

## 4'-Methylchalcone

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The molecule of the title compound [systematic name: 3-(4-methylphenyl)-1-phenylprop-2-enone],  $C_{16}H_{14}O$ , displays a significant deviation from planarity; the torsion angle of the carbonyl oxygen and the three enone C atoms is  $16.3(3)^\circ$ , while the dihedral angle between the two benzene rings is  $50.7(2)^\circ$ .

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## Key indicators

Single-crystal X-ray study

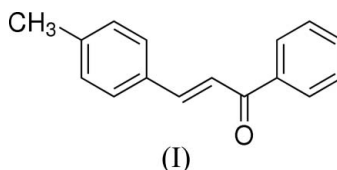
 $T = 298\text{ K}$ Mean  $\sigma(C-C) = 0.003\text{ \AA}$  $R$  factor = 0.050 $wR$  factor = 0.148

Data-to-parameter ratio = 12.2

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

## Comment

In our preparation of a series of chalcones, we obtained pale-yellow crystals of 3-(4-methylphenyl)-1-phenylprop-2-enone, (I). While the crystal structures of the related *p*-methylchalcone and *p,p'*-dimethylchalcone have been determined (Toda *et al.*, 1998; Rabinovich & Shakked, 1974), the structure of (I) has not been reported.



As in other chalcone structures, the enone unit in (I) (Fig. 1) is arranged in a *cisoid* relationship, and effects of the conjugation are seen in the longer  $C=C$  and shorter  $C-C$  bonds (Rabinovich, 1970; Ravishankar *et al.*, 2003; Selvi *et al.*, 2003; Toda *et al.*, 1998) (Table 1). The enone unit is not planar, with an  $O1-C1-C2-C3$  torsion angle of  $16.3(3)^\circ$ . The two benzene rings are not coplanar with the enone system; there is a  $11.0(4)^\circ$  angle between the C4-benzene ring and the enone system ( $C2-C3-C4-C5$ ) and a  $25.4(3)^\circ$  angle between the 1-benzene ring and the enone system ( $C2-C1-C10-C15$ ). This non-linearity is commonly observed in other *p'*-substituted chalcones (Rabinovich & Schmidt, 1970; Rabinovich *et*

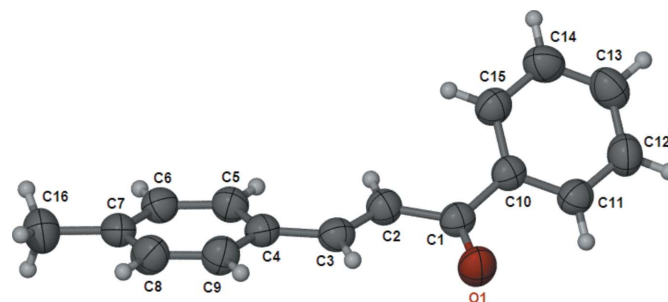


Figure 1

The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level.

*al.*, 1973; Warshel *et al.*, 1974; Toda *et al.*, 1998; Li *et al.*, 1992), and is likely due to the accommodation of the bulky 4-substituent within the crystal structure.

### Experimental

To a solution of acetophenone (1.6 ml, 0.014 mol) in 95% ethanol (10 ml) was added *p*-tolualdehyde (1.4 ml, 0.012 mol), and the mixture was stirred for 6 min. Water (10 ml) was added and the crude product collected by vacuum filtration; recrystallization from hot ethanol by slow cooling gave 1.39 g (52% yield) of the chalcone as pale-yellow crystals (m.p. 367.0–369.3 K).

#### Crystal data

$C_{16}H_{14}O$	$Z = 4$
$M_r = 222.27$	$D_x = 1.203 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
$a = 5.8601 (6) \text{ \AA}$	$\mu = 0.57 \text{ mm}^{-1}$
$b = 16.732 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 12.5363 (16) \text{ \AA}$	Block, pale yellow
$\beta = 93.522 (9)^\circ$	$0.48 \times 0.16 \times 0.12 \text{ mm}$
$V = 1226.9 (2) \text{ \AA}^3$	

#### Data collection

Bruker P4 diffractometer	1398 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$R_{\text{int}} = 0.069$
Absorption correction: numerical ( <i>XPREP</i> ; Bruker, 1999)	$\theta_{\text{max}} = 61.8^\circ$
$T_{\text{min}} = 0.760$ , $T_{\text{max}} = 0.934$	3 standard reflections
2693 measured reflections	every 97 reflections
1886 independent reflections	intensity decay: none

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0728P)^2 + 0.2602P]$
$R[F^2 > 2\sigma(F^2)] = 0.050$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.148$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
1886 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
155 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

C1–C2	1.474 (3)	C2–C3	1.326 (3)
C1–C10	1.493 (3)	C3–C4	1.459 (3)
O1–C1–C2–C3	16.3 (3)	C2–C1–C10–C11	–157.5 (2)
O1–C1–C10–C11	23.2 (3)	C2–C1–C10–C15	25.4 (3)
O1–C1–C10–C15	–153.9 (2)	C4–C3–C2–C1	–176.8 (2)
C2–C3–C4–C5	11.0 (4)	C10–C1–C2–C3	–163.0 (2)
C2–C3–C4–C9	–171.4 (2)		

All H atoms were treated as riding, with C–H distances of 0.93–0.96  $\text{\AA}$ , and with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$  or  $1.5 U_{\text{eq}}(\text{methyl C})$ .

Data collection: *XSCANS* (Bruker, 1999); cell refinement: *XSCANS*; data reduction: *XPREP* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *X-SEED*.

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