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2-Hydroxy-5-methylbenzene-1,3-dicarbaldehyde

Deng-Tai Chen,[a] Lai-Jin Tian[a]* and Hai-Long Wang[b]

[a]Department of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China, and [b]Department of Chemistry, Shandong University, Jinan 250100, People's Republic of China
Correspondence e-mail: laijintian@163.com

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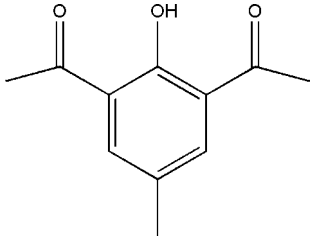
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.144; data-to-parameter ratio = 15.4.

The title compound, $C_{11}H_{12}O_3$, was synthesized by the acetylation of 4-methylphenol in the presence of aluminium trichloride. The molecule is essentially planar (r.m.s. deviation for all non-H atoms = 0.012 Å). There is a strong intramolecular hydrogen bond between the hydroxy group and the O atom of a carbonyl group.

Related literature

For related literature, see: Borisova *et al.* (2007); Khanjin & Menger (1997); Mandal & Nag (1983); Nanda *et al.* (1998); Ray & Gupta (1986).



Experimental

Crystal data

$C_{11}H_{12}O_3$
M_r = 192.21
Monoclinic, $P2_1/c$
a = 9.1404 (3) Å
b = 16.0798 (5) Å
c = 7.2639 (2) Å
β = 109.601 (2)°
V = 1005.75 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.22 × 0.16 × 0.03 mm

Data collection

Bruker SMART APEX detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.974, T_{max} = 0.990
17406 measured reflections
1966 independent reflections
1417 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.144
S = 1.05
1966 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.78	2.516 (2)	148

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2648).

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supplementary materials

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2-Hydroxy-5-methylbenzene-1,3-dicarbaldehyde

D.-T. Chen, L.-J. Tian and H.-L. Wang

Comment

The title compound is a important compound used to construct Schiff base ligand, especially macrocyclic Schiff base ligand, and the corresponding metal complexes (Borisova *et al.*, 2007; Khanjin & Menger, 1997; Mandal & Nag, 1983; Nanda *et al.*, 1998). We herein report its crystal structure (Fig. 1).

The bond lengths and angles are within normal ranges (Ray & Gupta, 1986). There is a strong intramolecular hydrogen bond between the hydroxy group (O2–H2) and the oxygen (O1) of a carbonyl group (Table 1). Because of the O2—H2···O1 interaction, the C═O distance [1.236 (2) Å] between C2 and O1 is longer than the C═O length [1.204 (3) Å] between C10 and O3. The title compound is essentially planar, with maximum deviation of 0.0296 (27) Å for methyl C11 atom of a acetyl group. In the crystal, the separation between two adjacent molecular planes is 3.502 Å.

Experimental

The title compound was synthesized by the acetylation of 4-methylphenol (5.4 g, 0.05 mol) with acetyl chloride (7.85 g, 0.1 mol) in the presence of aluminium trichloride in nitrobenzene (60 ml) according to the reported method (Mandal & Nag,1983). Colorless plate like crystals were obtained by slow evaporation of the ether solution at room temperature.

Refinement

The H atoms were placed at calculated positions and were included in the refinement in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic H atoms, C—H = 0.96 Å and U_{iso}(H) = 1.5Ueq(C) for methyl H atoms, and O—H = 0.82 Å and U_{iso}(H) = 1.5Ueq(O) for the hydroxy H atom.

Figures

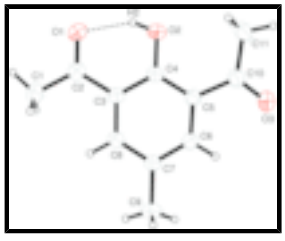

Fig. 1. The molecular structure of the title compound, with displacement ellipsoids are drawn at the 30% probability level. The hydrogen bond is indicated by a dashed line.

2-Hydroxy-5-methylbenzene-1,3-dicarbaldehyde

Crystal data

$C_{11}H_{12}O_3$ F_{000} = 408

M_r = 192.21	D_x = 1.269 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4532 reflections
a = 9.1404 (3) Å	θ = 2.5–23.8º
b = 16.0798 (5) Å	μ = 0.09 mm^{-1}
c = 7.2639 (2) Å	T = 295 (2) K
β = 109.601 (2)º	Plate, colorless
V = 1005.75 (5) Å^3	0.22 × 0.16 × 0.03 mm
Z = 4	

Data collection

Bruker SMART APEX detector diffractometer	1966 independent reflections
Radiation source: fine-focus sealed tube	1417 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 295(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −11→9
T_{min} = 0.974, T_{max} = 0.990	k = −17→19
17406 measured reflections	l = −8→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	H-atom parameters constrained
$wR(F^2)$ = 0.144	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.3303P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1966 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
128 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.55595 (18)	0.07936 (10)	0.6888 (3)	0.0887 (5)
O2	0.58456 (15)	0.23486 (9)	0.6841 (3)	0.0753 (5)
H2	0.5436	0.1899	0.6892	0.113*
O3	0.8741 (2)	0.43432 (10)	0.7143 (3)	0.1101 (7)
C1	0.7565 (3)	−0.01684 (14)	0.7204 (4)	0.0945 (8)
H1A	0.6757	−0.0559	0.7148	0.142*
H1B	0.8405	−0.0235	0.8415	0.142*
H1C	0.7936	−0.0267	0.6133	0.142*
C2	0.6942 (2)	0.06921 (13)	0.7073 (3)	0.0677 (5)
C3	0.7953 (2)	0.14150 (11)	0.7159 (3)	0.0542 (5)
C4	0.7344 (2)	0.22292 (11)	0.7045 (3)	0.0533 (4)
C5	0.8321 (2)	0.29126 (11)	0.7151 (3)	0.0540 (4)
C6	0.9857 (2)	0.27648 (12)	0.7345 (3)	0.0590 (5)
H6	1.0499	0.3220	0.7401	0.071*
C7	1.0489 (2)	0.19765 (12)	0.7458 (3)	0.0590 (5)
C8	0.9516 (2)	0.13103 (12)	0.7364 (3)	0.0574 (5)
H8	0.9913	0.0774	0.7441	0.069*
C9	1.2178 (2)	0.18455 (15)	0.7649 (4)	0.0869 (7)
H9A	1.2810	0.1867	0.9004	0.130*
H9B	1.2497	0.2274	0.6946	0.130*
H9C	1.2294	0.1312	0.7119	0.130*
C10	0.7809 (2)	0.38034 (13)	0.7063 (3)	0.0668 (5)
C11	0.6192 (3)	0.40390 (15)	0.6887 (4)	0.0879 (7)
H11A	0.6139	0.4628	0.7064	0.132*
H11B	0.5896	0.3753	0.7867	0.132*
H11C	0.5500	0.3887	0.5615	0.132*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0627 (9)	0.0737 (10)	0.1362 (15)	−0.0098 (7)	0.0421 (9)	0.0041 (9)
O2	0.0509 (8)	0.0701 (9)	0.1097 (12)	0.0068 (7)	0.0333 (8)	0.0048 (9)
O3	0.0883 (12)	0.0526 (9)	0.191 (2)	−0.0035 (8)	0.0496 (13)	−0.0004 (11)
C1	0.0787 (16)	0.0559 (13)	0.145 (2)	−0.0104 (11)	0.0317 (15)	−0.0035 (14)
C2	0.0600 (12)	0.0613 (12)	0.0821 (14)	−0.0049 (9)	0.0240 (10)	0.0010 (10)
C3	0.0500 (10)	0.0540 (10)	0.0582 (11)	−0.0004 (8)	0.0176 (8)	0.0005 (8)
C4	0.0456 (9)	0.0593 (11)	0.0551 (10)	0.0036 (8)	0.0170 (8)	0.0012 (8)
C5	0.0518 (10)	0.0525 (10)	0.0558 (10)	0.0039 (8)	0.0154 (8)	0.0009 (8)
C6	0.0506 (10)	0.0574 (11)	0.0659 (11)	−0.0050 (8)	0.0156 (8)	0.0007 (9)
C7	0.0471 (10)	0.0601 (11)	0.0679 (12)	0.0022 (8)	0.0169 (8)	−0.0005 (9)
C8	0.0511 (10)	0.0523 (10)	0.0671 (12)	0.0051 (8)	0.0174 (9)	0.0003 (8)
C9	0.0491 (12)	0.0871 (16)	0.123 (2)	0.0048 (11)	0.0269 (13)	−0.0010 (14)

C10	0.0682 (13)	0.0553 (11)	0.0736 (13)	0.0042 (10)	0.0192 (10)	−0.0002 (9)
C11	0.0780 (15)	0.0657 (14)	0.1142 (19)	0.0227 (11)	0.0248 (14)	−0.0002 (13)

Geometric parameters (Å, °)

O1—C2	1.236 (2)	C5—C10	1.502 (3)
O2—C4	1.341 (2)	C6—C7	1.384 (3)
O2—H2	0.8200	C6—H6	0.9300
O3—C10	1.204 (3)	C7—C8	1.380 (3)
C1—C2	1.487 (3)	C7—C9	1.517 (3)
C1—H1A	0.9600	C8—H8	0.9300
C1—H1B	0.9600	C9—H9A	0.9600
C1—H1C	0.9600	C9—H9B	0.9600
C2—C3	1.474 (3)	C9—H9C	0.9600
C3—C8	1.395 (2)	C10—C11	1.488 (3)
C3—C4	1.414 (2)	C11—H11A	0.9600
C4—C5	1.402 (3)	C11—H11B	0.9600
C5—C6	1.384 (3)	C11—H11C	0.9600
C4—O2—H2	109.5	C8—C7—C6	117.28 (17)
C2—C1—H1A	109.5	C8—C7—C9	121.09 (18)
C2—C1—H1B	109.5	C6—C7—C9	121.63 (18)
H1A—C1—H1B	109.5	C7—C8—C3	122.12 (17)
C2—C1—H1C	109.5	C7—C8—H8	118.9
H1A—C1—H1C	109.5	C3—C8—H8	118.9
H1B—C1—H1C	109.5	C7—C9—H9A	109.5
O1—C2—C3	120.31 (18)	C7—C9—H9B	109.5
O1—C2—C1	119.06 (18)	H9A—C9—H9B	109.5
C3—C2—C1	120.63 (18)	C7—C9—H9C	109.5
C8—C3—C4	119.13 (16)	H9A—C9—H9C	109.5
C8—C3—C2	120.97 (17)	H9B—C9—H9C	109.5
C4—C3—C2	119.89 (16)	O3—C10—C11	119.1 (2)
O2—C4—C5	120.13 (16)	O3—C10—C5	118.68 (19)
O2—C4—C3	120.44 (16)	C11—C10—C5	122.19 (19)
C5—C4—C3	119.43 (16)	C10—C11—H11A	109.5
C6—C5—C4	118.47 (16)	C10—C11—H11B	109.5
C6—C5—C10	117.35 (17)	H11A—C11—H11B	109.5
C4—C5—C10	124.18 (17)	C10—C11—H11C	109.5
C5—C6—C7	123.56 (17)	H11A—C11—H11C	109.5
C5—C6—H6	118.2	H11B—C11—H11C	109.5
C7—C6—H6	118.2		
O1—C2—C3—C8	−179.9 (2)	C4—C5—C6—C7	−0.7 (3)
C1—C2—C3—C8	0.0 (3)	C10—C5—C6—C7	179.54 (18)
O1—C2—C3—C4	0.5 (3)	C5—C6—C7—C8	0.2 (3)
C1—C2—C3—C4	−179.6 (2)	C5—C6—C7—C9	179.40 (19)
C8—C3—C4—O2	179.81 (17)	C6—C7—C8—C3	0.2 (3)
C2—C3—C4—O2	−0.6 (3)	C9—C7—C8—C3	−179.02 (19)
C8—C3—C4—C5	−0.4 (3)	C4—C3—C8—C7	−0.1 (3)
C2—C3—C4—C5	179.23 (17)	C2—C3—C8—C7	−179.69 (18)
O2—C4—C5—C6	−179.46 (17)	C6—C5—C10—O3	0.8 (3)

C3—C4—C5—C6	0.7 (3)	C4—C5—C10—O3	−179.0 (2)
O2—C4—C5—C10	0.3 (3)	C6—C5—C10—C11	−179.08 (19)
C3—C4—C5—C10	−179.49 (17)	C4—C5—C10—C11	1.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	1.78	2.516 (2)	148

Fig. 1