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# 1-(2-Naphthyl)-3-(4-nitrophenyl)prop-2-en-1-one†

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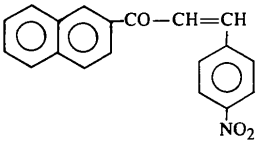
## Abstract

The crystal structure of the title compound, $C_{19}H_{13}NO_3$, has been solved by direct methods and refined to a final *R* value of 0.058. The molecule is found to have an *s-cis* conformation for the ketone system, with a torsion angle of −19.4 (6)°. The molecules are packed *via* van der Waals-type 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 (Pianka & Edwards, 1963). A crystal structure study of the title compound, (I), was undertaken in order to establish the structure and conformation of the various groups.



(I)

An *ORTEP*II (Johnson, 1976) plot of the title molecule is shown in Fig. 1. The molecule assumes an *s-cis* conformation for the ketone system as seen from the conformational angle O20—C11—C12—C13 of −19.4 (6)°. A similar kind of situation is observed with α,β-unsaturated ketone systems (Tokuno *et al.*, 1986; Eswaramoorthy, Ponnuswamy, Raju, Nanjundan & Krishnasamy, 1994). The C=O bond length [C11=O20 1.222 (4) Å] is comparable to values reported in the literature (Zabel, Watson, Cassels & Langs, 1980). The unsaturated ketone group is not strictly in a planar conformation, as can been seen from the torsion angles C1—C2—C11—C12 162.0 (3), C2—C11—C12—C13 161.5 (4), C11—C12—C13—C14 175.5 (4) and C12—C13—C14—C15 174.8 (4)°. It is significant that the π-electron conjugation and the non-planarity of the molecule are interrelated.

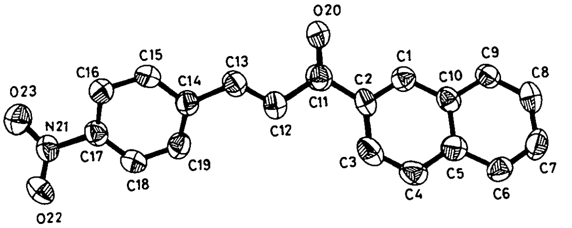


Fig. 1. *ORTEP*II (Johnson, 1976) plot of the title molecule with the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level.

The naphthalene ring is planar [maximum deviation ±0.021 (4) Å] and at an angle of 135.8 (1)° with respect to the phenyl group. The short contact H3···H12 [2.22 (4) Å] should open up the C2—C11—C12 angle or result in torsional rotation around the C2—C11 bond [observed at 18°]. Also, the H12···H19 contact [2.44 (2) Å] should result either in an opening of the C12—C13—C14 angle or in a rotation of the nitrophenyl group around the C13—C14 bond. Since the torsion angle C12—C13—C14—C19 is only −7.9 (5)°, it is clear that some of the strain induced by the short contact is being adjusted by the opening of the C12—C13—C14 angle [128.2 (4)°]. The reason for the different behaviour at different locations of the molecule could be because of the interplay between the conjugational forces and the intramolecular interactions. The structure packs in a linear fashion along the **c** direction. It is interesting to observe two C—H···O-type hydrogen bonds (Table 3) (Desiraju, 1989).

## Experimental

Pale-yellow needle-shaped crystals were grown from a 1:2 chloroform–methanol mixture.

*Crystal data*

$C_{19}H_{13}NO_3$
$M_r = 303.32$
Triclinic
$P\bar{1}$
$a = 6.060\,(2)$ Å
$b = 7.185\,(3)$ Å
$c = 16.872\,(6)$ Å
$\alpha = 101.44\,(3)°$
$\beta = 91.93\,(3)°$
$\gamma = 86.93\,(4)°$
$V = 718.8\,(5)$ Å$^3$
$Z = 2$
$D_x = 1.40$ Mg m$^{-3}$
$D_m$ not measured

Cu *K*α radiation
$\lambda = 1.5418$ Å
Cell parameters from 13 reflections
$\theta = 18–26°$
$\mu = 0.738$ mm$^{-1}$
$T = 298$ K
Needle
0.25 × 0.22 × 0.16 mm
Pale yellow

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† DCB contribution No. 874.

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: empirical *via* $\psi$ scans (North, Phillips & Mathews, 1968)
$T_{\min} = 0.832$, $T_{\max} = 0.973$
2732 measured reflections
2531 independent reflections
2128 observed reflections [$I > 3\sigma(I)$]
$R_{\rm int} = 0.034$
$\theta_{\max} = 70°$
$h = -7 \rightarrow 7$
$k = 0 \rightarrow 8$
$l = -20 \rightarrow 20$
3 standard reflections monitored every 200 reflections
frequency: 120 min
intensity decay: 1.2%

*Refinement*

Refinement on $F$
$R = 0.058$
$wR = 0.064$
$S = 2.16$
2128 reflections
260 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) + 0.0001F^2]$
$(\Delta/\sigma)_{\max} = 0.012$
$\Delta\rho_{\max} = 0.24$ e Å$^{-3}$
$\Delta\rho_{\min} = 0.15$ e Å$^{-3}$
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å$^2$)*

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

| | $x$ | $y$ | $z$ | $B_{\rm eq}$ |
|---|---|---|---|---|
| C1 | −0.0332 (4) | 0.6851 (3) | −0.1474 (1) | 3.69 (5) |
| C2 | 0.1102 (4) | 0.7424 (4) | −0.0838 (1) | 3.90 (7) |
| C3 | 0.3179 (4) | 0.8086 (4) | −0.0991 (2) | 4.38 (9) |
| C4 | 0.3719 (4) | 0.8180 (4) | −0.1754 (2) | 4.31 (8) |
| C5 | 0.2279 (4) | 0.7591 (3) | −0.2421 (2) | 3.81 (5) |
| C6 | 0.2807 (5) | 0.7640 (4) | −0.3232 (2) | 4.52 (9) |
| C7 | 0.1364 (5) | 0.7027 (4) | −0.3852 (2) | 4.89 (9) |
| C8 | −0.0675 (5) | 0.6332 (4) | −0.3704 (2) | 4.63 (8) |
| C9 | −0.1236 (4) | 0.6250 (4) | −0.2942 (1) | 3.95 (7) |
| C10 | 0.0204 (4) | 0.6891 (3) | −0.2274 (1) | 3.58 (5) |
| C11 | 0.0376 (5) | 0.7388 (4) | −0.0007 (2) | 4.35 (8) |
| C12 | 0.2071 (5) | 0.7439 (4) | 0.0657 (2) | 4.50 (8) |
| C13 | 0.1458 (4) | 0.7928 (4) | 0.1417 (2) | 4.06 (8) |
| C14 | 0.2818 (4) | 0.7946 (3) | 0.2153 (1) | 3.57 (5) |
| C15 | 0.1858 (4) | 0.8666 (4) | 0.2893 (1) | 3.86 (7) |
| C16 | 0.2963 (4) | 0.8632 (4) | 0.3613 (1) | 3.82 (7) |
| C17 | 0.5114 (4) | 0.7896 (3) | 0.3582 (1) | 3.63 (5) |
| C18 | 0.6164 (4) | 0.7198 (3) | 0.2863 (1) | 3.84 (5) |
| C19 | 0.4996 (4) | 0.7211 (4) | 0.2154 (1) | 3.98 (7) |
| O20 | −0.1580 (3) | 0.7293 (3) | 0.0126 (1) | 5.75 (7) |
| N21 | 0.6327 (4) | 0.7858 (3) | 0.4350 (1) | 4.54 (6) |
| O22 | 0.8326 (3) | 0.7908 (4) | 0.4358 (1) | 6.32 (7) |
| O23 | 0.5273 (4) | 0.7800 (4) | 0.4941 (1) | 6.82 (7) |

Table 2. *Selected geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C2—C11 | 1.489 (4) | C13—C14 | 1.465 (4) |
| C11—C12 | 1.491 (5) | N21—O22 | 1.213 (3) |
| C11—O20 | 1.222 (4) | N21—O23 | 1.211 (3) |
| C12—C13 | 1.321 (5) | | |
| C2—C11—O20 | 120.4 (3) | C12—C13—C14 | 128.2 (4) |
| C2—C11—C12 | 119.1 (4) | C13—C14—C19 | 123.7 (4) |
| C12—C11—O20 | 120.5 (3) | C13—C14—C15 | 118.2 (3) |
| C11—C12—C13 | 119.5 (7) | C15—C14—C19 | 118.1 (3) |
| C1—C2—C11—C12 | 162.0 (3) | C2—C11—C12—C13 | 161.5 (4) |
| C1—C2—C11—O20 | −17.0 (6) | O20—C11—C12—C13 | −19.4 (6) |
| C3—C2—C11—C12 | −20.1 (6) | C11—C12—C13—C14 | 175.5 (4) |
| C3—C2—C11—O20 | 160.8 (4) | C12—C13—C14—C15 | 174.8 (4) |

Table 3. *Hydrogen-bonding geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···O23$^{\rm i}$ | 0.98 (4) | 2.55 (4) | 3.314 (3) | 135 (3) |
| C16—H16···O22$^{\rm ii}$ | 0.98 (3) | 2.69 (3) | 3.225 (3) | 115 (2) |

Symmetry codes: (i) $x, y, z - 1$; (ii) $x - 1, y, z$.

A total of 2128 reflections out of 2531 unique reflections were found to be observed with $|F_o| > 6\sigma(|F_o|)$ and used for structure analysis and least-squares refinement. The structure was solved by direct methods and refinement was carried out by full-matrix least-squares procedures. The $R$ value was observed to be 0.058 and $wR$ 0.064 in the final refinement.

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: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *PLUTO* (Motherwell & Clegg, 1978) and *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

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Lists of structure factors, least-squares-planes data, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: DE1029). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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