

Qiao-Zhen Zhang,* Yan-Li Zhao,
Xin Chen and Ming YuCollege of Sciences, Tianjin University of
Science and Technology, Tianjin 300222,
People's Republic of ChinaCorrespondence e-mail:
zhang_qiaozhen@163.com

Key indicators

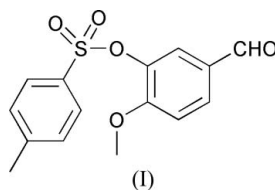
Single-crystal X-ray study
 $T = 294\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.048
 wR factor = 0.146
Data-to-parameter ratio = 15.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.5-Formyl-2-methoxyphenyl 4-methylbenzene-
sulfonate

In the title compound, $\text{C}_{15}\text{H}_{14}\text{O}_5\text{S}$, the isovanillin group makes a dihedral angle of $49.63(10)^\circ$ with the benzene ring. The crystal structure is stabilized by a weak non-classical intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond that forms a centrosymmetric dimer.

Received 6 November 2006
Accepted 24 November 2006

Comment

The background to this study has been described in an earlier paper (Zhang *et al.*, 2006).



Bond lengths and angles in the title compound, (I), are within normal ranges (Allen *et al.*, 1987). The isovanillin group (atoms C8–C14/O3/O4) is essentially planar (Fig. 1), with an r.m.s. deviation for fitted atoms of 0.0084 \AA . This group makes a dihedral angle of $49.63(10)^\circ$ with the benzene ring (C1–C6). The crystal structure is stabilized by a weak non-classical intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond (Table 1) that forms a centrosymmetric dimer (Fig. 2).

Experimental

An anhydrous benzene solution (100 ml) of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a benzene solution (100 ml) of 4-methylbenzene-1-sulfonyl chloride (1.91 g, 10 mmol) and pyridine (0.79 g, 10 mmol) and the mixture refluxed for

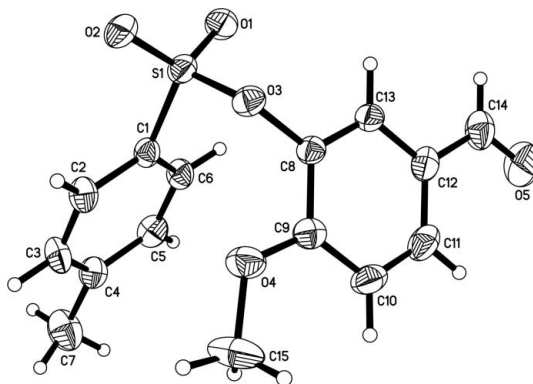


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

24 h under nitrogen. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The white precipitate was isolated, recrystallized from acetonitrile and then dried in a vacuum to give pure compound (I) in 56% yield. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

C₁₅H₁₄O₅S
M_r = 306.33
 Monoclinic, *P*2₁/*c*
a = 7.6465 (19) Å
b = 8.843 (2) Å
c = 22.000 (6) Å
 β = 99.457 (5)°
V = 1467.4 (6) Å³
Z = 4
D_x = 1.387 Mg m⁻³
 Mo *K*α radiation
 μ = 0.24 mm⁻¹
T = 294 (2) K
 Block, colorless
 0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.931, *T_{max}* = 0.958
 7922 measured reflections
 2994 independent reflections
 1622 reflections with *I* > 2σ(*I*)
R_{int} = 0.049
 θ_{max} = 26.5°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.048
wR(*F*²) = 0.146
S = 1.02
 2994 reflections
 191 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.2051P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.31 e Å⁻³
 Δρ_{min} = -0.33 e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C6–H6···O1 ⁱ	0.93	2.60	3.421 (3)	147

Symmetry code: (i) -*x*, -*y*, -*z* + 1.

H atoms were included in calculated positions (C–H = 0.93–0.96 Å) and refined as riding, with *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(methyl C).

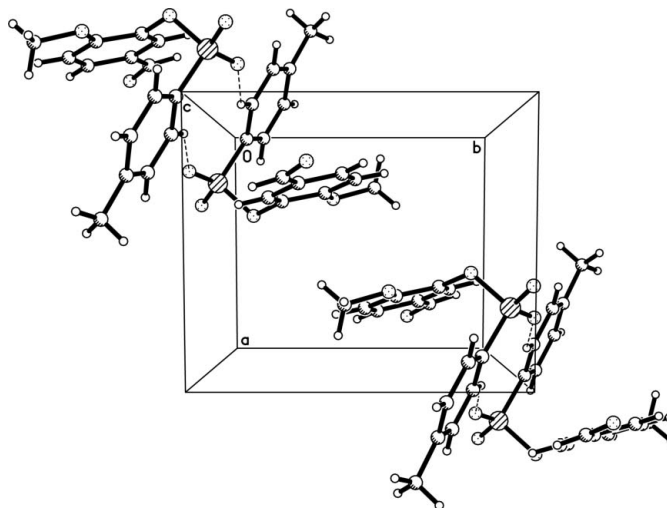


Figure 2

A partial packing diagram of (I), viewed along the *c* axis, with hydrogen bonds shown as dashed lines.

Data collection: SMART (Bruker, 1999); cell refinement: SAINTE (Bruker, 1999); data reduction: SAINTE; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
 Bruker (1999). SMART (Version 5.0) and SAINTE (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). SHELXTL. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
 Zhang, Q.-Z., Zhao, Y.-L., Chen, X. & Yu, M. (2006). *Acta Cryst. E* **62**, o5711–o5712.