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Structure of 5-(4-Methoxybenzylidene)-1,3-thiazolidine-2,4-dione

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Abstract. $C_{11}H_9NO_3S$, $M_r = 235{\cdot}26$, orthorhombic, $Pna2_1$, $a = 13{\cdot}156$ (1), $b = 12{\cdot}223$ (1), $c = 6{\cdot}461$ (1) Å, $V = 1039{\cdot}0$ (3) Å^3, $D_m = 1{\cdot}48$, $D_x = 1{\cdot}50$ g cm^{-3}, $Z = 4$, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 26{\cdot}6$ cm^{-1}, $F(000) = 488$, $T = 297$ K, final $R = 0{\cdot}026$, $wR = 0{\cdot}029$ for 1046 independent reflections. The molecule is made up of two planar fragments: the 1,3-thiazolidine-2,4-dione ring and the methoxybenzylidene moiety with an angle of 5·9 (5)° between them. Bond distances and angles are normal and intermolecular hydrogen bonding occurs between N(3) and the methoxy O(14) from neighbouring molecules in a 'head-to-tail' order [N(3)—H(3)···O(14)′ = 2·916 (1) Å, N(3)—H(3)—O(14)′ = 169·8 (3)°; (′) = 0·5 − x, 0·5 + y, 0·5 + z].

Experimental. The compound was prepared in the condensation reaction of 2,4-dioxotetrahydro-1,3-thiazole with 4-methoxybenzaldehyde using morpholine as a catalyst. A pale-yellow needle-like single crystal (0·64 × 0·20 × 0·16 mm) was mounted on a glass fiber. D_m by flotation. Diffraction data were collected on an Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Cu $K\alpha$ radiation, ω–2θ scan mode, lattice parameters from 23 reflections ($12 < \theta < 23°$), three standard reflections measured every hour, no loss of intensity. A total of 4296 reflections were measured (h −16→16, k −14→14, l 0→7) with $\theta < 70°$, 4035 with $I > 3\sigma(I)$, of which 1074 were independent ($R_{int} = 0{\cdot}011$). Data were corrected for Lorentz and polarization effects, absorption correction applied (*DIFABS*; Walker & Stuart, 1983); max. and min. transmission factors 1·00 and 0·86. Solution of the structure by direct methods (*SHELXS*86; Sheldrick, 1986) and refinement by full-matrix least squares based on F, $w = 1/\sigma^2(I)$, using the Enraf–Nonius *SDP* V3.1 program package (Frenz, 1985); scattering factors were in *SDP*. Non-H atoms were refined anisotropically; the H atoms were located in a ΔF map and refined isotropically. Final $R = 0{\cdot}026$, $wR = 0{\cdot}029$, $S = 2{\cdot}67$ for 1046 observations and 181 variables in the last cycle, final difference map with no features greater than 0·2 e Å^{-3}; extinction coefficient $g = 5{\cdot}2 \times 10^{-7}$. $(\Delta/\sigma)_{max} = 0{\cdot}00001$. The atomic coordinates and equivalent isotropic temperature factors of the non-H atoms are given in Table 1;* bond lengths and angles are listed in Table 2; Fig. 1 shows the molecule.

Related literature. For detailed preparation of the compound and a discussion of the results, see Popov-Pergal, Čeković & Pergal (1987). For the structure of a similar compound, 5-[(4-methoxyphenyl)-methylene]imidazolidine-2,4-dione, see Drew, Mok, Ang & Tan (1987). For the structure of thiazolidine-2,4-dione see Form, Raper & Downie (1975).

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances and angles involving H atoms, least-squares planes and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53953 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters*

$B_{eq} = (4/3)\sum_i\sum_j \beta_{ij} \mathbf{a}_i . \mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
S(1)	0·6270 (1)	0·0148 (1)	0·935*	3·55 (1)
C(2)	0·6539 (2)	0·0933 (2)	1·1599 (4)	3·63 (4)
N(3)	0·7563 (1)	0·1000 (2)	1·1882 (3)	3·47 (3)
C(4)	0·8191 (2)	0·0498 (2)	1·0459 (4)	3·11 (4)
C(5)	0·7567 (2)	−0·0042 (1)	0·8845 (3)	2·94 (4)
C(6)	0·8018 (2)	−0·0585 (2)	0·7279 (4)	3·04 (4)
C(7)	0·7571 (1)	−0·1175 (2)	0·5565 (4)	2·94 (4)
C(8)	0·8227 (1)	−0·1601 (2)	0·4060 (3)	3·11 (4)
C(9)	0·7862 (2)	−0·2171 (2)	0·2359 (3)	3·18 (4)
C(10)	0·6829 (2)	−0·2339 (2)	0·2152 (3)	2·83 (3)
C(11)	0·6158 (1)	−0·1933 (2)	0·3640 (4)	3·31 (4)
C(12)	0·6531 (2)	−0·1366 (2)	0·5327 (4)	3·36 (4)
C(13)	0·5471 (2)	−0·3155 (2)	0·0225 (4)	4·61 (5)
O(14)	0·6526 (1)	−0·2899 (1)	0·0432 (2)	3·53 (3)
O(15)	0·5901 (1)	0·1330 (2)	1·2687 (3)	5·34 (4)
O(16)	0·9112 (1)	0·0512 (1)	1·0545 (3)	4·18 (3)

* Origin-defining.

Table 2. *Bond distances* (Å) *and bond angles* (°)

S(1)—C(5)	1·752 (2)	C(5)—C(6)	1·348 (3)
S(1)—C(2)	1·779 (2)	C(6)—C(7)	1·446 (4)
O(14)—C(10)	1·365 (3)	C(7)—C(8)	1·400 (3)
O(14)—C(13)	1·429 (3)	C(7)—C(12)	1·397 (3)
O(15)—C(2)	1·198 (3)	C(8)—C(9)	1·387 (3)
O(16)—C(4)	1·213 (3)	C(9)—C(10)	1·380 (3)
N(3)—C(2)	1·363 (3)	C(10)—C(11)	1·396 (3)
N(3)—C(4)	1·380 (3)	C(11)—C(12)	1·382 (3)
C(4)—C(5)	1·483 (3)		

C(2)—S(1)—C(5)	91·7 (2)	C(5)—C(6)—C(7)	130·0 (2)
C(2)—N(3)—C(4)	118·4 (2)	C(6)—C(7)—C(8)	117·8 (2)
C(10)—O(14)—C(13)	118·0 (2)	C(6)—C(7)—C(12)	124·4 (2)
S(1)—C(2)—O(15)	124·0 (2)	C(8)—C(7)—C(12)	117·7 (2)
S(1)—C(2)—N(3)	109·9 (2)	C(7)—C(8)—C(9)	121·6 (2)
O(15)—C(2)—N(3)	126·2 (2)	C(8)—C(9)—C(10)	119·6 (2)
O(16)—C(4)—N(3)	124·1 (3)	C(9)—C(10)—C(11)	120·2 (2)
O(16)—C(4)—C(5)	126·3 (3)	C(9)—C(10)—C(14)	116·2 (2)
N(3)—C(4)—C(5)	109·6 (2)	C(11)—C(10)—C(14)	123·7 (2)
S(1)—C(5)—C(4)	110·5 (1)	C(10)—C(11)—C(12)	119·8 (2)
S(1)—C(5)—C(6)	129·3 (2)	C(7)—C(12)—C(11)	121·2 (2)
C(4)—C(5)—C(6)	120·2 (2)		

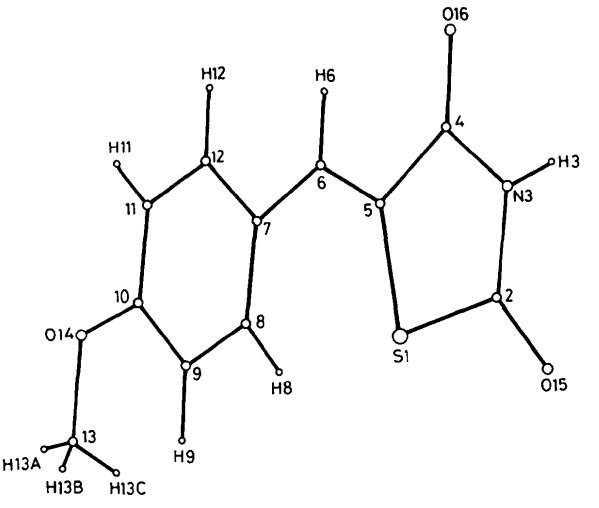

Fig. 1. The structure of the molecule with the atom-numbering scheme (C atoms where no label appears).

thiazolidine-2,4-dione see Form, Raper & Downie (1975).

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Structure of 2,3-Di(2-pyridyl)-6,7-dimethylquinoxaline

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Abstract. $C_{20}H_{16}N_4$, $M_r = 312·37$, monoclinic, $C2/c$, $a = 16·474$ (1), $b = 13·132$ (1), $c = 7·638$ (1) Å, $\beta = 99·24$ (1)°, $V = 1630·9$ (3) Å^3, $Z = 4$, $D_x = 1·272$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 5·78$ cm^{-1}, $F(000) = 656$, $T = 291$ K, $R = 0·0450$ for 1021 unique reflections. The structure consists of molecules oriented about the twofold axes. The angle between the least-squares planes for the quinoxaline part of the molecule and the pyridyl fragment is 39·65 (5)°.

Experimental. Crystals of the title compound were grown from acetonitrile. A Syntex $P2_1$ diffractometer was used with graphite-monochromatized Cu $K\alpha$

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