| N1—C1 | 1.345 (6) | C6—H6C | 0.96 |
| N2—C1 | 1.335 (6) | C7—H7A | 0.96 |
| N2—C2 | 1.342 (6) | C7—H7B | 0.96 |
| C2—C3 | 1.384 (6) | C7—H7C | 0.96 |
| C1—S1—C5 | 101.7 (2) | S1—C5—H5B | 109.5 |
| C4—O1—C6 | 116.8 (3) | H5A—C5—H5B | 109.5 |
| C2—O2—C7 | 116.7 (3) | S1—C5—H5C | 109.5 |
| C4—N1—C1 | 114.4 (4) | H5A—C5—H5C | 109.5 |
| C1—N2—C2 | 114.5 (4) | H5B—C5—H5C | 109.5 |
| N2—C1—N1 | 127.9 (4) | O1—C6—H6A | 109.5 |
| N2—C1—S1 | 118.9 (3) | O1—C6—H6B | 109.5 |
| N1—C1—S1 | 113.2 (3) | H6A—C6—H6B | 109.5 |
| N2—C2—O2 | 118.4 (4) | O1—C6—H6C | 109.5 |
| N2—C2—C3 | 124.5 (4) | H6A—C6—H6C | 109.5 |
| O2—C2—C3 | 117.1 (4) | H6B—C6—H6C | 109.5 |
| C2—C3—C4 | 114.4 (4) | O2—C7—H7A | 109.5 |
| C2—C3—H3A | 122.8 | O2—C7—H7B | 109.5 |
| C4—C3—H3A | 122.8 | H7A—C7—H7B | 109.5 |
| N1—C4—O1 | 118.6 (4) | O2—C7—H7C | 109.5 |
| N1—C4—C3 | 124.4 (4) | H7A—C7—H7C | 109.5 |
| O1—C4—C3 | 117.0 (4) | H7B—C7—H7C | 109.5 |
| S1—C5—H5A | 109.5 | | |
| C2—N2—C1—N1 | 0.9 (7) | C7—O2—C2—C3 | −179.4 (4) |
| C2—N2—C1—S1 | −179.3 (3) | N2—C2—C3—C4 | −0.3 (7) |
| C4—N1—C1—N2 | −1.1 (7) | O2—C2—C3—C4 | 179.6 (4) |
| C4—N1—C1—S1 | 179.1 (3) | C1—N1—C4—O1 | −179.7 (4) |
| C5—S1—C1—N2 | 1.6 (4) | C1—N1—C4—C3 | 0.4 (6) |
| C5—S1—C1—N1 | −178.5 (3) | C6—O1—C4—N1 | 0.9 (6) |
| C1—N2—C2—O2 | 179.9 (4) | C6—O1—C4—C3 | −179.3 (4) |
| C1—N2—C2—C3 | −0.2 (7) | C2—C3—C4—N1 | 0.1 (7) |
| C7—O2—C2—N2 | 0.4 (6) | C2—C3—C4—O1 | −179.7 (4) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7A···N1$^{i}$ | 0.96 | 2.62 | 3.573 (6) | 171 |

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

**Fig. 1**

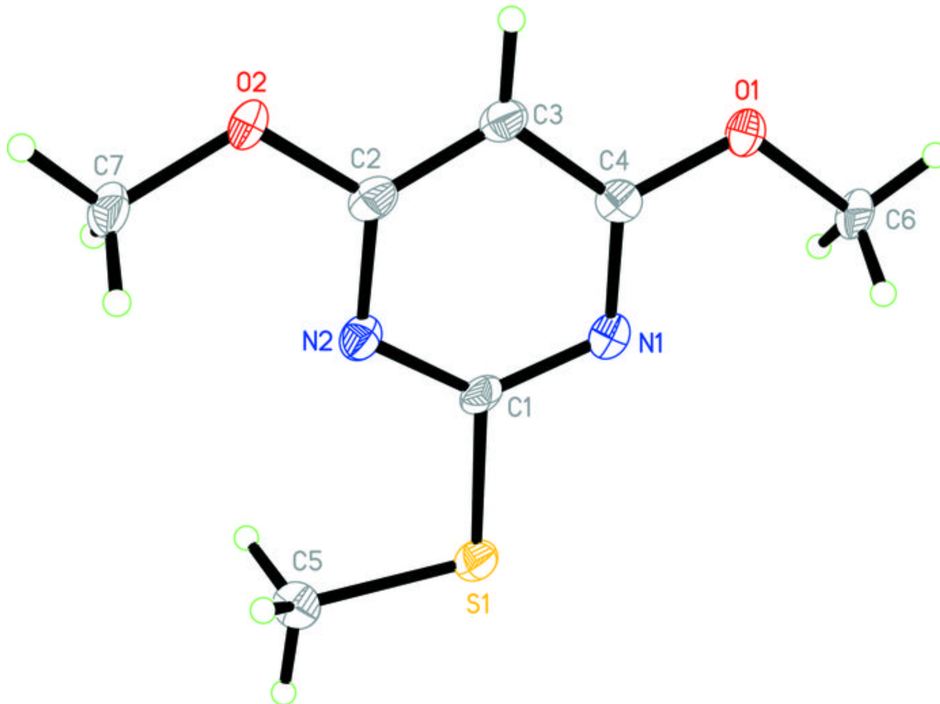


Fig. 2