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3-Amino-4*H*-pyrido[2,3-e]-1,2,4-thiadiazine 1,1-dioxide

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The title compound, $C_6H_6N_4O_2S$, was prepared for structural comparison with diazoxide (7-chloro-3-methyl-4*H*-1,2,4-benzothiadiazine 1,1-dioxide) and other 3-alkylaminopyridothiadiazine 1,1-dioxides known to be potassium channel openers. Particular attention was paid to the tautomeric conformation adopted by the compound in the crystalline state, which is found to be the 4*H*-form.

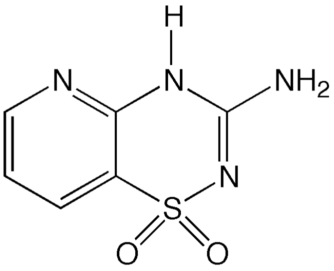
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.032
wR factor = 0.090
Data-to-parameter ratio = 8.4

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

Comment

Although most of the published X-ray data on pyridothiadiazine dioxides are related to compounds with the pyridinic nitrogen in the 7-position of the pyridothiadiazine ring, this example, (I), of a compound with the N atom in the 5-position will complete our information on the influence of this position on the tautomeric behaviour of pyridothiadiazine dioxides. It confirms the predominance of the 4*H*-tautomeric form. These results may help to establish in such molecules which are the important chemical and geometrical parameters required (pharmacophore) for their biological activity.



(I)

Experimental

The title compound was synthesized at the Laboratory of Medicinal Chemistry of Liège, according to the method of Kotovskaya *et al.* (1979). Cystals were obtained by slow evaporation of a methanol solution.

Crystal data

$C_6H_6N_4O_2S$
M_r = 198.21
Orthorhombic, *Pbca*
a = 9.7545 (6) Å
b = 12.0427 (9) Å
c = 13.5242 (18) Å
V = 1588.7 (3) Å^3
Z = 8
D_x = 1.657 Mg m^{-3}

Cu $K\alpha$ radiation
Cell parameters from 34 reflections
θ = 24.7–40.7°
μ = 3.43 mm^{-1}
T = 293 (2) K
Prism, colourless
0.34 × 0.23 × 0.11 mm

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Data collection

Stoe–Siemens AED four-circle diffractometer
ω scans
Absorption correction: ψ-scan (*EMPIR*; Stoe & Cie, 1987)
$T_{\min} = 0.388$, $T_{\max} = 0.704$
1077 measured reflections
1077 independent reflections
829 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 57.4^\circ$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 13$
$l = 0 \rightarrow 14$
2 standard reflections frequency: 60 min intensity decay: 3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.090$
$S = 0.96$
1077 reflections
128 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0560P)^2 + 0.7861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0043 (4)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N4—H4$\cdots$N2$^{\rm i}$	0.84 (3)	2.22 (3)	3.047 (3)	172 (3)
N11—H112$\cdots$O1$^{\rm i}$	0.92 (3)	1.96 (3)	2.868 (3)	173 (3)
N11—H111$\cdots$N6$^{\rm ii}$	0.86 (3)	2.13 (3)	2.997 (3)	177 (3)

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

H atoms were constrained (included as riding atoms) except those on N4 and N11, which were refined, with isotropic displacement parameters fixed at $1.2U_{\rm eq}$ of the parent atom.

Data collection: *DIF*4 (Stoe & Cie, 1987); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

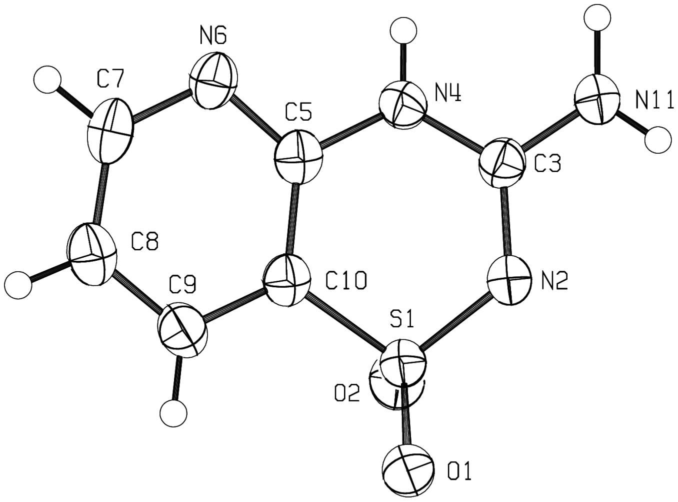

Figure 1
The molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are shown at the 50% probability level and H atoms are shown as small circles or arbitrary radii.

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