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3-(4-Chlorophenyl)-1-(2-naphthyl)prop-2-enone†

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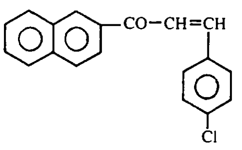
Abstract

The title molecule, $C_{19}H_{13}ClO$, has an *s-cis* conformation for the ketone system, with a torsion angle of −20.8 (4)°. The structure is stabilized by van der Waals interactions.

Comment

The chalcones derived from acetonaphthones are potential germicides, fungicides and anticarcinogens (Misra, Tewari & Nath, 1971). The carbonyl system plays an important role in the antibacterial activity of chalcones (Pinaka & Edwards, 1963). The present crystal structure study was undertaken to establish the structure and conformation of the chalcone (I).



(I)

The title molecule assumes an *s-cis* conformation for the ketone system as evidenced by the value of the O20—C11—C12—C13 torsion angle [−20.8 (4)°]. A similar conformation is observed in α,β-unsaturated ketone systems (Tokuno *et al.*, 1986; Eswaramoorthy, Ponnuswamy, Raju, Nanjundan & Krishnasamy, 1994). The C═O bond length of C11—O20 [1.213 (3) Å] is comparable to values reported in the literature (Zabel, Watson, Cassels & Langs, 1980; Shanmuga Sundara Raj, Ponnuswamy, Shanmugam & Nanjundan, 1996). The unsaturated ketone system is not strictly planar as can be seen from the values of the relevant torsion angles. The molecules run in a linear fashion along the **c** direction. The structure is stabilized by van der Waals interactions.

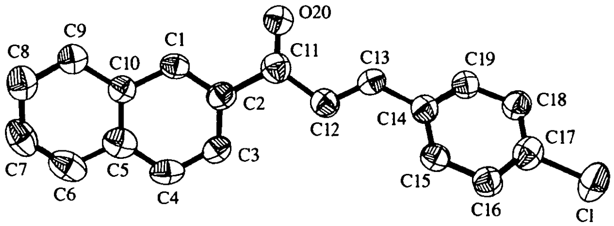


Fig. 1. *ORTEP*II (Johnson, 1976) plot of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

Experimental

The method of Jacobs & Singer (1952) was used for the preparation of the title compound.

Crystal data

$C_{19}H_{13}ClO$
$M_r = 292.74$
Triclinic
$P\bar{1}$
$a = 5.911\ (4)$ Å
$b = 7.474\ (3)$ Å
$c = 16.366\ (3)$ Å
$\alpha = 100.55\ (3)°$
$\beta = 91.90\ (3)°$
$\gamma = 91.62\ (4)°$
$V = 710.0\ (6)$ Å^3
$Z = 2$
$D_x = 1.369$ Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 18 reflections
$\theta = 16$–$23°$
$\mu = 2.327$ mm^{-1}
$T = 293\ (2)$ K
Needle
0.20 × 0.15 × 0.12 mm
Transparent

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2533 measured reflections
2351 independent reflections
2017 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.0850$
$\theta_{\rm max} = 65°$
$h = -6 \rightarrow 5$
$k = 0 \rightarrow 8$
$l = -19 \rightarrow 18$
3 standard reflections
frequency: 60 min
intensity decay: <1.5%

Refinement

Refinement on F^2
$R(F) = 0.0563$
$wR(F^2) = 0.1730$
$S = 1.066$
2351 reflections
242 parameters
All H atoms refined
$w = 1/[\sigma^2(F_o^2) + (0.1189P)^2 + 0.141P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} = -0.065$
$\Delta\rho_{\rm max} = 0.359$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.244$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

C2—C11	1.495 (3)	C12—C13	1.319 (4)
C11—O20	1.213 (3)	C13—C14	1.463 (3)
C11—C12	1.483 (4)	C17—Cl	1.748 (2)
C3—C2—C11	122.6 (2)	C12—C11—C2	118.5 (2)
O20—C11—C12	121.2 (2)	C13—C12—C11	120.4 (3)
O20—C11—C2	120.2 (2)	C12—C13—C14	128.2 (3)

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C10—C1—C2—C11	179.3 (2)	C11—C12—C13—C14	176.3 (2)
O20—C11—C12—C13	−20.8 (4)	C12—C13—C14—C19	170.8 (2)
C2—C11—C12—C13	160.2 (2)		

Data collection: *SDP* (Frenz, 1978). Cell refinement: *SDP*. Data reduction: *SDP*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1049). Services for accessing these data are described at the back of the journal.

References

Eswaramoorthy, S., Ponnuswamy, M. N., Raju, K. S., Nanjundan, S. & Krishnasamy, V. (1994). *Z. Kristallogr.* **209**, 669–672.

Frenz, B. A. (1978). *The Enraf–Nonius CAD-4 SDP – a Real-Time System for Concurrent X-ray Data Collection and Crystal Structure Solution. Computing in Crystallography*, edited by H. Schenk, R. Olthof-Hazekamp, H. van Koningsveld & G. C. Bassi, pp. 64–71. Delft University Press.

Jacobs, T. L. & Singer, S. (1952). *J. Org. Chem.* **17**, 475–481.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Misra, S. S., Tewari, R. S. & Nath, B. (1971). *Indian J. Appl. Chem.* **34**, 260–264.

Pinaka, M. & Edwards, J. (1963). *J. Sci. Food Agric.* **14**, 48–51.

Shanmuga Sundara Raj, S., Ponnuswamy, M. N., Shanmugam, G. & Nanjundan, S. (1996). *Acta Cryst.* **C52**, 3145–3146.

Sheldrick, G. M. (1985). *SHELXS*86. *Program for the Solution of Crystal Structures*. University of Göttingen, Germany.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

Tokuno, K., Matsui, M., Miyoshi, F., Asao, Y., Ohashi, T. & Kihara, K. (1986). *Acta Cryst.* **C42**, 85–88.

Zabel, V., Watson, W. H., Cassels, B. K. & Langs, D. A. (1980). *Cryst. Struct. Commun.* **9**, 461–467.

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3,4-Diiodo-2,5-dimethylhexa-2,4-diene

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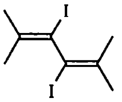
Abstract

The title compound, $C_8H_{12}I_2$, displays crystallographic twofold symmetry. The two double bonds are not conjugated [torsion angle −78.8 (5)° about the central single bond]. Intermolecular I···I contacts of 4.098 (1) Å connect the molecules into layers parallel to the *xy* plane.

Comment

As part of our general investigations on structural and spectroscopic features of π-systems (Hopf, Hänel & Traetteberg, 1994; Hopf & Hänel, 1994), we have recently become interested in orthogonal butadienes (*i.e.* those in which the planes of the π-bond systems are orthogonal). An example is provided by 2,3-di-*tert*-butyl-1,3-butadiene, for which the orthogonal structure has been established by electron diffraction (Hopf, Traetteberg & Hänel, 1994) and X-ray structure analysis (at 110 K, torsion angle 84°; Roth, Adamczak, Breuckmann, Lennartz & Boese, 1991).

The title compound, (I) (Fig. 1), displays crystallographic twofold symmetry. It can be seen that even the iodine substituents, which are only moderately bulky compared with *tert*-butyl groups, can force the two double bonds almost completely out of conjugation; the dihedral angle C2—C3—C3^i—C2^i is −78.8 (5)° [symmetry code: (i) $1-x, y, \frac{1}{2}-z$]. The central C3—C3^i bond is, at 1.469 (5) Å, closer to the standard value for non-conjugated C_{sp^2}—C_{sp^2} (1.478 *cf.* 1.455 Å in conjugated systems; Allen *et al.*, 1987) and C2—C3 is, at 1.334 (4) Å, close to the standard value of 1.331 Å for $R_2C{=}CR_2$.



(I)

Several bond angles display marked deviations from ideal values: C1—C2—C4 113.8 (3), C1—C2—C3 125.6 (3) and C3^i—C3—I 112.74 (15)°. This presumably reflects steric pressure, although it is surprising that the angle between the methyl groups is so narrow.

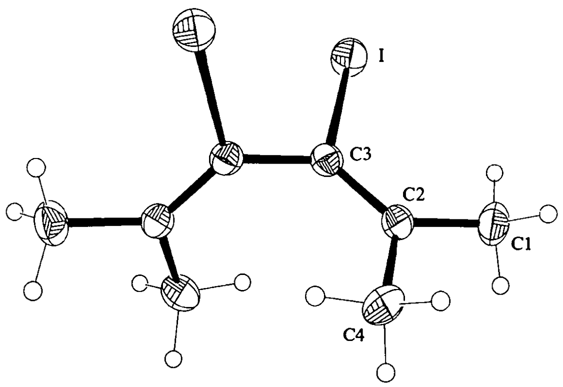


Fig. 1. The molecule of the title compound in the crystal. Ellipsoids represent 50% probability levels. Only the asymmetric unit is numbered. H-atom radii are arbitrary.

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