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# 2,3,4-Trimethoxy-6-methylbenzaldehyde

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**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.041
*wR* factor = 0.119
Data-to-parameter ratio = 15.5

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



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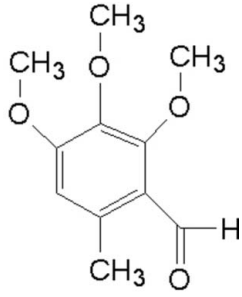
In the title compound, $C_{11}H_{14}O_4$, the aldehyde group and non-H atoms of the methoxy group at the *para* position are nearly coplanar with the benzene ring.

## Comment

The crystal structure of the title compound, (I), has been determined in order to elucidate the molecular conformation.



(I)

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters in Table 1.

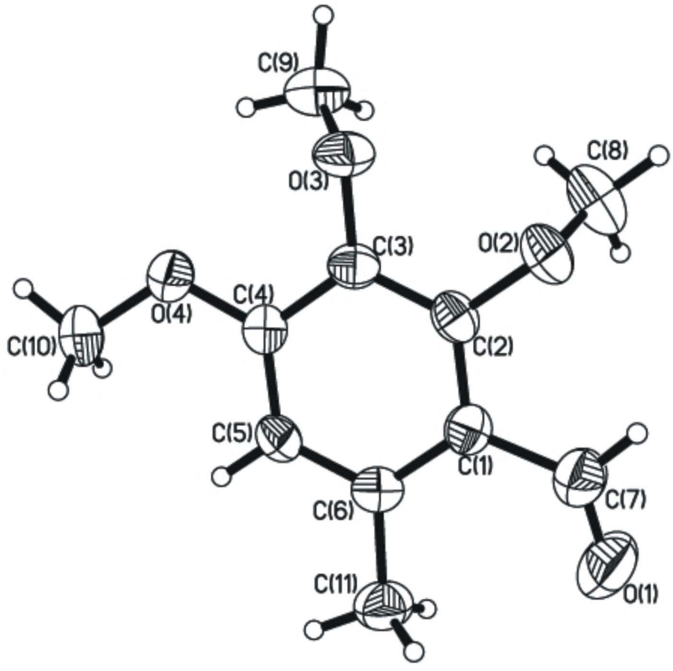



**Figure 1**
A view of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

## Experimental

Compound (I) was prepared according to the method of Ishii *et al.* (1992). To a stirred solution of 3,4,5-trimethoxytoluene (18.2 g, 100 mmol) and dimethylformamide (7.3 g, 100 mmol) in chloroform (200 ml) at room temperature was added phosphorus oxychloride (16 g, 100 mmol). The mixture was stirred for 1 h. The chloroform layer was washed with water three times, dried over $Na_2SO_4$ and concentrated. Compound (I) was recrystallized from petroleum ether (m.p. 333 K). Spectroscopic analysis: IR (KBr, $\nu$, $cm^{-1}$): 1680.

*Crystal data*

$C_{11}H_{14}O_4$
$M_r$ = 210.22
Monoclinic, $P2_1/n$
$a$ = 9.239 (2) Å
$b$ = 7.3884 (15) Å
$c$ = 15.649 (3) Å
$\beta$ = 92.329 (3)°
$V$ = 1067.3 (4) Å$^3$
$Z$ = 4
$D_x$ = 1.308 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1636 reflections
$\theta$ = 2.6–26.3°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 294 (2) K
Prism, colourless
0.20 × 0.14 × 0.12 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.972, $T_{max}$ = 0.988
5806 measured reflections
2180 independent reflections
1368 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 26.4°
$h = -11 \rightarrow 11$
$k = -9 \rightarrow 4$
$l = -19 \rightarrow 19$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.119
$S$ = 1.03
2180 reflections
141 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.1632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.019 (3)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C7 | 1.194 (2) | O4—C4 | 1.3551 (19) |
| O2—C2 | 1.380 (2) | C1—C7 | 1.472 (2) |
| O3—C3 | 1.3760 (19) | C11—C6 | 1.508 (2) |
| | | | |
| C2—O2—C8 | 114.36 (14) | C4—O4—C10 | 118.34 (14) |
| C3—O3—C9 | 115.72 (13) | O1—C7—C1 | 127.1 (2) |
| | | | |
| C10—O4—C4—C5 | −0.1 (2) | C8—O2—C2—C3 | −85.60 (19) |
| C9—O3—C3—C4 | −67.5 (2) | C6—C1—C7—O1 | 8.7 (3) |

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.96 Å). For the CH and $CH_2$ groups, $U_{iso}$(H) values were set equal to $1.2U_{eq}$(C) and for the methyl groups they were set equal to $1.5U_{eq}$(C).

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

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