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Key indicators

Single-crystal X-ray study

$T = 180$ K

Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å

R factor = 0.069

wR factor = 0.195

Data-to-parameter ratio = 20.7

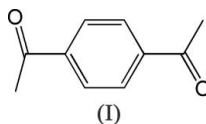
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

1,4-Diacetylbenzene

The asymmetric unit of the title compound, $\text{C}_{10}\text{H}_{10}\text{O}_2$, contains two half-molecules, each molecule being located on a centre of inversion. The dihedral angle between the planes of the two independent molecules is $39.67(4)^\circ$.

Comment

1,4-Diacetylbenzene is used in polymerization reactions to obtain polymers of quinoline derivatives (Bracke, 1969; Imai *et al.*, 1975). We report here the crystal structure of the title compound, (I).



The asymmetric unit of (I) contains two half-molecules, each molecule being located on a centre of inversion (Fig. 1). Selected geometric parameters are listed in Table 1. Corresponding bond lengths and angles in the two independent molecules agree with each other. Both the molecules are essentially planar; the dihedral angle between the planes of the two molecules is $39.67(4)^\circ$. No π - π stacking interactions or hydrogen bonds are observed in the crystal structure (Fig. 2).

Experimental

p-Ethylacetophenone (14.825 g, 0.1 mol) was added dropwise to a mixture of magnesium oxide (10.0 g, 0.25 mol), water (258 ml), concentrated nitric acid (34 ml, 0.53 mol) and potassium permanganate (39.5 g, 0.25 mol), with stirring at 332–334 K. The mixture was stirred further at 331–335 K for 4.5 h and then cooled, filtered by vacuum and dried. The powdered residue was dissolved in hot benzene (300 ml) to extract the crude product. This was slurried with cold anhydrous diethyl ether (70 ml), filtered, and dried to obtain white crystals of the title compound (13.3 g). Single crystals suitable for X-ray diffraction were obtained by dissolving the compound (2.0 g, 12.3 mmol) in benzene (25 ml) and allowing the solution to evaporate at room temperature for about 15 d.

Crystal data

$\text{C}_{10}\text{H}_{10}\text{O}_2$
 $M_r = 162.18$
 Monoclinic, $P2_1/n$
 $a = 12.699(3)$ Å
 $b = 5.4604(11)$ Å
 $c = 12.950(3)$ Å
 $\beta = 114.07(3)^\circ$
 $V = 819.9(4)$ Å³
 $Z = 4$

$D_x = 1.314$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 2627 reflections
 $\theta = 1.7$ – 31.1°
 $\mu = 0.09$ mm⁻¹
 $T = 180(2)$ K
 Prism, colourless
 $0.24 \times 0.15 \times 0.09$ mm

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Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2002)
 $T_{\min} = 0.979$, $T_{\max} = 0.992$
 6624 measured reflections

2297 independent reflections
 1979 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\text{max}} = 31.3^\circ$
 $h = -18 \rightarrow 18$
 $k = -7 \rightarrow 6$
 $l = -16 \rightarrow 17$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.069$
 $wR(F^2) = 0.195$
 $S = 1.16$
 2297 reflections
 111 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0962P)^2 + 0.1961P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.29 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e } \text{\AA}^{-3}$

Table 1Selected geometric parameters (\AA , $^\circ$).

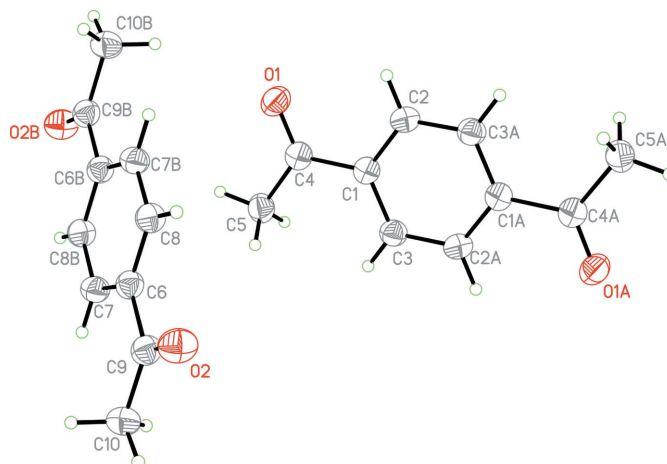
O1–C4	1.221 (2)	O2–C9	1.218 (2)
O1–C4–C1	119.89 (15)	O2–C9–C10	121.12 (15)
O1–C4–C5	121.29 (14)	O2–C9–C6	120.23 (15)

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C–H distances of 0.95 (aromatic) or 0.97 (methyl) \AA , and with $U_{\text{iso}}(\text{H}) = 1.2$ or 1.5 (methyl) times $U_{\text{eq}}(\text{C})$.

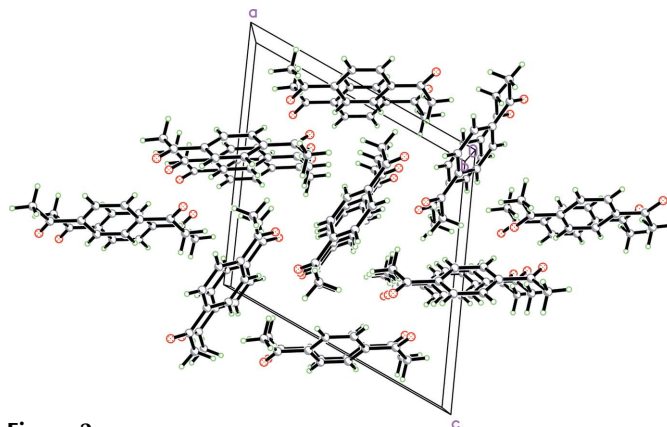
Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

References

- Bracke, W. (1969). *Macromolecules*, **2**, 286–289.
 Bruker (2001). SMART, SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
 Imai, Y., Johnson, E. F., Katto, T., Katto, T., Kurihara, M. & Stille, J. K. (1975). *J. Polym. Sci.* **13**, 2233–2249.

**Figure 1**

The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms labeled with the suffixes A and B are generated by the symmetry operations $(1 - x, -y, -z)$ and $(2 - x, -y, -z)$, respectively.

**Figure 2**

The crystal structure of (I).

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