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# 2-(4-Nitrophenyl)-6-phenyltetrahydropyran-4-one

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**Key indicators**

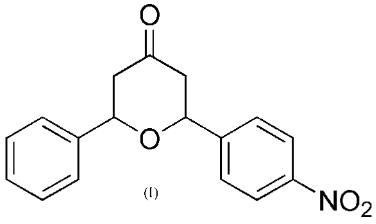
Single-crystal X-ray study
*T* = 297 K
Mean $\sigma$(C–C) = 0.003 Å
*R* factor = 0.059
*wR* factor = 0.152
Data-to-parameter ratio = 17.3

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

The crystal structure of the title compound, $C_{17}H_{15}NO_4$, is stabilized by intermolecular C—H···O interactions.

## Comment

Derivatives of tetrahydropyran have many applications; they occur in many natural products exhibiting important biological activities. These units can be found in monocyclic and polycyclic structures, such as laulimalide, the bryostatins, the phorboxazoles, and ratjadone (Gouverneur & Reiter, 2005). We report here the structure of the title tetrahydropyran derivative, (I) (Fig. 1), in which the bond lengths and angles present no unusual features. The two aromatic substituents are *syn* with respect to the tetrahydropyran system.



(I)

In the crystal structure, C—H···O hydrogen bonds (Table 1) link the molecules into chains along the *c* axis (Fig. 2).

## Experimental

The title compound was synthesized according to the procedure of Li *et al.* (2006). Crystals appropriate for data collection were obtained by slow evaporation of an $^{i}$PrOH solution at 283 K.

*Crystal data*

$C_{17}H_{15}NO_4$
$M_r$ = 297.10
Monoclinic, $P2_1/c$
$a$ = 9.2600 (9) Å
$b$ = 12.8916 (13) Å
$c$ = 12.7775 (13) Å
$\beta$ = 107.687 (2)°
$V$ = 1453.2 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 297 (2) K
0.30 × 0.20 × 0.20 mm

*Data collection*

Bruker SMART 4 K CCD area-detector diffractometer
Absorption correction: none
12630 measured reflections
3439 independent reflections
2743 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.028

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.152
$S$ = 1.04
3439 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{\rm min}$ = −0.18 e Å$^{-3}$

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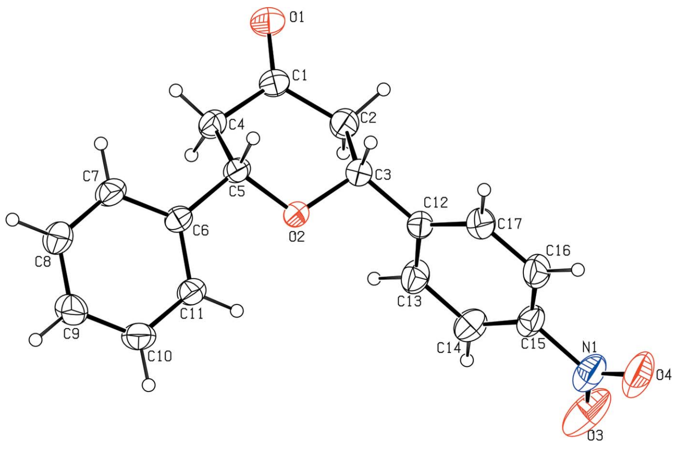

**Figure 1**
The molecular structure of compound (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Table 1**
Hydrogen-bond geometry (Å, °).

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
|---|---|---|---|---|
| C2—H2*A*⋯O4$^{i}$ | 0.97 | 2.56 | 3.381 (3) | 143 |

Symmetry code: (i) $-x+1, -y, -z+2$.

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry with C—H distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.95–1.00 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

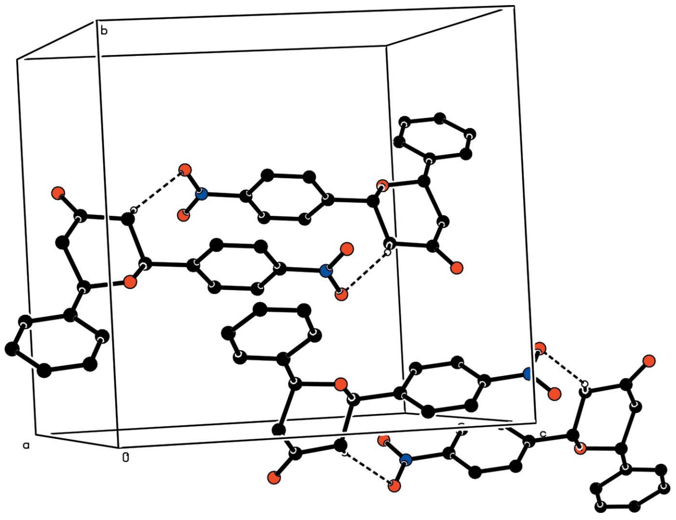

**Figure 2**
The molecular packing of (I). Hydrogen bonds are drawn as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

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