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1-(2-Hydroxy-4,6-dimethylphenyl)-ethanone

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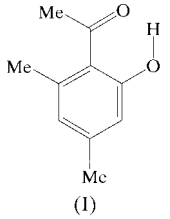
In the crystal of the title compound, $C_{10}H_{12}O_2$, there are two symmetry-independent molecules, which are essentially superimposable. Each molecule exhibits an intramolecular O—H···O hydrogen bond, with O···O separations of 2.483 (4) and 2.468 (4) Å.

Comment

Bismuth(III) β-diketonates are commonly used as precursor compounds in the synthesis of bismuth oxide-based materials (Fujiwara *et al.*, 1999; Ling, 1999; Barreca *et al.*, 1998; Boivin & Mairesse, 1998). For example, $Bi(dpm)_3$ (dpmH is 2,2,6,6-tetramethyl-3,5-heptanedione) has already been adopted as a source for the preparation of Bi_2O_3 films *via* CVD because of its high volatility and monomeric structure.

These compounds are also very attractive precursors in the sol-gel processing of materials. In this case, the organic fraction of the starting compounds should be kept at a minimum to avoid contamination of the final product. Accordingly, the synthesis of $Bi(acac)_3$ (acacH is 2,4-pentanedione) was planned following the same procedure used for the preparation of $Bi(dpm)_3$, *i.e.* starting from $Bi(C_6H_5)_3$ and acetylacetone. The reaction yielded the air-stable title compound, (I), which was fully characterized by IR and X-ray diffraction.



(I)

The asymmetric unit comprises two well separated perfectly superimposable molecules (r.m.s. of only 0.05 Å when the fitting is performed on the 12 non-H atoms). In each molecule (strictly planar, apart from the methyl H atoms), an effective intramolecular O—H···O hydrogen bond is present. It recalls those present in three substituted 2-hydroxy-4,6-dimethylchalcones (Satish Goud *et al.*, 1995); in particular, the angle at hydrogen is 146°.

Experimental

Anhydrous white solid $Bi(C_6H_5)_3$ (Aldrich) was added to colourless liquid acetylacetone (Aldrich) and the mixture warmed for 10 h at 403 K. The product, obtained by the reaction

$$2C_5H_8O_2 \rightarrow C_{10}H_{12}O_2 + 2H_2O,$$

?tpbgc=^st_head3_bgcolour]>was recrystallized from benzene.

Crystal data

$C_{10}H_{12}O_2$	$Z = 4$
$M_r = 164.20$	$D_x = 1.234$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.431$ (4) Å	Cell parameters from 50 reflections
$b = 7.604$ (3) Å	$\theta = 8.1$–$13.3°$
$c = 16.007$ (6) Å	$\mu = 0.085$ mm^{-1}
$\alpha = 93.61$ (3)°	$T = 293$ (2) K
$\beta = 95.50$ (4)°	Parallelepiped, pale yellow
$\gamma = 99.89$ (4)°	0.30 × 0.20 × 0.10 mm
$V = 884.0$ (7) Å^3	

Data collection

Nicolet *R*3*m*/*V* diffractometer	$h = 0 \rightarrow 8$
ω–2θ scans	$k = -8 \rightarrow 8$
2932 measured reflections	$l = -19 \rightarrow 19$
2917 independent reflections	2 standard reflections
1334 reflections with $I > 2\sigma(I)$	every 150 reflections
$R_{int} = 0.004$	intensity decay: none
$\theta_{max} = 25.57°$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1115P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.147$	$\Delta\rho_{max} = 0.27$ e Å^{-3}
$S = 0.913$	$\Delta\rho_{min} = -0.21$ e Å^{-3}
2917 reflections	Extinction correction: *SHELXL*93
218 parameters	Extinction coefficient: 0.0725 (89)
H-atom parameters constrained	

H atoms were refined using a riding model; methyl and hydroxyl protons were refined with 1.5 times, and for the phenyl H atoms with 1.2 times, the U_{eq} value of the parent atom.

Data collection, cell refinement and data reduction: *P*3/*P*4-*PC Diffractometer Control Program* (Siemens, 1991) program(s) used to solve structure: *SHELXTL*/*PC* (Sheldrick, 1994); program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993); software used to prepare material for publication: *SHELXTL*/*PC*.

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