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2,4-Dimethyl-1,5-diphenylpenta-1,4-dien-3-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.099
Data-to-parameter ratio = 7.0

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

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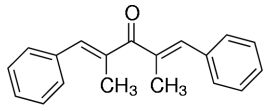
In the crystal structure of the title compound, $C_{19}H_{18}O$, there is one-half molecule in the asymmetric unit and the carbonyl group is located on a crystallographic twofold rotation axis. The olefinic bond is in an *anti* configuration.

Comment

α,β-Unsaturated ketones have attracted considerable interest because they are versatile intermediates in organic synthesis, especially in the synthesis of natural and bioactive products (Fuchs & Paquette, 1994).



(I)

The molecule of the title compound, (I), lies on a crystallographic twofold rotation axis (Fig. 1). The olefinic bond is in an *anti* configuration. Some unexpected bond angles (Table 1) may be the result of steric repulsions in the molecule. The molecules are stretched into an undulating ribbon structure along the *c* axis and pack into infinite chains parallel to each other along the *b* axis (Fig. 2).

Experimental

Pentan-3-one (0.86 g, 10 mmol) and benzaldehyde (1.06 g, 10 mmol) were dissolved in ethanol (25 ml). To the mixture was added 10% aqueous NaOH (10 ml, 25 mmol). The mixture was stirred at room temperature for 2 h. The reaction mixture was extracted with CH_2Cl_2, dried with anhydrous $MgSO_4$ and recrystallized from ethanol to produce the title compound, (I) (Concellon & Huerta, 2003).

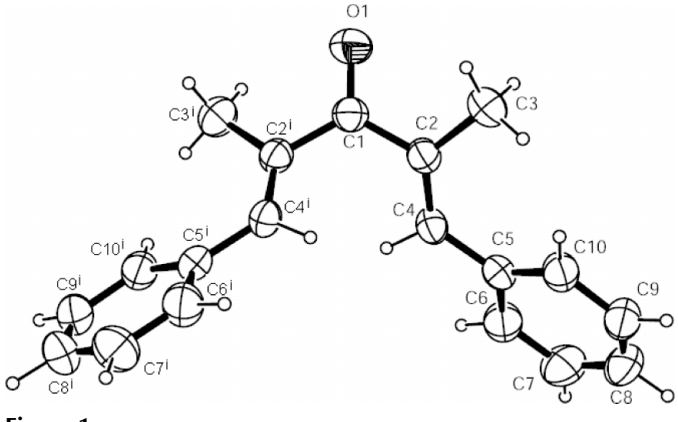


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids. [Symmetry code: (i) $1-x, y, -z$.]

Crystal data

$C_{19}H_{18}O$	D_x = 1.199 Mg m^{-3}
M_r = 262.35	Mo Kα radiation
Monoclinic, *C*2	Cell parameters from 2926 reflections
a = 10.5362 (6) Å	θ = 3.7–27.3°
b = 6.5254 (2) Å	μ = 0.07 mm^{-1}
c = 10.6656 (4) Å	*T* = 296 (1) K
β = 97.790 (1)°	Chunk, colorless
V = 726.52 (5) Å^3	0.33 × 0.30 × 0.17 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	904 independent reflections
ω scans	715 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.027
T_{min} = 0.953, T_{max} = 0.988	θ_{max} = 27.4°
3380 measured reflections	$h = -13 \rightarrow 13$
	$k = -8 \rightarrow 8$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[0.0019F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.099	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.10 e Å^{-3}
715 reflections	Extinction correction: (Larson, 1970)
93 parameters	
H-atom parameters constrained	Extinction coefficient: 3.0 (5) × 10^2

Table 1
Selected geometric parameters (°).

O1—C1—C2	119.1 (1)	C2—C4—C5	128.8 (2)
C1—C2—C3	114.4 (2)	C4—C5—C10	124.2 (2)
C1—C2—C4	119.7 (2)	C4—C5—C6	117.9 (2)
C4—C2—C3	125.5 (2)		
C3—C2—C4—C5	−0.8 (2)	C2—C4—C5—C10	−31.5 (2)

In the absence of significant anomalous dispersion effects, Friedel-pair reflections were merged before the final refinement. The H atoms were positioned geometrically and treated as riding, with C—H distances of 0.97 Å and U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

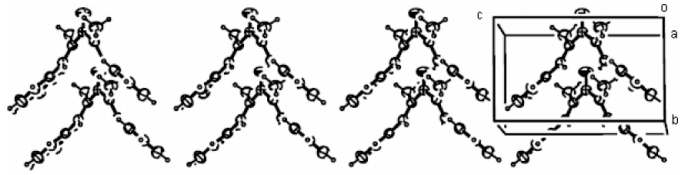


Figure 2
The crystal structure of (I).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.

Concellon, J. M. & Huerta, M. (2003). *Tetrahedron Lett.* **44**, 1931–1934.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Fuchs, K. & Paquette, L. A. (1994). *J. Org. Chem.* **59**, 528–532.

Higashi, T. (1995). *ABSCOR.* Rigaku Corporation, Tokyo, Japan.

Larson, A. C. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 291–294. Copenhagen: Munksgaard.

Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2004). *CrystalStructure.* Version 3.6.0. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX, USA 77381–5209.

Watkin, D. J., Prout, C. K., Carruthers, J. R. & Betteridge, P. W. (1996). *CRYSTALS.* Issue 10. Chemical Crystallography Laboratory, Oxford, England.