

## *trans*-2-(2-Nitro-1-phenylethyl)cyclohexanone

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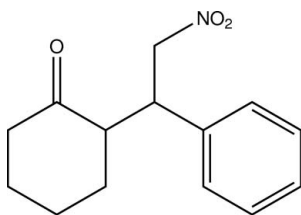
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 Key indicators: single-crystal X-ray study;  $T = 173$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.090; data-to-parameter ratio = 16.0.

In the title compound,  $\text{C}_{14}\text{H}_{17}\text{NO}_3$ , the plane of the phenyl ring and the least-squares plane of the cyclohexyl moiety enclose an angle of  $89.14(6)^\circ$ . The cyclohexyl ring adopts a chair conformation. In the crystal, the molecules are linked by weak  $\text{C}-\text{H}\cdots\text{O}$  bonds, with each of the nitro-O atoms accepting two such interactions.

### Related literature

For the history and synthesis of nitroalkenes, see: Tsogoeva *et al.* (2007); Sulzer-Mosse & Alexakis (2007); Mukherjee *et al.* (2007); Kempf *et al.* (2003); Blarer *et al.* (1982); Juaristi *et al.* (1993). For related structures, see: Cobb *et al.* (2005), Xu *et al.* (2007*a,b*).



### Experimental

#### Crystal data

 $\text{C}_{14}\text{H}_{17}\text{NO}_3$ 
 $M_r = 247.29$ 

 Monoclinic,  $P2_1/c$ 
 $a = 13.4567(6)$  Å

 $b = 8.3618(4)$  Å

 $c = 11.3668(5)$  Å

 $\beta = 91.734(4)^\circ$ 
 $V = 1278.43(10)$  Å<sup>3</sup>
 $Z = 4$ 

 Mo  $K\alpha$  radiation

 $\mu = 0.09$  mm<sup>-1</sup>
 $T = 173$  K

 $0.38 \times 0.27 \times 0.18$  mm

#### Data collection

Oxford Xcalibur diffractometer

Absorption correction: multi-scan

 (*CrysAlis PRO*; Oxford Diffraction, 2006)

 $T_{\min} = 0.986$ ,  $T_{\max} = 1.000$ 

9360 measured reflections

2605 independent reflections

 1829 reflections with  $I > 2\sigma(I)$ 
 $R_{\text{int}} = 0.026$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.036$ 
 $wR(F^2) = 0.090$ 
 $S = 0.98$ 

2605 reflections

163 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.17$  e Å<sup>-3</sup>
 $\Delta\rho_{\text{min}} = -0.17$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                                      | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C1}-\text{H1B}\cdots\text{O2}^{\text{i}}$   | 0.99  | 2.57        | 3.4403 (14) | 146           |
| $\text{C5}-\text{H5A}\cdots\text{O2}^{\text{ii}}$  | 0.99  | 2.47        | 3.4312 (16) | 165           |
| $\text{C8}-\text{H8A}\cdots\text{O1}^{\text{iii}}$ | 0.99  | 2.53        | 3.3536 (16) | 140           |
| $\text{C10}-\text{H10}\cdots\text{O2}^{\text{i}}$  | 0.95  | 2.50        | 3.4289 (15) | 165           |

 Symmetry codes: (i)  $x, -y + \frac{1}{2}, z - \frac{1}{2}$ ; (ii)  $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (iii)  $x, y - 1, z$ .

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2009).

The authors thank Prof. Thomas M. Klapötke for generous allocation of diffractometer time.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5052).

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**supplementary materials**

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## ***trans*-2-(2-Nitro-1-phenylethyl)cyclohexanone**

**I. Zenz, H. Mayr and P. Mayer**

### **Comment**

Nitroalkenes are important reagents in organic chemistry and they are the most prominent Michael acceptors used in organocatalytic reactions [Tsogoeva *et al.* (2007), Sulzer-Mosse *et al.* (2007), Mukherjee *et al.* (2007)]. During our studies on the electrophilic reactivity of *trans*- $\beta$ -nitrostyrenes, we employed enamines of known nucleophilic reactivities and, hence, obtained the title compound from a reaction of *trans*- $\beta$ -nitrostyrene and 1-pyrrolidinocyclohexene [Kempf *et al.* (2003), Blarer *et al.* (1982), Juaristi *et al.* (1993)].

In the title compound, the 1'-Phenyl-2'-nitro-ethyl moiety occupies an equatorial binding site in 2-position of the cyclohexanone ring (see Fig. 1). The plane of the phenyl ring and the least-square plane of the cyclohexyl moiety enclose an angle of 89.14 (6) $^{\circ}$  which is close to the angles found in enantiopure crystals of the title compound (87.1 (3) $^{\circ}$  at 180 K (Cobb *et al.* (2005)), 87.40 (8) $^{\circ}$  at 296 K (Xu *et al.*, 2007a,b)). The plane through the nitro group and the adjacent C1 atom encloses an angle of 68.81 (7) $^{\circ}$  with the phenyl ring.

Taking into account merely interactions with hydrogen-acceptor distances at least 0.1 Å shorter than the sum of van-der-Waals radii, the molecules are linked by very weak contacts of the type C—H $\cdots$ O with nitro-O atoms as acceptors (see Fig. 2). The molecular structure of the title compound is stabilized by these contacts as well, as the involved hydrogen atoms are located in the cyclohexyl ring, the phenyl ring and the nitro-ethyl side chain. The keto group is not involved in hydrogen bonding.  $\pi$ -stacking and C—H $\cdots$  $\pi$ -interactions are not observed.

### **Experimental**

*trans*-2-[1'-Phenyl-2'-nitro-ethyl]-cyclohexanone has been obtained by dissolving *trans*- $\beta$ -nitrostyrene (4.05 mmol, 604 mg) in dry diethylether (40 ml) and dropwise addition of 1-pyrrolidinocyclohexene (4.05 mmol, 612 mg) at -78  $^{\circ}$ C. After stirring the reaction at RT for 2 h, 60 ml water, 60 ml ethanol and 5 ml 1M HCl have been added, and the mixture was stirred for 30 min at 60  $^{\circ}$ C. After removing the solvent *in vacuo*, a white solid has been obtained (3.01 mmol, 745 mg, 74%).

Crystallization procedure: The title compound was dissolved in ethanol and heated to the boiling point. The solvent was allowed to cool slowly to room temperature. After 24 h, colourless crystals had formed that were suitable for X-ray analysis; mp 108  $^{\circ}$ C.

### **Refinement**

All H atoms were calculated in ideal geometry and refined in a riding model.

## Figures

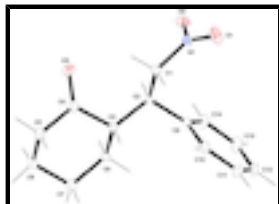


Fig. 1. The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at 50% probability level) for non-H atoms.

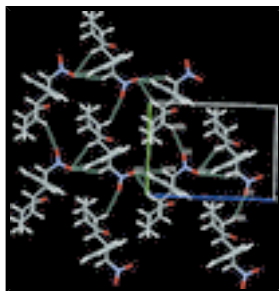


Fig. 2. Weak intermolecular interactions in the crystal structure of the title compound viewed along [100].

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### Crystal data

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Hall symbol: -P 2ybc

$a = 13.4567$  (6) Å

$b = 8.3618$  (4) Å

$c = 11.3668$  (5) Å

$\beta = 91.734$  (4)°

$V = 1278.43$  (10) Å<sup>3</sup>

$Z = 4$

$F(000) = 528$

$D_x = 1.285$  (1) Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3796 reflections

$\theta = 4.3$ – $26.3$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 173$  K

Block, colourless

$0.38 \times 0.27 \times 0.18$  mm

### Data collection

Oxford Xcalibur  
diffractometer

Radiation source: fine-focus sealed tube  
graphite

$\omega$  scans

Absorption correction: multi-scan  
(*CrysAlis PRO*; Oxford Diffraction, 2006)

$T_{\min} = 0.986$ ,  $T_{\max} = 1.000$

9360 measured reflections

2605 independent reflections

1829 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 26.4$ °,  $\theta_{\min} = 4.3$ °

$h = -16 \rightarrow 16$

$k = -10 \rightarrow 10$

$l = -14 \rightarrow 14$

*Refinement*

|                                 |  |
|---------------------------------|--|
| Refinement on $F^2$             | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full      | Secondary atom site location: difference Fourier map           |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | Hydrogen site location: inferred from neighbouring sites       |
| $wR(F^2) = 0.090$               | H-atom parameters constrained                                  |
| $S = 0.98$                      | $w = 1/[\sigma^2(F_o^2) + (0.0503P)^2]$                        |
| 2605 reflections                | where $P = (F_o^2 + 2F_c^2)/3$                                 |
| 163 parameters                  | $(\Delta/\sigma)_{\max} < 0.001$                               |
| 0 restraints                    | $\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$          |
|                                 | $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$         |

*Special details*

**Experimental.** CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.33.41 (release 06-05-2009 CrysAlis171 .NET) (compiled May 6 2009, 17:20:42) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

|     | <i>x</i>     | <i>y</i>      | <i>z</i>     | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| O1  | 0.27791 (8)  | 0.45264 (12)  | 0.27671 (8)  | 0.0497 (3)                       |
| O2  | 0.30532 (7)  | 0.25646 (11)  | 0.39600 (7)  | 0.0361 (3)                       |
| O3  | 0.46549 (7)  | -0.07785 (11) | 0.20442 (8)  | 0.0378 (3)                       |
| N1  | 0.30166 (8)  | 0.31433 (13)  | 0.29688 (9)  | 0.0272 (3)                       |
| C1  | 0.32921 (9)  | 0.20990 (14)  | 0.19718 (10) | 0.0243 (3)                       |
| H1A | 0.4012       | 0.1854        | 0.2029       | 0.029*                           |
| H1B | 0.3155       | 0.2661        | 0.1218       | 0.029*                           |
| C2  | 0.26933 (9)  | 0.05426 (14)  | 0.20005 (10) | 0.0214 (3)                       |
| H2  | 0.2817       | 0.0036        | 0.2788       | 0.026*                           |
| C3  | 0.30432 (9)  | -0.06309 (14) | 0.10615 (10) | 0.0217 (3)                       |
| H3  | 0.2931       | -0.0124       | 0.0272       | 0.026*                           |
| C4  | 0.41304 (9)  | -0.11083 (15) | 0.11829 (11) | 0.0258 (3)                       |
| C5  | 0.44795 (10) | -0.21687 (16) | 0.02103 (11) | 0.0333 (3)                       |
| H5A | 0.5197       | -0.2403       | 0.0330       | 0.040*                           |
| H5B | 0.4383       | -0.1623       | -0.0558      | 0.040*                           |
| C6  | 0.38803 (10) | -0.37313 (16) | 0.02159 (11) | 0.0333 (3)                       |
| H6A | 0.4068       | -0.4406       | -0.0458      | 0.040*                           |
| H6B | 0.4037       | -0.4330       | 0.0950       | 0.040*                           |
| C7  | 0.27722 (9)  | -0.33748 (16) | 0.01310 (11) | 0.0325 (3)                       |
| H7A | 0.2397       | -0.4386       | 0.0205       | 0.039*                           |
| H7B | 0.2605       | -0.2914       | -0.0653      | 0.039*                           |
| C8  | 0.24528 (10) | -0.22137 (15) | 0.10807 (11) | 0.0279 (3)                       |
| H8A | 0.2551       | -0.2724       | 0.1862       | 0.033*                           |
| H8B | 0.1735       | -0.1978       | 0.0966       | 0.033*                           |
| C9  | 0.15860 (9)  | 0.08735 (14)  | 0.18614 (10) | 0.0220 (3)                       |

## supplementary materials

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|     |               |              |              |            |
|-----|---------------|--------------|--------------|------------|
| C10 | 0.11872 (9)   | 0.16173 (15) | 0.08584 (10) | 0.0298 (3) |
| H10 | 0.1618        | 0.1982       | 0.0268       | 0.036*     |
| C11 | 0.01755 (10)  | 0.18327 (17) | 0.07092 (12) | 0.0358 (3) |
| H11 | -0.0082       | 0.2349       | 0.0021       | 0.043*     |
| C12 | -0.04660 (10) | 0.13068 (16) | 0.15475 (12) | 0.0368 (4) |
| H12 | -0.1163       | 0.1439       | 0.1434       | 0.044*     |
| C13 | -0.00848 (11) | 0.05889 (17) | 0.25497 (13) | 0.0393 (4) |
| H13 | -0.0521       | 0.0231       | 0.3136       | 0.047*     |
| C14 | 0.09322 (10)  | 0.03820 (16) | 0.27118 (11) | 0.0316 (3) |
| H14 | 0.1186        | -0.0103      | 0.3415       | 0.038*     |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$   | $U^{22}$   | $U^{33}$   | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|------------|------------|------------|-------------|-------------|-------------|
| O1  | 0.0667 (8) | 0.0264 (6) | 0.0566 (7) | 0.0132 (5)  | 0.0092 (5)  | -0.0020 (5) |
| O2  | 0.0429 (6) | 0.0418 (6) | 0.0236 (5) | -0.0013 (5) | 0.0033 (4)  | -0.0039 (4) |
| O3  | 0.0260 (5) | 0.0419 (6) | 0.0449 (6) | 0.0040 (4)  | -0.0083 (4) | -0.0096 (5) |
| N1  | 0.0240 (6) | 0.0270 (6) | 0.0306 (6) | -0.0007 (5) | 0.0020 (4)  | -0.0046 (5) |
| C1  | 0.0260 (7) | 0.0258 (7) | 0.0212 (6) | -0.0004 (6) | 0.0048 (5)  | -0.0022 (5) |
| C2  | 0.0215 (6) | 0.0223 (7) | 0.0204 (6) | 0.0001 (5)  | 0.0014 (5)  | 0.0015 (5)  |
| C3  | 0.0202 (6) | 0.0225 (7) | 0.0224 (6) | 0.0013 (5)  | -0.0008 (5) | 0.0007 (5)  |
| C4  | 0.0233 (7) | 0.0234 (7) | 0.0308 (7) | -0.0014 (6) | 0.0026 (5)  | 0.0010 (5)  |
| C5  | 0.0247 (7) | 0.0381 (8) | 0.0373 (7) | 0.0055 (6)  | 0.0055 (6)  | -0.0061 (6) |
| C6  | 0.0321 (8) | 0.0299 (8) | 0.0377 (7) | 0.0080 (6)  | -0.0019 (6) | -0.0082 (6) |
| C7  | 0.0309 (8) | 0.0269 (7) | 0.0395 (8) | 0.0019 (6)  | -0.0040 (6) | -0.0070 (6) |
| C8  | 0.0215 (7) | 0.0253 (7) | 0.0368 (7) | -0.0004 (6) | 0.0004 (5)  | -0.0035 (6) |
| C9  | 0.0222 (7) | 0.0183 (6) | 0.0255 (6) | 0.0010 (5)  | 0.0011 (5)  | -0.0044 (5) |
| C10 | 0.0270 (7) | 0.0326 (8) | 0.0299 (7) | 0.0017 (6)  | 0.0018 (5)  | 0.0017 (6)  |
| C11 | 0.0315 (8) | 0.0384 (8) | 0.0371 (8) | 0.0066 (7)  | -0.0052 (6) | 0.0032 (6)  |
| C12 | 0.0202 (7) | 0.0360 (8) | 0.0540 (9) | 0.0061 (6)  | -0.0015 (6) | -0.0032 (7) |
| C13 | 0.0274 (8) | 0.0412 (9) | 0.0500 (8) | 0.0009 (7)  | 0.0126 (6)  | 0.0048 (7)  |
| C14 | 0.0277 (7) | 0.0332 (8) | 0.0340 (7) | 0.0031 (6)  | 0.0053 (6)  | 0.0060 (6)  |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|        |             |         |             |
|--------|-------------|---------|-------------|
| O1—N1  | 1.2198 (13) | C6—H6A  | 0.9900      |
| O2—N1  | 1.2258 (12) | C6—H6B  | 0.9900      |
| O3—C4  | 1.2210 (14) | C7—C8   | 1.5234 (17) |
| N1—C1  | 1.4865 (15) | C7—H7A  | 0.9900      |
| C1—C2  | 1.5316 (16) | C7—H7B  | 0.9900      |
| C1—H1A | 0.9900      | C8—H8A  | 0.9900      |
| C1—H1B | 0.9900      | C8—H8B  | 0.9900      |
| C2—C9  | 1.5192 (17) | C9—C14  | 1.3888 (17) |
| C2—C3  | 1.5343 (16) | C9—C10  | 1.3919 (16) |
| C2—H2  | 1.0000      | C10—C11 | 1.3786 (18) |
| C3—C4  | 1.5187 (17) | C10—H10 | 0.9500      |
| C3—C8  | 1.5442 (16) | C11—C12 | 1.3770 (19) |
| C3—H3  | 1.0000      | C11—H11 | 0.9500      |
| C4—C5  | 1.5035 (18) | C12—C13 | 1.3732 (19) |

|             |              |                 |              |
|-------------|--------------|-----------------|--------------|
| C5—C6       | 1.5355 (19)  | C12—H12         | 0.9500       |
| C5—H5A      | 0.9900       | C13—C14         | 1.3862 (19)  |
| C5—H5B      | 0.9900       | C13—H13         | 0.9500       |
| C6—C7       | 1.5209 (18)  | C14—H14         | 0.9500       |
| O1—N1—O2    | 123.37 (10)  | C7—C6—H6B       | 109.6        |
| O1—N1—C1    | 118.92 (10)  | C5—C6—H6B       | 109.6        |
| O2—N1—C1    | 117.70 (10)  | H6A—C6—H6B      | 108.1        |
| N1—C1—C2    | 109.84 (9)   | C6—C7—C8        | 112.15 (10)  |
| N1—C1—H1A   | 109.7        | C6—C7—H7A       | 109.2        |
| C2—C1—H1A   | 109.7        | C8—C7—H7A       | 109.2        |
| N1—C1—H1B   | 109.7        | C6—C7—H7B       | 109.2        |
| C2—C1—H1B   | 109.7        | C8—C7—H7B       | 109.2        |
| H1A—C1—H1B  | 108.2        | H7A—C7—H7B      | 107.9        |
| C9—C2—C1    | 110.98 (10)  | C7—C8—C3        | 112.33 (10)  |
| C9—C2—C3    | 111.39 (9)   | C7—C8—H8A       | 109.1        |
| C1—C2—C3    | 110.85 (9)   | C3—C8—H8A       | 109.1        |
| C9—C2—H2    | 107.8        | C7—C8—H8B       | 109.1        |
| C1—C2—H2    | 107.8        | C3—C8—H8B       | 109.1        |
| C3—C2—H2    | 107.8        | H8A—C8—H8B      | 107.9        |
| C4—C3—C2    | 114.83 (9)   | C14—C9—C10      | 117.75 (12)  |
| C4—C3—C8    | 105.55 (10)  | C14—C9—C2       | 120.91 (10)  |
| C2—C3—C8    | 111.68 (10)  | C10—C9—C2       | 121.29 (11)  |
| C4—C3—H3    | 108.2        | C11—C10—C9      | 120.93 (12)  |
| C2—C3—H3    | 108.2        | C11—C10—H10     | 119.5        |
| C8—C3—H3    | 108.2        | C9—C10—H10      | 119.5        |
| O3—C4—C5    | 122.47 (12)  | C12—C11—C10     | 120.70 (12)  |
| O3—C4—C3    | 123.05 (11)  | C12—C11—H11     | 119.7        |
| C5—C4—C3    | 114.19 (11)  | C10—C11—H11     | 119.7        |
| C4—C5—C6    | 108.84 (11)  | C13—C12—C11     | 119.17 (13)  |
| C4—C5—H5A   | 109.9        | C13—C12—H12     | 120.4        |
| C6—C5—H5A   | 109.9        | C11—C12—H12     | 120.4        |
| C4—C5—H5B   | 109.9        | C12—C13—C14     | 120.48 (13)  |
| C6—C5—H5B   | 109.9        | C12—C13—H13     | 119.8        |
| H5A—C5—H5B  | 108.3        | C14—C13—H13     | 119.8        |
| C7—C6—C5    | 110.30 (11)  | C13—C14—C9      | 120.94 (12)  |
| C7—C6—H6A   | 109.6        | C13—C14—H14     | 119.5        |
| C5—C6—H6A   | 109.6        | C9—C14—H14      | 119.5        |
| O1—N1—C1—C2 | -128.32 (12) | C6—C7—C8—C3     | 56.07 (15)   |
| O2—N1—C1—C2 | 52.56 (14)   | C4—C3—C8—C7     | -56.14 (13)  |
| N1—C1—C2—C9 | 61.75 (12)   | C2—C3—C8—C7     | 178.44 (10)  |
| N1—C1—C2—C3 | -173.91 (9)  | C1—C2—C9—C14    | -122.22 (12) |
| C9—C2—C3—C4 | -176.37 (10) | C3—C2—C9—C14    | 113.75 (13)  |
| C1—C2—C3—C4 | 59.53 (13)   | C1—C2—C9—C10    | 60.49 (14)   |
| C9—C2—C3—C8 | -56.26 (13)  | C3—C2—C9—C10    | -63.53 (15)  |
| C1—C2—C3—C8 | 179.64 (9)   | C14—C9—C10—C11  | -1.04 (19)   |
| C2—C3—C4—O3 | 10.01 (17)   | C2—C9—C10—C11   | 176.33 (11)  |
| C8—C3—C4—O3 | -113.44 (13) | C9—C10—C11—C12  | -0.4 (2)     |
| C2—C3—C4—C5 | -176.03 (10) | C10—C11—C12—C13 | 1.2 (2)      |

## supplementary materials

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|             |             |                 |              |
|-------------|-------------|-----------------|--------------|
| C8—C3—C4—C5 | 60.52 (13)  | C11—C12—C13—C14 | -0.6 (2)     |
| O3—C4—C5—C6 | 112.56 (13) | C12—C13—C14—C9  | -0.9 (2)     |
| C3—C4—C5—C6 | -61.43 (14) | C10—C9—C14—C13  | 1.68 (19)    |
| C4—C5—C6—C7 | 55.04 (14)  | C2—C9—C14—C13   | -175.70 (12) |
| C5—C6—C7—C8 | -53.99 (14) |                 |              |

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

| $D-H\cdots A$                     | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------------|-------|-------------|-------------|---------------|
| C1—H1B $\cdots$ O2 <sup>i</sup>   | 0.99  | 2.57        | 3.4403 (14) | 146           |
| C5—H5A $\cdots$ O2 <sup>ii</sup>  | 0.99  | 2.47        | 3.4312 (16) | 165           |
| C8—H8A $\cdots$ O1 <sup>iii</sup> | 0.99  | 2.53        | 3.3536 (16) | 140           |
| C10—H10 $\cdots$ O2 <sup>i</sup>  | 0.95  | 2.50        | 3.4289 (15) | 165           |

Symmetry codes: (i)  $x, -y+1/2, z-1/2$ ; (ii)  $-x+1, y-1/2, -z+1/2$ ; (iii)  $x, y-1, z$ .



Fig. 1

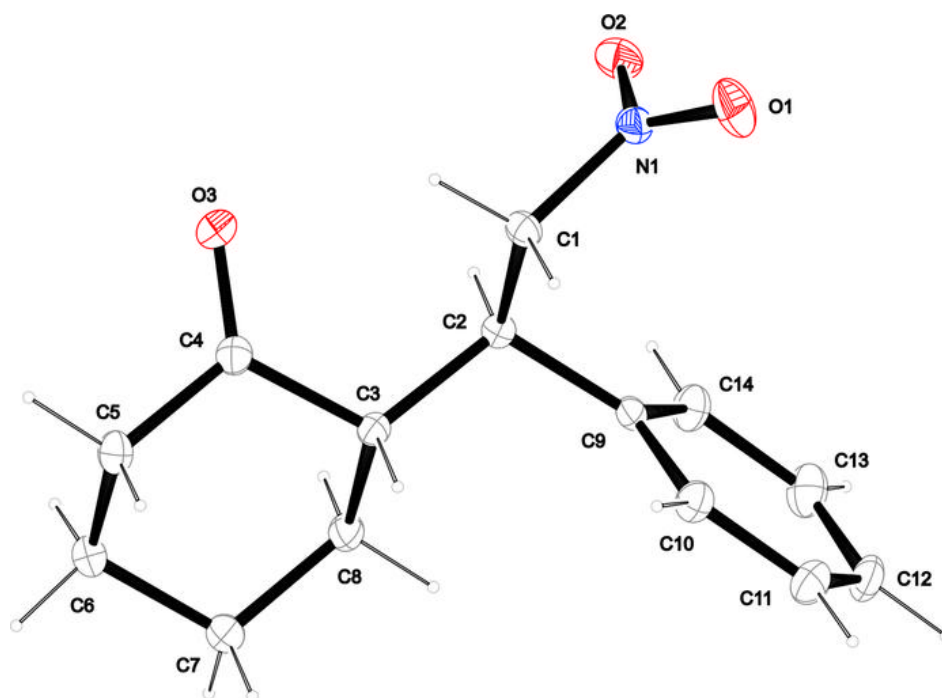


Fig. 2

