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## Structure Reports

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**(E)-2-(4-Nitrobenzylideneamino)-benzamide**

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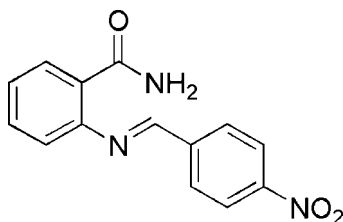
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.093; data-to-parameter ratio = 12.0.

The title compound,  $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}_3$ , adopts an *E* conformation, with a dihedral angle of  $41.8(1)^\circ$  between the mean planes of the two benzene rings. One of the amino H atoms forms an intramolecular hydrogen bond with the amide N atom, while the other H atom forms an intermolecular hydrogen bond with the carbonyl O atom of an adjacent molecule, forming dimers about inversion centers. A non-classical intermolecular C—H $\cdots$ O hydrogen bond also links adjacent molecules into dimers.

## Related literature

For Schiff bases complexes with metal ions, see: Kannan & Ramesh (2006); Lv *et al.* (2006); Maurya *et al.* (2006); Parekh *et al.* (2006); Vanco *et al.* (2004).



## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_{11}\text{N}_3\text{O}_3$   
 $M_r = 269.26$ Monoclinic,  $P2_1/c$   
 $a = 7.3863(2)$  Å $b = 12.2657(3)$  Å  
 $c = 14.1414(4)$  Å  
 $\beta = 97.248(1)^\circ$   
 $V = 1270.95(6)$  Å<sup>3</sup>  
 $Z = 4$ Mo  $K\alpha$  radiation  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.45 \times 0.29 \times 0.16$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: none  
9505 measured reflections2278 independent reflections  
1809 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.034$   
 $wR(F^2) = 0.093$   
 $S = 1.04$   
2278 reflections  
190 parametersH atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.14$  e Å<sup>-3</sup>**Table 1**  
Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                              | $D-H$      | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------------|------------|-------------|-------------|---------------|
| $\text{C13}-\text{H13A}\cdots\text{O2}^i$  | 0.93       | 2.44        | 3.1903 (19) | 138           |
| $\text{N1}-\text{H1B}\cdots\text{O3}^{ii}$ | 0.904 (18) | 2.059 (19)  | 2.9581 (17) | 173.3 (15)    |
| $\text{N1}-\text{H1A}\cdots\text{N2}$      | 0.877 (18) | 1.999 (18)  | 2.7027 (18) | 136.4 (15)    |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

We are grateful to the National Natural Science Foundation of China (20802061), the Natural Science Foundation (08KJD150019) and the Qing Lan Project (08QLT001) of Jiangsu Education Committee for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2166).

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**supplementary materials**

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## (*E*)-2-(4-Nitrobenzylideneamino)benzamide

S.-L. Wang, K. Yang, X.-S. Wang and S.-J. Tu

### Comment

Schiff bases are well known as ligands for many metal ions, such as copper(II) (Vanco *et al.*, 2005), Vanadium(IV, V) (Maurya *et al.*, 2006) and ruthenium(III) (Kannan & Ramesh, 2006). Some of metal Schiff base complexes possess biological activities. For example, it was reported that oxovanadium(IV) complexes with Schiff bases had antifungal activity (Parekh *et al.*, 2006), cobalt(II) and copper(II) complexes of valine-derived Schiff bases possessed antimicrobial activity (Lv *et al.*, 2006). We have synthesized the title compound, (I), by the reaction of 4-nitrobenzaldehyde, 2-aminobenzamide in an ionic liquid at room temperature which is reported in this article.

The X-ray crystal structure determination indicates that the title compound adopts an *E*-configuration (Fig. 1). The plane defined as the atoms of C7, C8, C9, N2 and H8A is nearly parallel to the benzene ring (C9—C14), forming a dihedral angle of 0.8 (1)°. The dihedral angle between the basal plane (atoms C7, C8, C9, N2 and H8A) and the other benzene ring (C2—C7) is 41.1 (1)°. The benzene rings make a dihedral angle of 41.8 (1)°.

The classical (N—H···O) and unclassical (C—H···O) hydrogen bonds are present in the crystal structure of (I) (Table 1). One of the hydrogen atoms (H1A) on the amino group forms an intra-molecular hydrogen bond (N1—H1A···N2) with the atom N2, while the other hydrogen atom (H1B) forms an inter-molecular hydrogen bond of the type N—H···O with the atom O3 in the adjacent molecule, forming dimmers. An unclassical intermolecular hydrogen bond (C13—H13A···O2) also links the adjacent molecules into dimmers (Fig. 2). The above inter-molecular hydrogen bonds link the molecules into polymers.

### Experimental

The title compound, (I), was prepared by the reaction of 4-nitrobenzaldehyde (2 mmol, 0.302 g) and 2-aminobenzamide (2 mmol, 0.272 g) in an ionic liquid of [Bmim]Br (Bmim = 1-butyl-3-methylimidazolium) (2 ml) at 353 K; m.p. 457–458 K. The single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

### Refinement

The H atoms bonded to C atoms were calculated geometrically and refined as riding, with C—H = 0.93 Å while the amino H-atoms were allowed to refine;  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ .

### Figures

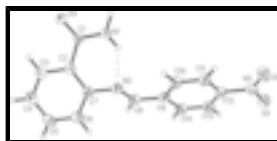


Fig. 1. The molecular structure of (I) showing 50% probability of displacement ellipsoids and the atom-numbering scheme.

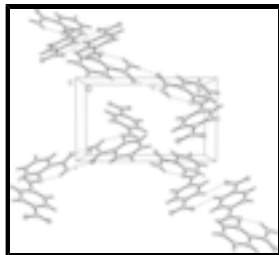


Fig. 2. The molecular packing diagram showing the hydrogen-bonding network in the crystal for (I).

## (E)-2-(4-Nitrobenzylideneamino)benzamide

### Crystal data

$C_{14}H_{11}N_3O_3$

$M_r = 269.26$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.3863$  (2) Å

$b = 12.2657$  (3) Å

$c = 14.1414$  (4) Å

$\beta = 97.2480$  (10)°

$V = 1270.95$  (6) Å<sup>3</sup>

$Z = 4$

$F_{000} = 560$

$D_x = 1.407$  Mg m<sup>-3</sup>

Melting point = 457–458 K

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 3148 reflections

$\theta = 2.2$ – $25.8$ °

$\mu = 0.10$  mm<sup>-1</sup>

$T = 296$  K

Block, yellow

$0.45 \times 0.29 \times 0.16$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$  K

$\phi$  and  $\omega$  scans

Absorption correction: none

9505 measured reflections

2278 independent reflections

1809 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.026$

$\theta_{max} = 25.2$ °

$\theta_{min} = 2.2$ °

$h = -8$ → $8$

$k = -14$ → $14$

$l = -16$ → $16$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.093$

$S = 1.04$

2278 reflections

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.1992P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.14$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.14$  e Å<sup>-3</sup>

190 parameters

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.046 (3)

Secondary atom site location: difference Fourier map

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

|      | <i>x</i>      | <i>y</i>     | <i>z</i>      | $U_{iso}^*/U_{eq}$ |
|------|---------------|--------------|---------------|--------------------|
| N2   | 0.29424 (15)  | 0.81888 (9)  | 0.04882 (9)   | 0.0480 (3)         |
| O2   | 0.66701 (16)  | 0.86265 (9)  | 0.54680 (8)   | 0.0669 (3)         |
| O3   | -0.03944 (14) | 0.58880 (8)  | -0.10923 (7)  | 0.0556 (3)         |
| C9   | 0.39628 (18)  | 0.86357 (11) | 0.21085 (11)  | 0.0459 (4)         |
| C2   | 0.10787 (17)  | 0.76078 (11) | -0.09651 (10) | 0.0413 (3)         |
| C1   | 0.06905 (17)  | 0.64827 (11) | -0.06033 (10) | 0.0412 (3)         |
| N3   | 0.66097 (17)  | 0.79210 (10) | 0.48528 (10)  | 0.0525 (3)         |
| C12  | 0.56915 (18)  | 0.81749 (11) | 0.38992 (10)  | 0.0445 (4)         |
| C7   | 0.20752 (18)  | 0.84286 (11) | -0.04369 (11) | 0.0445 (3)         |
| N1   | 0.15232 (19)  | 0.61634 (11) | 0.02351 (10)  | 0.0536 (4)         |
| C8   | 0.30111 (19)  | 0.88799 (12) | 0.11590 (11)  | 0.0503 (4)         |
| H8A  | 0.2447        | 0.9554       | 0.1046        | 0.060*             |
| C14  | 0.3976 (2)    | 0.93889 (11) | 0.28377 (11)  | 0.0521 (4)         |
| H14A | 0.3381        | 1.0053       | 0.2721        | 0.063*             |
| C13  | 0.4860 (2)    | 0.91691 (11) | 0.37357 (11)  | 0.0518 (4)         |
| H13A | 0.4892        | 0.9684       | 0.4220        | 0.062*             |
| C3   | 0.0323 (2)    | 0.78476 (12) | -0.18910 (11) | 0.0497 (4)         |
| H3A  | -0.0348       | 0.7314       | -0.2248       | 0.060*             |
| C11  | 0.5690 (2)    | 0.74035 (12) | 0.31915 (13)  | 0.0540 (4)         |
| H11A | 0.6261        | 0.6734       | 0.3318        | 0.065*             |
| C10  | 0.4840 (2)    | 0.76367 (12) | 0.23011 (12)  | 0.0552 (4)         |
| H10A | 0.4844        | 0.7124       | 0.1817        | 0.066*             |
| O1   | 0.72849 (17)  | 0.70200 (9)  | 0.49945 (9)   | 0.0717 (4)         |
| C4   | 0.0538 (2)    | 0.88540 (14) | -0.22967 (12) | 0.0592 (4)         |
| H4A  | 0.0017        | 0.8994       | -0.2918       | 0.071*             |
| C5   | 0.1527 (2)    | 0.96491 (14) | -0.17769 (13) | 0.0645 (5)         |
| H5A  | 0.1680        | 1.0329       | -0.2047       | 0.077*             |
| C6   | 0.2289 (2)    | 0.94391 (12) | -0.08568 (13) | 0.0590 (4)         |

## supplementary materials

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|     |           |             |             |            |
|-----|-----------|-------------|-------------|------------|
| H6A | 0.2957    | 0.9981      | -0.0510     | 0.071*     |
| H1A | 0.226 (2) | 0.6618 (14) | 0.0573 (13) | 0.067 (5)* |
| H1B | 0.121 (2) | 0.5508 (15) | 0.0458 (11) | 0.060 (5)* |

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

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| N2  | 0.0529 (7)  | 0.0391 (6)  | 0.0509 (8)  | -0.0056 (5) | 0.0025 (6)  | -0.0035 (6) |
| O2  | 0.0898 (8)  | 0.0617 (7)  | 0.0489 (7)  | -0.0009 (6) | 0.0074 (6)  | -0.0088 (6) |
| O3  | 0.0673 (6)  | 0.0468 (6)  | 0.0495 (7)  | -0.0128 (5) | -0.0050 (5) | -0.0018 (5) |
| C9  | 0.0473 (7)  | 0.0400 (7)  | 0.0507 (9)  | -0.0063 (6) | 0.0079 (6)  | -0.0063 (7) |
| C2  | 0.0418 (7)  | 0.0405 (7)  | 0.0421 (8)  | 0.0023 (5)  | 0.0079 (6)  | 0.0007 (6)  |
| C1  | 0.0440 (7)  | 0.0399 (7)  | 0.0404 (8)  | -0.0003 (6) | 0.0076 (6)  | -0.0039 (6) |
| N3  | 0.0589 (7)  | 0.0471 (7)  | 0.0530 (9)  | -0.0034 (6) | 0.0135 (6)  | -0.0007 (7) |
| C12 | 0.0464 (7)  | 0.0428 (8)  | 0.0452 (9)  | -0.0052 (6) | 0.0091 (6)  | -0.0023 (7) |
| C7  | 0.0477 (7)  | 0.0388 (7)  | 0.0472 (9)  | 0.0022 (6)  | 0.0066 (6)  | 0.0012 (6)  |
| N1  | 0.0678 (8)  | 0.0412 (7)  | 0.0484 (8)  | -0.0137 (6) | -0.0058 (7) | 0.0056 (6)  |
| C8  | 0.0544 (8)  | 0.0396 (7)  | 0.0568 (10) | -0.0013 (6) | 0.0067 (7)  | -0.0037 (7) |
| C14 | 0.0666 (9)  | 0.0358 (7)  | 0.0544 (10) | 0.0019 (6)  | 0.0098 (8)  | -0.0051 (7) |
| C13 | 0.0696 (9)  | 0.0390 (8)  | 0.0482 (10) | -0.0030 (7) | 0.0130 (8)  | -0.0091 (7) |
| C3  | 0.0507 (8)  | 0.0529 (8)  | 0.0456 (9)  | 0.0022 (6)  | 0.0066 (7)  | 0.0024 (7)  |
| C11 | 0.0569 (8)  | 0.0431 (8)  | 0.0610 (10) | 0.0080 (6)  | 0.0041 (7)  | -0.0095 (7) |
| C10 | 0.0620 (9)  | 0.0466 (8)  | 0.0553 (11) | 0.0055 (7)  | 0.0014 (8)  | -0.0167 (7) |
| O1  | 0.0907 (8)  | 0.0550 (7)  | 0.0685 (8)  | 0.0134 (6)  | 0.0062 (7)  | 0.0070 (6)  |
| C4  | 0.0638 (9)  | 0.0637 (10) | 0.0506 (10) | 0.0091 (8)  | 0.0089 (8)  | 0.0151 (8)  |
| C5  | 0.0774 (11) | 0.0480 (9)  | 0.0693 (12) | 0.0043 (8)  | 0.0140 (9)  | 0.0188 (9)  |
| C6  | 0.0702 (10) | 0.0384 (8)  | 0.0683 (12) | -0.0041 (7) | 0.0080 (8)  | 0.0019 (8)  |

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

|            |             |              |             |
|------------|-------------|--------------|-------------|
| N2—C8      | 1.2684 (19) | N1—H1A       | 0.877 (18)  |
| N2—C7      | 1.4131 (19) | N1—H1B       | 0.904 (18)  |
| O2—N3      | 1.2238 (16) | C8—H8A       | 0.9300      |
| O3—C1      | 1.2299 (15) | C14—C13      | 1.379 (2)   |
| C9—C14     | 1.384 (2)   | C14—H14A     | 0.9300      |
| C9—C10     | 1.397 (2)   | C13—H13A     | 0.9300      |
| C9—C8      | 1.466 (2)   | C3—C4        | 1.379 (2)   |
| C2—C3      | 1.389 (2)   | C3—H3A       | 0.9300      |
| C2—C7      | 1.4053 (19) | C11—C10      | 1.365 (2)   |
| C2—C1      | 1.5118 (19) | C11—H11A     | 0.9300      |
| C1—N1      | 1.3241 (19) | C10—H10A     | 0.9300      |
| N3—O1      | 1.2186 (16) | C4—C5        | 1.375 (2)   |
| N3—C12     | 1.4645 (19) | C4—H4A       | 0.9300      |
| C12—C13    | 1.372 (2)   | C5—C6        | 1.375 (2)   |
| C12—C11    | 1.377 (2)   | C5—H5A       | 0.9300      |
| C7—C6      | 1.392 (2)   | C6—H6A       | 0.9300      |
| C8—N2—C7   | 121.60 (12) | C13—C14—C9   | 120.91 (14) |
| C14—C9—C10 | 118.75 (14) | C13—C14—H14A | 119.5       |

|               |              |                 |              |
|---------------|--------------|-----------------|--------------|
| C14—C9—C8     | 120.25 (13)  | C9—C14—H14A     | 119.5        |
| C10—C9—C8     | 120.99 (13)  | C12—C13—C14     | 118.60 (13)  |
| C3—C2—C7      | 118.09 (13)  | C12—C13—H13A    | 120.7        |
| C3—C2—C1      | 116.21 (12)  | C14—C13—H13A    | 120.7        |
| C7—C2—C1      | 125.67 (13)  | C4—C3—C2        | 121.88 (14)  |
| O3—C1—N1      | 121.61 (13)  | C4—C3—H3A       | 119.1        |
| O3—C1—C2      | 119.27 (12)  | C2—C3—H3A       | 119.1        |
| N1—C1—C2      | 119.12 (12)  | C10—C11—C12     | 118.97 (14)  |
| O1—N3—O2      | 123.15 (14)  | C10—C11—H11A    | 120.5        |
| O1—N3—C12     | 118.47 (13)  | C12—C11—H11A    | 120.5        |
| O2—N3—C12     | 118.38 (12)  | C11—C10—C9      | 120.79 (14)  |
| C13—C12—C11   | 121.95 (14)  | C11—C10—H10A    | 119.6        |
| C13—C12—N3    | 119.32 (13)  | C9—C10—H10A     | 119.6        |
| C11—C12—N3    | 118.73 (13)  | C5—C4—C3        | 119.60 (15)  |
| C6—C7—C2      | 119.41 (14)  | C5—C4—H4A       | 120.2        |
| C6—C7—N2      | 121.19 (13)  | C3—C4—H4A       | 120.2        |
| C2—C7—N2      | 119.27 (12)  | C4—C5—C6        | 119.97 (15)  |
| C1—N1—H1A     | 119.1 (12)   | C4—C5—H5A       | 120.0        |
| C1—N1—H1B     | 117.8 (10)   | C6—C5—H5A       | 120.0        |
| H1A—N1—H1B    | 122.9 (15)   | C5—C6—C7        | 121.04 (15)  |
| N2—C8—C9      | 121.19 (13)  | C5—C6—H6A       | 119.5        |
| N2—C8—H8A     | 119.4        | C7—C6—H6A       | 119.5        |
| C9—C8—H8A     | 119.4        |                 |              |
| C3—C2—C1—O3   | -7.15 (18)   | C10—C9—C14—C13  | 1.0 (2)      |
| C7—C2—C1—O3   | 170.60 (13)  | C8—C9—C14—C13   | 179.76 (13)  |
| C3—C2—C1—N1   | 173.09 (13)  | C11—C12—C13—C14 | 1.0 (2)      |
| C7—C2—C1—N1   | -9.2 (2)     | N3—C12—C13—C14  | -178.97 (12) |
| O1—N3—C12—C13 | 177.42 (13)  | C9—C14—C13—C12  | -1.6 (2)     |
| O2—N3—C12—C13 | -2.95 (19)   | C7—C2—C3—C4     | 0.5 (2)      |
| O1—N3—C12—C11 | -2.57 (19)   | C1—C2—C3—C4     | 178.39 (13)  |
| O2—N3—C12—C11 | 177.05 (13)  | C13—C12—C11—C10 | 0.1 (2)      |
| C3—C2—C7—C6   | -0.8 (2)     | N3—C12—C11—C10  | -179.88 (13) |
| C1—C2—C7—C6   | -178.46 (13) | C12—C11—C10—C9  | -0.7 (2)     |
| C3—C2—C7—N2   | -176.60 (12) | C14—C9—C10—C11  | 0.2 (2)      |
| C1—C2—C7—N2   | 5.7 (2)      | C8—C9—C10—C11   | -178.58 (14) |
| C8—N2—C7—C6   | 41.8 (2)     | C2—C3—C4—C5     | 0.0 (2)      |
| C8—N2—C7—C2   | -142.45 (14) | C3—C4—C5—C6     | -0.2 (2)     |
| C7—N2—C8—C9   | -178.08 (12) | C4—C5—C6—C7     | -0.1 (3)     |
| C14—C9—C8—N2  | -178.12 (14) | C2—C7—C6—C5     | 0.6 (2)      |
| C10—C9—C8—N2  | 0.6 (2)      | N2—C7—C6—C5     | 176.34 (14)  |

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

| <i>D</i> —H $\cdots$ <i>A</i>     | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|-----------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C13—H13A $\cdots$ O2 <sup>i</sup> | 0.93        | 2.44                | 3.1903 (19)                | 138                           |
| N1—H1B $\cdots$ O3 <sup>ii</sup>  | 0.904 (18)  | 2.059 (19)          | 2.9581 (17)                | 173.3 (15)                    |
| N1—H1A $\cdots$ N2                | 0.877 (18)  | 1.999 (18)          | 2.7027 (18)                | 136.4 (15)                    |

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

Fig. 1

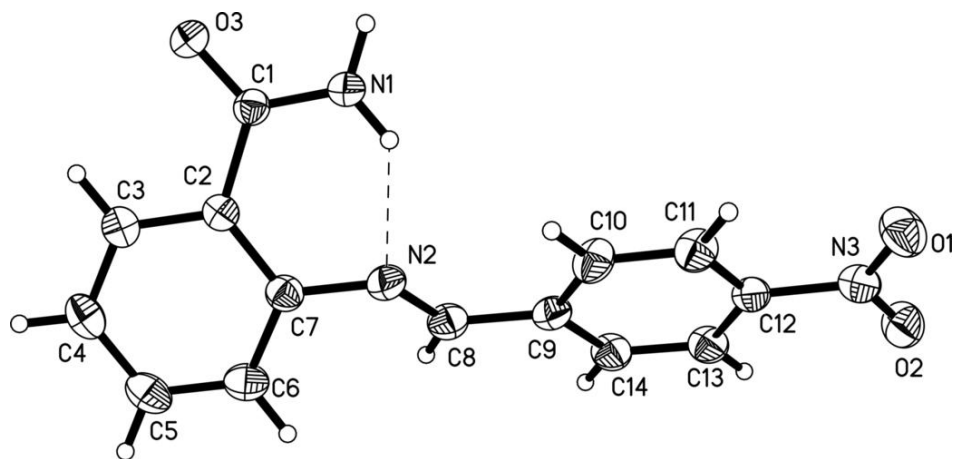




Fig. 2

