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# 2,4,5-Trimethoxybenzaldehyde monohydrate

**Abdullah M. Asiri,[a,b] Salman A. Khan[b] and M. Nawaz Tahir[c]***

[a]The Center of Excellence for Advanced Materials Research, King Abdul Aziz University, Jeddah 21589, PO Box 80203, Saudi Arabia, [b]Department of Chemistry, Faculty of Science, King Abdul Aziz University, Jeddah 21589, PO Box 80203, Saudi Arabia, and [c]Department of Physics, University of Sargodha, Sargodha, Pakistan
Correspondence e-mail: dmntahir_uos@yahoo.com

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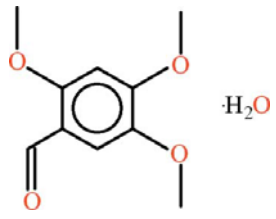
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.060; $wR$ factor = 0.212; data-to-parameter ratio = 12.9.

In the title compound, $C_{10}H_{12}O_4\cdot H_2O$, the 2,4,5-trimethoxybenzaldehyde molecule is almost planar (rms deviation = 0.0183 Å). There is an $R_1^2(5)$ ring motif due to O—H···O hydrogen bonding. In the crystal, the molecules are stabilized in the form of one-dimensional polymeric chains extending along [010] due to O—H···O hydrogen bonding with adjacent water molecules. The H atoms involved in intermolecular hydrogen bonding are disordered over two sets of sites of equal occupancy.

## Related literature

For related background and related structures, see: Asiri *et al.* (2010*a*,*b*), Hussain *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



## Experimental

### Crystal data

$C_{10}H_{12}O_4\cdot H_2O$
$M_r$ = 214.21
Monoclinic, $P2_1/c$
$a$ = 18.084 (5) Å
$b$ = 4.2456 (10) Å
$c$ = 14.600 (4) Å
$\beta$ = 108.290 (9)°
$V$ = 1064.3 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 296 K
0.22 × 0.10 × 0.08 mm

### Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.992, $T_{max}$ = 0.995
8287 measured reflections
1915 independent reflections
983 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.066

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.212
$S$ = 1.05
1915 reflections
148 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.22 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O5—H51···O2 | 0.85 (4) | 2.54 (5) | 3.181 (5) | 133 (4) |
| O5—H51···O3 | 0.85 (4) | 2.19 (4) | 3.006 (5) | 160 (4) |
| O5—H52···O5$^{i}$ | 0.83 (10) | 1.89 (10) | 2.710 (6) | 174 (19) |
| O5—H53···O5$^{ii}$ | 0.86 (10) | 1.86 (10) | 2.714 (6) | 169 (7) |

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2621).

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