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2*H*-Thiochromen-2-one

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Key indicators

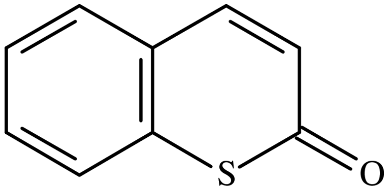
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.072
Data-to-parameter ratio = 13.0

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

The crystal structure of the title compound, C_9H_6OS, also known as 2*H*-thiochromen-2-one, has been determined as monoclinic in the space group *Pc* at room temperature. The molecule is essentially planar and the crystal is a candidate for second harmonic generation (SHG) effects.

Comment

Coumarins, simple organic molecules, have featured in several areas of synthetic chemistry, medicinal chemistry and photochemistry. The most important of these applications is the formation of [2+2] cycloaddition products upon irradiation (Vishnumurthy *et al.*, 2001). Several substituted coumarin derivatives find application in the dye industry. Coumarins have also been studied extensively as laser dyes and have shown state-dependent variation in their static dipole moments. They have been employed as probes for examination of ultrafast solvation effects (Maroncelli & Fleming, 1987). Theoretical calculations using semi-empirical methods demonstrate that coumarins (which are labeled differently depending on the nature of the substitution as, for example, coumarin 4, coumarin 138, coumarin 153 and coumarin 343) possess pronounced dipole moments. For example, coumarin itself has a ground-state dipole moment of 4.8 Debye.



(I)

These features make coumarin and its derivatives excellent candidates for organic SHG materials. Here we report the structure of 2*H*-thiochromen-2-one, (I). It crystallizes in a non-centrosymmetric space group. The molecular structure of (I) is illustrated in Fig. 1. Fig. 2 shows the packing of the molecules in the crystal structure.

Experimental

The title compound was synthesized according to a reported procedure (Meth-Cohn & Tarnowski, 1978). It was obtained from *o*-nitrobenzaldehyde *via* a three-step reaction. Crystals were grown by slow evaporation, at low temperature, from chloroform and hexene (1:4) as pale pink blocks (m.p. 354 K).

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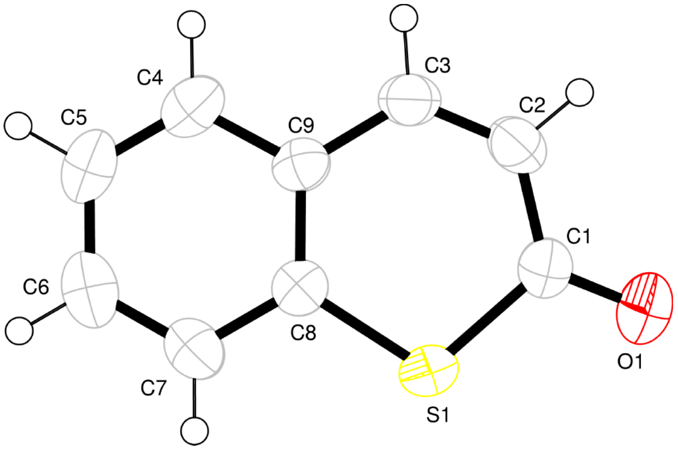

Figure 1
View of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

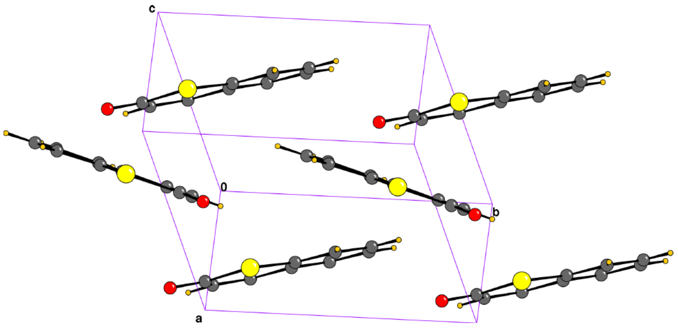

Figure 2
Packing diagram of the title compound.

Crystal data

C_9H_6OS
$M_r = 162.20$
Monoclinic, *Pc*
$a = 3.8899\ (5)$ Å
$b = 8.4355\ (11)$ Å
$c = 11.4569\ (15)$ Å
$\beta = 96.530\ (5)^\circ$
$V = 373.50\ (8)$ Å^3
$Z = 2$
$D_x = 1.442$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2232 reflections
$\theta = 2.4$–24.9°
$\mu = 0.36$ mm^{-1}
$T = 293\ (2)$ K
Block, pale pink
0.40 × 0.21 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
3453 measured reflections
1304 independent reflections
1253 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\rm max} = 25.0^\circ$
$h = -4 \rightarrow 4$
$k = -10 \rightarrow 9$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.072$
$S = 1.05$
1304 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.18$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}
Absolute structure: Flack (1983); 644 Friedel pairs
Flack parameter = −0.03 (8)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 for Windows (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *PLATON* (Spek, 1990) and *SHELXL*.

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