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2,4-Diacetylbenzene-1,3-diol

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In the crystal structure of the title compound, $C_{10}H_{10}O_4$, there are two independent molecules in the asymmetric unit. Each molecule is characterized by intramolecular O—H···O hydrogen bonding. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds and π–π interactions.

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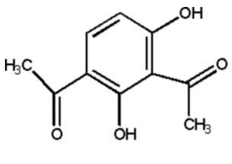
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.004 Å
R factor = 0.064
wR factor = 0.149
Data-to-parameter ratio = 10.5

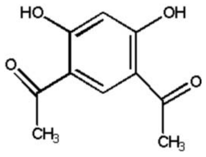
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Compounds containing the symmetrical resodiacetophenone, RDP (II), unit are of considerable interest for exploration of the basic coordination chemistry of metal complexes (Taha, 2003). In our attempts to prepare 1,3-diacetyl-4,6-dihydroxybenzene, (II), the unsymmetrical title compound, (I), was obtained instead; its melting point is 392 K. The melting point of (II) reported in the literature is 452 K (Emara & Abou-Hussen, 2006). Our interest in synthesizing simple molecules with potential hydrogen-bond donor and acceptor groups and examining their solid state structures to interpret their physical properties has prompted us to carry out a single-crystal X-ray diffraction study of (I) (Fig. 1).



(I)



(II)

In the crystal structure of (I) there are two independent molecules in the asymmetric unit. Excluding methyl H atoms, each molecule is essentially planar. The C═O bond lengths [1.246 (3)–1.250 (3) Å] are somewhat longer than those reported for 1,4-diacetylbenzene [1.221 (2) and 1.218 (2) Å; Liu *et al.*, 2006]. Each molecule exhibits intramolecular O—H···O hydrogen bonding (Fig. 1 and Table 1).

The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds (Table 1). The molecules pack in stacks parallel to the a axis. If the C1 molecule is a and the C1B molecule is b, then the stacks contain almost parallel molecules, alternating $ababab\cdots$. For the π–π interactions, the centroid(a)···centroid(b)($-x, \frac{1}{2}+y, \frac{1}{2}-z$) distance is 3.649 Å; the centroid(a)···centroid(b)($1-x, \frac{1}{2}+y, \frac{1}{2}-z$) distance is 3.727 Å.

Experimental

The title compound was prepared according to the previously described elegant one-pot procedure (Emara & Abou-Hussen, 2006).

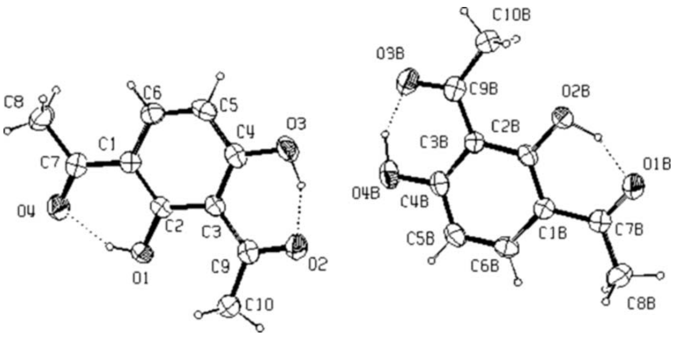


Figure 1
The asymmetric unit of (I), showing displacement ellipsoids at the 50% probability level for non-H atoms. Dotted lines indicate hydrogen bonds.

Rather than the formation of (II), having a melting point of 452 K, (I) was obtained in good yield (65%, m.p. 392 K). Orange needle crystals were obtained from an ethanol solution. Elemental analysis calculated for $C_{10}H_{10}O_4$: C 61.85, H 5.19%; found: C 60.27, H 4.39%.

Crystal data

$C_{10}H_{10}O_4$
$M_r = 194.18$
Monoclinic, $P2_1/c$
$a = 6.9666$ (3) Å
$b = 10.6786$ (7) Å
$c = 24.0792$ (14) Å
$\beta = 95.215$ (4)°
$V = 1783.92$ (17) Å^3
$Z = 8$
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 173$ (2) K
0.1 × 0.05 × 0.02 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
9562 measured reflections
3482 independent reflections
2097 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.082$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.149$
$S = 1.04$
3482 reflections
333 parameters
All H-atom parameters refined
$\Delta\rho_{\rm max} = 0.25$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1X···O4	0.88 (4)	1.69 (4)	2.506 (3)	153 (4)
O2B—H2Y···O1B	1.01 (4)	1.55 (4)	2.499 (3)	146 (4)
O3—H3X···O2	0.98 (4)	1.57 (4)	2.492 (3)	155 (4)
O4B—H4Y···O3B	1.06 (4)	1.50 (4)	2.475 (3)	150 (4)
C6B—H6B···O4$B^{\rm i}$	0.96 (3)	2.52 (3)	3.310 (4)	140 (2)
C8B—H8D···O3$B^{\rm ii}$	1.04 (4)	2.54 (4)	3.336 (4)	133 (3)
C10B—H10E···O1$B^{\rm iii}$	1.01 (3)	2.52 (3)	3.505 (4)	167 (2)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$; (iii) $-x+1, -y, -z+1$.

All H atoms were located in difference Fourier maps and refined freely. Refined distances are O—H = 0.88 (4)–1.06 (4) Å; C(ar)—H = 0.92 (3)–0.98 (3) Å; C(methyl) = 0.96 (3)–1.03 (5) Å. The range of refined $U_{\rm iso}$(H) values is 0.033 (7)–0.15 (2) Å^2.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor 1997); 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: *WinGX* (Farrugia, 1999).

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