

(2E)-3-(Biphenyl-4-yl)-1-(4-methoxyphenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study

$T = 296\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$

R factor = 0.057

wR factor = 0.145

Data-to-parameter ratio = 8.5

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

The title compound, $\text{C}_{22}\text{H}_{18}\text{O}_2$, was prepared from biphenyl-4-carbaldehyde and 4-methoxyacetophenone. The molecule deviates significantly from planarity.

Comment

For a structurally simple group of compounds, chalcones have displayed an impressive array of biological activities, among which antimalarial (Liu *et al.*, 2003), antiprotozoal (Nielson *et al.*, 1998), nitric oxide inhibition (Rajas *et al.*, 2002) and anti-cancer activities (Dinkova-Kostova *et al.*, 1998) have been cited in the literature. Among several organic compounds reported for non-linear optical (NLO) properties, chalcone derivatives are notable materials for their excellent blue-light transmittance and good crystallizability. They provide the necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002; Sarojini *et al.*, 2006). Substitution on either of the benzene rings greatly influences the non-centrosymmetric crystal packing. It is speculated that, in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of non-centrosymmetric crystals (Fichou *et al.*, 1988). The molecular hyperpolarizability is strongly influenced, not only by the electronic effect, but also by the steric effect of the substituent (Cho *et al.*, 1996). Prompted by this, and in a continuation of our quest to synthesize new materials which can find use in the photonics industry, we have synthesized new chalcones and studied their SHG (second harmonic generation) efficiency. In a continuation of our work on chalcones (Harrison *et al.*, 2005; Harrison, Yathirajan, Sarojini, Narayana & Vijaya Raj, 2006; Harrison, Yathirajan, Sarojini, Narayana & Indira, 2006; Harrison, Yathirajan, Anilkumar *et al.*, 2006), the present paper reports the crystal structure of a newly synthesized chalcone, (I), which was synthesized from biphenyl-4-carbaldehyde and 4-methoxyacetophenone.

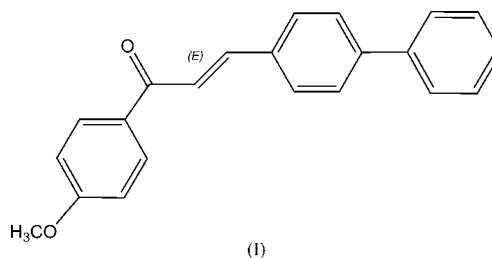


Fig. 1 shows the molecular structure of (I). The geometry of the molecule is unexceptional. The molecule deviates signifi-

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cantly from planarity, with dihedral angles of 8.51 (13)° between the rings of the biphenyl group and 54.14 (12)° between the C7–C12 ring and the C16–C21 ring.

Experimental

4-Methoxyacetophenone (1.5 g, 0.01 mol) in methanol (20 ml) was mixed with biphenyl-4-carbaldehyde (1.82 g, 0.01 mol) and the mixture was treated with 30% potassium hydroxide solution (3 ml) at 278 K. The reaction mixture was then brought to room temperature and stirred for 3 h. The solid precipitate was filtered off, washed with water, dried and recrystallized from acetone (m.p. 419–421 K). Analysis (%) for C₂₂H₁₈O₂ found (calculated): C 83.94 (84.05), H 5.66 (5.77).

Crystal data

| | |
|--|---|
| C ₂₂ H ₁₈ O ₂ | $V = 1633.08 (18) \text{ \AA}^3$ |
| $M_r = 314.38$ | $Z = 4$ |
| Monoclinic, Cc | Mo $K\alpha$ radiation |
| $a = 35.232 (3) \text{ \AA}$ | $\mu = 0.08 \text{ mm}^{-1}$ |
| $b = 7.4972 (5) \text{ \AA}$ | $T = 296 \text{ K}$ |
| $c = 6.2113 (3) \text{ \AA}$ | $0.58 \times 0.33 \times 0.12 \text{ mm}$ |
| $\beta = 95.509 (6)^\circ$ | |

Data collection

| | |
|---------------------------------------|--|
| Bruker–Nonius KappaCCD diffractometer | 1843 independent reflections |
| Absorption correction: none | 1408 reflections with $I > 2\sigma(I)$ |
| 10464 measured reflections | $R_{\text{int}} = 0.048$ |

Refinement

| | |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.057$ | 217 parameters |
| $wR(F^2) = 0.145$ | H-atom parameters constrained |
| $S = 1.12$ | $\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$ |
| 1843 reflections | $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$ |

Due to the absence of significant anomalous dispersion effects, Friedel pairs were merged prior to refinement. H atoms were placed at calculated positions and refined as riding on the respective carrier atom, with C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for Csp^2 or C–H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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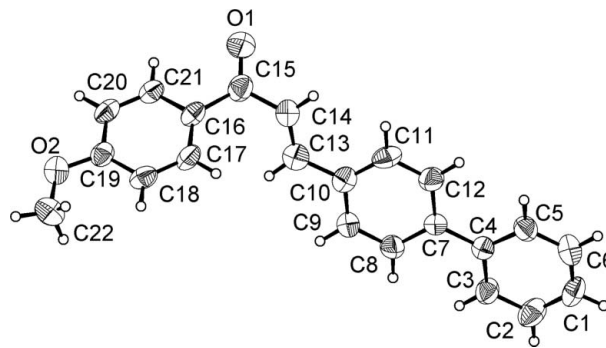


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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References

- Brandenburg, K. (2006). *DIAMOND*. Release 3.1d. Crystal Impact GbR, Bonn, Germany.
- Cho, B. R., Je, J. T., Kim, H. S., Jean, S. J., Song, O. K. & Wang, C. H. (1996). *Bull. Korean Chem. Soc.* **17**, 693–695.
- Dinkova-Kostova, A. T., Abey-Gunawardana, C. & Talalay, P. (1998). *J. Med. Chem.* **41**, 5287–5296.
- Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
- Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
- Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn. J. Appl. Phys.* **27**, 429–430.
- Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
- Harrison, W. T. A., Yathirajan, H. S., Anilkumar, H. G., Sarojini, B. K. & Narayana, B. (2006). *Acta Cryst. E* **62**, o3251–o3253.
- Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Anilkumar, H. G. (2005). *Acta Cryst. C* **61**, o728–o730.
- Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Indira, J. (2006). *Acta Cryst. E* **62**, o1647–o1649.
- Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Vijaya Raj, K. K. (2006). *Acta Cryst. E* **62**, o1578–o1579.
- Indira, J., Karat, P. P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
- Liu, M., Wilairat, P., Croft, S. L., Tan, A. L. C. & Go, M. I. (2003). *Bioorg. Med. Chem.* **11**, 2729–2738.
- Nielson, S. F., Christensen, S. B., Cruciani, G., Kharazmi, A. & Liljefors, T. (1998). *J. Med. Chem.* **41**, 4819–4832.
- Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Rajas, J., Paya, M., Domingues, J. N. & Ferrandiz, M. L. (2002). *Bioorg. Med. Chem. Lett.* **12**, 1951–1954.
- Sarojini, B. K., Narayana, B., Ashalatha, B. V., Indira, J. & Lobo, K. J. (2006). *J. Cryst. Growth*, **295**, 54–59.
- Sheldrick, G. M. (1997). *SHELXS97 and SHELXL97*. University of Göttingen, Germany.
- Tam, W., Guerin, B., Calabrese, J. C. & Stevenson, S. H. (1989). *Chem. Phys. Lett.* **154**, 93–96.
- Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.
- Westrip, S. P. (2007). *publCIF*. In preparation.