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4-Hydroxy-6-methyl-2-(sulfonatoethylsulfanyl)pyrimidin-1-ium monohydrate

Daniel E. Lynch[a]* and Ian McClenaghan[b]

[a]School of Science and the Environment, Coventry University, Coventry CV1 5FB, England, and [b]Key Organics Ltd, Highfield Industrial Estate, Camelford, Cornwall PL32 9QZ, England

Correspondence e-mail: apx106@coventry.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.032
wR factor = 0.082
Data-to-parameter ratio = 11.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the structure of the title compound, $C_7H_{10}N_2O_4S_2\cdot H_2O$, the 4-hydroxy group hydrogen bonds to the water O atom, which in turn associates *via* one water H atom with one sulfonate O atom to create an intramolecular $R_2^2(12)$ hydrogen-bonded ring. The other water H atom and the pyrimidinium H atom associate with adjacent and separate sulfonate O atoms.

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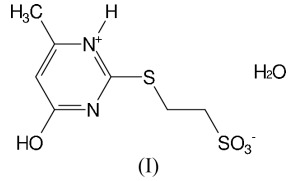
Comment

Recent investigations into the synthesis and structures of 2-(alkylthio)pyrimidines, such as the 4,6-dichloro-2-(methylthio)- (Lynch & McClenaghan, 2000), 6-chloro-2-(methylthio)-4-[(2-phenylethyl)amino]- (Lynch & McClenaghan, 2001*a*), 4-chloro-2-(methylthio)-6-(1-piperidyl)- (Lynch & McClenaghan, 2001*b*), and 4,6-dichloro-2-(methylthio)-5-phenyl- (Lynch & McClenaghan, 2001*c*) analogues, have led to the synthesis and structural investigation of the title compound, (I). The structure of (I) reveals a non-planar zwitterionic molecule that crystallizes with one water molecule (Fig. 1). The 4-hydroxy group hydrogen bonds to the water O atom, which in turn associates *via* one water H atom with one sulfonate O atom to create an intramolecular $R_2^2(12)$ hydrogen-bonded ring. The other water H atom and the pyrimidinium H atom associate with adjacent and separate sulfonate O atoms. Hydrogen-bonding associations and C—H···O/N close contacts are listed in Table 1.



(I)

The short O41—H41···O1*W* contact gives rise to two short H···H contacts [of 2.01 (5) Å each] from H41 to both of the water H atoms. It is interesting to note that the nearest structural comparison to (I) is [(4,6-dimethyl-2-pyrimidinyl)-thio]acetic acid, which also crystallizes with one water molecule (Zhu *et al.*, 1993), although the hydrogen-bonding networks surrounding the two respective water molecules are totally different.

Experimental

The title compound was obtained from Key Organics Ltd and was crystallized from ethanol.

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Crystal data

$C_7H_{10}N_2O_4S_2\cdot H_2O$	D_x = 1.628 Mg m^{-3}
M_r = 268.31	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 7654 reflections
a = 6.1137 (2) Å	θ = 2.9–27.5°
b = 11.2202 (3) Å	μ = 0.50 mm^{-1}
c = 15.9632 (6) Å	T = 120 (2) K
β = 91.0483 (18)°	Prism, colourless
V = 1094.84 (6) Å^3	0.35 × 0.20 × 0.08 mm
Z = 4	

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	1920 independent reflections
	1619 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.052
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	θ_{max} = 25.0°
	$h = -7 \rightarrow 7$
T_{min} = 0.932, T_{max} = 0.961	$k = -13 \rightarrow 13$
11989 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 0.5029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.032	
$wR(F^2)$ = 0.082	
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
1920 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
162 parameters	$\Delta\rho_{min}$ = −0.49 e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O26^{i}	0.87 (3)	1.85 (3)	2.716 (2)	176 (2)
O41—H41···O1W	1.00 (4)	1.50 (4)	2.491 (2)	174 (3)
O1W—H1W···O27	0.83 (3)	1.92 (4)	2.747 (2)	177 (3)
O1W—H2W···O25^{ii}	0.88 (3)	1.84 (4)	2.720 (2)	178 (3)
C22—H222···N3	0.99	2.46	2.824 (3)	101
C23—H232···N3	0.99	2.70	3.229 (3)	114
C22—H221···O27^{iii}	0.99	2.42	3.268 (2)	144
C5—H5···O41^{iv}	0.95	2.51	3.320 (2)	144

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

All H atoms not involved in the strong hydrogen-bonding associations were included in the refinement at calculated positions, in the riding-model approximation, with C—H distances of 0.95 (aromatic H atoms), 0.98 (methyl H atoms) and 0.99 Å (CH_2 H atoms). The isotropic displacement parameters were set equal to $1.25U_{eq}$ of the carrier atom. The hydroxy H atom, the pyrimidinium H atom and the two water H atoms were located in difference syntheses and both their positional and displacement parameters were refined.

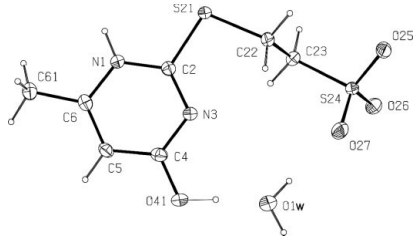

Figure 1
The molecular conformation and atomic numbering scheme for (I). Displacement ellipsoids are drawn at the 50% probability level.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO, SCALEPACK* (Otwinowski & Minor, 1997) and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

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