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1,4-Diphenylbutane-1,4-dione

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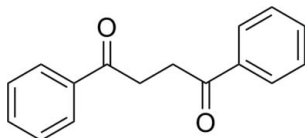
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å;
 R factor = 0.054; wR factor = 0.129; data-to-parameter ratio = 9.2.

The asymmetric unit of the title compound, $\text{C}_{16}\text{H}_{14}\text{O}_2$, contains one half-molecule, located on a twofold rotation axis. In the molecule, the two benzene rings form a dihedral angle of $72.28(2)^\circ$.

Related literature

For useful applications of 1,4-dicarbonyl compounds, see: Chiu & Sammes (1990); Greatrex *et al.* (2003); Nagarajan & Shechter (1984). For details of the synthesis, see Nevar *et al.* (2000).



Experimental

Crystal data

 $\text{C}_{16}\text{H}_{14}\text{O}_2$
 $M_r = 238.27$

 Orthorhombic, $P2_12_12$
 $a = 8.3781(13)$ Å

 $b = 14.161(2)$ Å

 $c = 5.3186(8)$ Å

 $V = 631.00(17)$ Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 0.08$ mm⁻¹
 $T = 298(2)$ K

 $0.20 \times 0.10 \times 0.10$ mm

Data collection

 Bruker SMART CCD area-detector
 diffractometer

Absorption correction: multi-scan

 (*SADABS*; Sheldrick, 1997)

 $T_{\min} = 0.984$, $T_{\max} = 0.992$

4063 measured reflections

762 independent reflections

 640 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.163$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.129$
 $S = 1.05$

762 reflections

83 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.20$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.22$ e Å⁻³

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The author is grateful to Ling Fan for a valuable discussion.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2479).

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supporting information

Acta Cryst. (2008). E64, o2423 [doi:10.1107/S1600536808038798]

1,4-Diphenylbutane-1,4-dione

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S1. Comment

1,4-Dicarbonyl compounds constitute key intermediates in various natural product syntheses, and they are important synthetic precursors of cyclopentenones, cyclopenta-1,3-diones, butenolides, and derivatives of furan and pyrrole (Chiu & Sammes, 1990; Greatrex *et al.*, 2003; Nagarajan & Shechter, 1984). Herewith we present the title compound (I) (Fig. 1). The asymmetric unit of (I) contains a half of the molecule located on a twofold rotational axis. Two benzene rings form a dihedral angle of 72.28 (2)°.

S2. Experimental

The title compound was synthesized as previously described by Nevar *et al.* (2000). Colourless crystals suitable for X-ray data collection were obtained by slow evaporation of a 1:3 ratio EtOAc:cyclohexane solution at room temperature.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding, allowing for free rotation of the methyl groups. The constraint $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ or $1.5 U_{\text{eq}}(\text{C})$ (methyl C) was applied. In the absence of anomalous scatterers, no attempt was made to establish the absolute configuration of the title compound, and 488 Friedel pairs were merged before the final refinement.

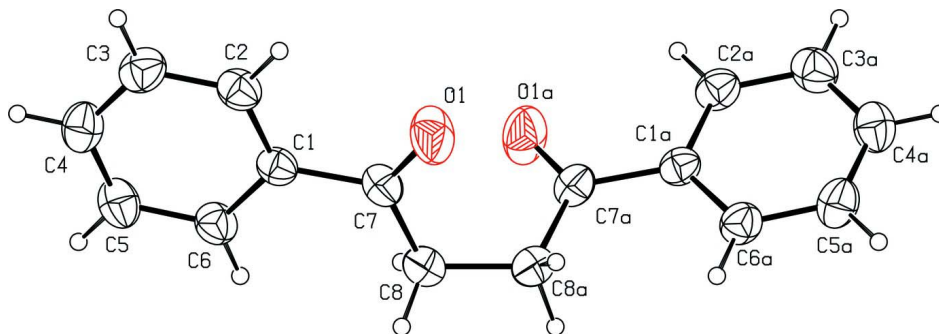


Figure 1

View of the title molecule showing the atom-labelling scheme. The displacement ellipsoids are drawn at the 30% probability level [symmetry code: (a) $-x, -y + 1, z$].

1,4-Diphenylbutane-1,4-dione

Crystal data

$\text{C}_{16}\text{H}_{14}\text{O}_2$

$M_r = 238.27$

Orthorhombic, $P2_12_12$

Hall symbol: P 2 2ab

$a = 8.3781$ (13) Å

$b = 14.161$ (2) Å

$c = 5.3186 (8) \text{ \AA}$
 $V = 631.00 (17) \text{ \AA}^3$
 $Z = 2$
 $F(000) = 252$
 $D_x = 1.254 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1423 reflections
 $\theta = 2.8\text{--}22.3^\circ$
 $\mu = 0.08 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Block, colourless
 $0.20 \times 0.10 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1997)
 $T_{\min} = 0.984$, $T_{\max} = 0.992$

4063 measured reflections
 762 independent reflections
 640 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.163$
 $\theta_{\max} = 26.0^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -10 \rightarrow 9$
 $k = -16 \rightarrow 17$
 $l = -6 \rightarrow 6$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.054$
 $wR(F^2) = 0.129$
 $S = 1.05$
 762 reflections
 83 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0734P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.012$
 $\Delta\rho_{\max} = 0.20 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$

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 $F^2 > \sigma(F^2)$ is used only for calculating 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1095 (3)	0.30567 (15)	0.2151 (4)	0.0508 (6)
C7	0.1070 (3)	0.40988 (16)	0.1653 (5)	0.0574 (7)
C4	0.1208 (3)	0.11385 (19)	0.3179 (6)	0.0699 (7)
H4	0.1241	0.0496	0.3532	0.084*
C8	0.0072 (4)	0.44647 (16)	-0.0468 (5)	0.0670 (7)
H8A	-0.0986	0.4191	-0.0354	0.080*
H8B	0.0540	0.4263	-0.2047	0.080*
C3	0.2031 (3)	0.17678 (17)	0.4670 (5)	0.0704 (8)
H3	0.2625	0.1548	0.6026	0.085*
C6	0.0283 (3)	0.24197 (17)	0.0654 (5)	0.0608 (7)

H6	-0.0307	0.2634	-0.0713	0.073*
C2	0.1980 (3)	0.27214 (16)	0.4163 (5)	0.0608 (7)
H2	0.2541	0.3142	0.5176	0.073*
O1	0.1843 (3)	0.46221 (13)	0.2966 (5)	0.0984 (8)
C5	0.0345 (3)	0.14619 (18)	0.1188 (6)	0.0712 (8)
H5	-0.0206	0.1037	0.0177	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0464 (11)	0.0571 (13)	0.0490 (11)	0.0054 (10)	0.0025 (10)	-0.0053 (10)
C7	0.0558 (13)	0.0561 (13)	0.0603 (14)	0.0011 (11)	-0.0034 (12)	-0.0105 (11)
C4	0.0636 (15)	0.0595 (13)	0.0867 (18)	0.0061 (13)	0.0053 (15)	0.0043 (15)
C8	0.0839 (17)	0.0614 (14)	0.0555 (13)	0.0048 (13)	-0.0040 (14)	-0.0074 (11)
C3	0.0658 (16)	0.0769 (17)	0.0686 (16)	0.0155 (14)	-0.0023 (15)	0.0091 (15)
C6	0.0613 (14)	0.0604 (13)	0.0607 (13)	-0.0011 (11)	-0.0092 (13)	-0.0065 (12)
C2	0.0560 (14)	0.0676 (14)	0.0589 (14)	0.0046 (12)	-0.0060 (12)	-0.0094 (12)
O1	0.1149 (17)	0.0632 (11)	0.1172 (17)	-0.0067 (11)	-0.0544 (16)	-0.0120 (12)
C5	0.0696 (17)	0.0597 (14)	0.0843 (17)	-0.0059 (13)	-0.0060 (16)	-0.0117 (14)

Geometric parameters (Å, °)

C1—C6	1.382 (3)	C8—H8A	0.9700
C1—C2	1.386 (3)	C8—H8B	0.9700
C1—C7	1.499 (3)	C3—C2	1.378 (3)
C7—O1	1.207 (3)	C3—H3	0.9300
C7—C8	1.496 (3)	C6—C5	1.387 (4)
C4—C5	1.361 (4)	C6—H6	0.9300
C4—C3	1.378 (3)	C2—H2	0.9300
C4—H4	0.9300	C5—H5	0.9300
C8—C8 ⁱ	1.521 (4)		
C6—C1—C2	119.0 (2)	H8A—C8—H8B	107.8
C6—C1—C7	122.3 (2)	C4—C3—C2	120.4 (2)
C2—C1—C7	118.74 (19)	C4—C3—H3	119.8
O1—C7—C8	121.5 (2)	C2—C3—H3	119.8
O1—C7—C1	119.7 (2)	C1—C6—C5	120.1 (2)
C8—C7—C1	118.8 (2)	C1—C6—H6	119.9
C5—C4—C3	119.7 (2)	C5—C6—H6	119.9
C5—C4—H4	120.1	C3—C2—C1	120.2 (2)
C3—C4—H4	120.1	C3—C2—H2	119.9
C7—C8—C8 ⁱ	112.9 (2)	C1—C2—H2	119.9
C7—C8—H8A	109.0	C4—C5—C6	120.6 (2)
C8 ⁱ —C8—H8A	109.0	C4—C5—H5	119.7
C7—C8—H8B	109.0	C6—C5—H5	119.7
C8 ⁱ —C8—H8B	109.0		
C6—C1—C7—O1	-177.5 (3)	C2—C1—C6—C5	0.7 (3)

C2—C1—C7—O1	1.7 (4)	C7—C1—C6—C5	179.8 (3)
C6—C1—C7—C8	2.8 (3)	C4—C3—C2—C1	0.2 (4)
C2—C1—C7—C8	-178.0 (2)	C6—C1—C2—C3	-0.6 (4)
O1—C7—C8—C8 ⁱ	-9.8 (4)	C7—C1—C2—C3	-179.9 (2)
C1—C7—C8—C8 ⁱ	169.9 (3)	C3—C4—C5—C6	-0.3 (4)
C5—C4—C3—C2	0.3 (4)	C1—C6—C5—C4	-0.2 (4)

Symmetry code: (i) $-x, -y+1, z$.