Jin-Qiang Liu*, Li Ji and Weizhou Wang

Crystal structure of 2-isopropylthioxanthone, $C_{16}H_{14}OS$

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Abstract

$C_{16}H_{14}OS$, monoclinic, $P2_1$ (no. 4), $a = 8.1588(5)$ Å, $b = 7.8670(4)$ Å, $c = 10.2161(5)$ Å, $V = 655.70(6)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0539$, $wR_{\text{ref}}(F^2) = 0.1312$, $T = 290$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was purchased from Sinopharm Chemical Reagent Co. Ltd. (Shanghai). Light yellow crystals suitable for X-ray diffraction study were obtained from a saturated toluene solution with cooling crystallization.

Experimental details

All of the non-hydrogen atoms were refined anisotropically. The hydrogen atoms were assigned with common isotropic

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	$0.27 \times 0.26 \times 0.25$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	0.23 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max} , completeness:	29.3° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	5364, 2923, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2582
$N(\text{param})_{\text{refined}}$:	165
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.50169(13)	0.3258(2)	0.50717(10)	0.0574(3)
O1	0.1820(4)	0.5895(6)	0.2193(3)	0.0821(11)
C1	0.7057(5)	0.3465(6)	0.3068(4)	0.0575(10)
H1	0.7759	0.2866	0.3622	0.069*
C2	0.7561(5)	0.3928(7)	0.1847(4)	0.0696(13)
H2	0.8622	0.3665	0.1591	0.084*
C3	0.6543(5)	0.4773(7)	0.0986(4)	0.0639(12)
C4	0.4980(5)	0.5176(5)	0.1393(4)	0.0542(10)
H4	0.4281	0.5747	0.0819	0.065*
C5	0.4414(5)	0.4752(5)	0.2646(3)	0.0451(8)
C6	0.2708(5)	0.5198(5)	0.2990(4)	0.0510(9)
C7	0.2099(4)	0.4795(5)	0.4315(3)	0.0447(8)
C8	0.0491(5)	0.5289(5)	0.4617(4)	0.0582(10)
H8	−0.0150	0.5829	0.3985	0.070*
C9	−0.0145(6)	0.4986(6)	0.5835(5)	0.0736(14)
H9	−0.1209	0.5327	0.6021	0.088*
C10	0.0790(6)	0.4172(7)	0.6790(5)	0.0708(13)
H10	0.0356	0.3982	0.7615	0.085*
C11	0.2351(5)	0.3651(5)	0.6515(4)	0.0582(11)
H11	0.2969	0.3088	0.7149	0.070*
C12	0.3019(5)	0.3966(5)	0.5278(3)	0.0452(8)
C13	0.5477(5)	0.3898(5)	0.3482(3)	0.0459(8)
C14	0.7167(7)	0.5189(9)	−0.0377(4)	0.0897(19)
H14	0.7875	0.4221	−0.0583	0.108*
C15	0.5995(8)	0.5186(9)	−0.1415(5)	0.100(2)
H15A	0.5429	0.4116	−0.1430	0.150*
H15B	0.6543	0.5352	−0.2232	0.150*
H15C	0.5221	0.6088	−0.1283	0.150*
C16	0.8335(7)	0.6665(9)	−0.0331(5)	0.0956(18)
H16A	0.7768	0.7661	−0.0034	0.143*
H16B	0.8760	0.6867	−0.1191	0.143*
H16C	0.9223	0.6411	0.0260	0.143*

*Corresponding author: Jin-Qiang Liu, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China, e-mail: liuque.zju@hotmail.com

Li Ji: Zhejiang Medicine Co., Ltd., R&D Center, Xinchang, Zhejiang Province 312500, P. R. China

Weizhou Wang: College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China

displacement factors $U_{\text{iso}}(\text{H}) = 1.2$ times $U_{\text{eq}}(\text{C, aromatic ring and methenyl})$, and $U_{\text{iso}}(\text{H}) = 1.5$ times $U_{\text{eq}}(\text{C, methyl})$. The final refinement by using geometrical restraints, with C–H = 0.93 Å (aromatic ring), C–H = 0.98 Å (methenyl), and C–H = 0.96 Å (methyl). The Flack parameter $x = 0.04(5)$ [4] was determined using 903 quotients $[(I+) - (I-)] / [(I+) + (I-)]$.

Comment

2-Isopropylthioxanthone (ITX), has been widely used in many processes such as printing inks, surface coatings, microelectronics, and photoresists [5]. Nevertheless, it was also widely used in UV curing to promote the polymerization of inks used in paper- or plastic-based packaging materials because of its high photoinitiation efficiency and absorption characteristics at near-UV range (370–385 nm) [6–9]. To obtain the basic experimental data of ITX, we had measured the solubility of ITX in seven different pure solvents from 299.15 to 329.85 K [10], which was very important for its large scale synthesis with high purity. When we completed that work, we found that the crystal structure of the title compound was not reported up to now.

A view of the molecular structure of the title compound is given in the Figure. The asymmetric unit contains one molecule of the title compound, which is constructed by the thioxanthone, and the isopropyl fragment. The whole thioxanthone is almost planar with the maximum deviation of 0.042 Å for C10. The bond lengths of C12–S1 and C13–S1 are 1.737(4) and 1.745(4) Å, respectively. The values are intermediate between the double and single bonds. The shortening of the C–S bonds showing the partial double-bond character. Bond lengths and angles are in accord with related structure [11].

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