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## Structure Reports

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***N'*-(2-Chlorobenzylidene)-4-nitrobenzohydrazide**

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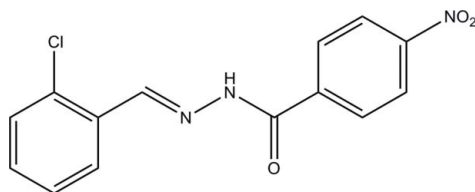
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.051;  $wR$  factor = 0.146; data-to-parameter ratio = 15.2.

In the title compound,  $\text{C}_{14}\text{H}_{10}\text{ClN}_3\text{O}_3$ , the dihedral angle between the benzene rings is  $6.64(13)^\circ$ . In the crystal, molecules are linked through  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming chains running along the  $c$  axis direction.

## Related literature

For general background to hydrazones, see: Rasras *et al.* (2010); Pyta *et al.* (2010); Angelusiu *et al.* (2010). For related structures, see: Fun *et al.* (2008); Singh & Singh (2010); Ahmad *et al.* (2010); Tang (2010, 2011). For reference bond-length data, see: Allen *et al.* (1987).



## Experimental

## Crystal data

 $\text{C}_{14}\text{H}_{10}\text{ClN}_3\text{O}_3$  $M_r = 303.70$ Monoclinic,  $P2_1/c$  $a = 11.2332(18)$  Å $b = 13.3778(18)$  Å $c = 8.9770(16)$  Å $\beta = 90.408(2)^\circ$  $V = 1349.0(4)$  Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.30$  mm<sup>-1</sup> $T = 298$  K $0.18 \times 0.17 \times 0.15$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\min} = 0.949$ ,  $T_{\max} = 0.957$ 

10640 measured reflections

2931 independent reflections

1882 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.045$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.051$  $wR(F^2) = 0.146$  $S = 1.03$ 

2931 reflections

193 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\max} = 0.36$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                   | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N2}-\text{H2}\cdots\text{O1}^i$ | 0.89 (1)     | 2.06 (1)           | 2.915 (3)   | 160 (3)              |

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); 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: SHELXL97.

Financial support from the Jiaying University research fund is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2353).

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**supplementary materials**

*Acta Cryst.* (2012). E68, o335 [ doi:10.1107/S1600536811055589 ]

## *N'*-(2-Chlorobenzylidene)-4-nitrobenzohydrazide

C.-B. Tang

### Comment

Hydrazone compounds have received much attention in biological and structural chemistry in the last few years (Rasras *et al.*, 2010; Pyta *et al.*, 2010; Angelusiu *et al.*, 2010; Fun *et al.*, 2008; Singh & Singh, 2010; Ahmad *et al.*, 2010). As a continuation of our work on the structural study on such compounds (Tang, 2010, 2011), we reports herein on the crystal structure of the title new hydrazone compound.

In the molecule of the title compound (Fig. 1), the dihedral angle between the two benzene rings is  $6.64(13)^\circ$ . Bond lengths in the compound are normal (Allen *et al.*, 1987) and comparable to those in the similar compounds (Tang, 2010; Tang, 2011).

In the crystal, molecules are linked through intermolecular N—H $\cdots$ O hydrogen bonds (Table 1), forming chains running along the *c* axis direction (Fig. 2).

### Experimental

2-Chlorobenzaldehyde (0.1 mmol, 14.1 mg) and 4-nitrobenzohydrazide (0.1 mmol, 18.2 mg) were dissolved in methanol (20 ml). The mixture was stirred at reflux for 10 min to give a clear yellow solution. Yellow needle-shaped crystals of the compound were formed by slow evaporation of the solvent over several days.

### Refinement

The amino H atom was located in a difference Fourier map and refined isotropically, with an N—H distance restraint of 0.90 (1) Å. C-bound H atoms were included in calculated positions and refined as riding atoms: C—H = 0.93 Å, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

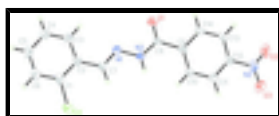


Fig. 1. The molecular structure of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

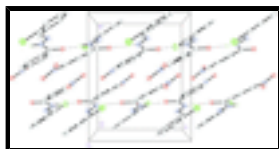


Fig. 2. Crystal packing of the title compound, viewed along the *b* axis, with hydrogen bonds shown as dashed lines.

## *N'*-(2-Chlorobenzylidene)-4-nitrobenzohydrazide

### *Crystal data*

|                                |   |
|--------------------------------|---|
| $C_{14}H_{10}ClN_3O_3$         | $F(000) = 624$  |
| $M_r = 303.70$                 | $D_x = 1.495 \text{ Mg m}^{-3}$                         |
| Monoclinic, $P2_1/c$           | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| $a = 11.2332 (18) \text{ \AA}$ | Cell parameters from 2464 reflections                   |
| $b = 13.3778 (18) \text{ \AA}$ | $\theta = 2.4\text{--}24.5^\circ$                       |
| $c = 8.9770 (16) \text{ \AA}$  | $\mu = 0.30 \text{ mm}^{-1}$                            |
| $\beta = 90.408 (2)^\circ$     | $T = 298 \text{ K}$                                     |
| $V = 1349.0 (4) \text{ \AA}^3$ | Cut from needle, yellow                                 |
| $Z = 4$                        | $0.18 \times 0.17 \times 0.15 \text{ mm}$               |

### *Data collection*

|  |  |
|--|--|
| Bruker SMART CCD area-detector diffractometer                        | 2931 independent reflections   |
| Radiation source: fine-focus sealed tube graphite                    | 1882 reflections with $I > 2\sigma(I)$                                 |
| $\omega$ scans   | $R_{\text{int}} = 0.045$   |
| Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996) | $\theta_{\text{max}} = 27.0^\circ$ , $\theta_{\text{min}} = 2.4^\circ$ |
| $T_{\text{min}} = 0.949$ , $T_{\text{max}} = 0.957$                  | $h = -14 \rightarrow 14$   |
| 10640 measured reflections   | $k = -14 \rightarrow 17$   |
|  | $l = -11 \rightarrow 11$   |

### *Refinement*

|                                 |  |
|---------------------------------|--|
| Refinement on $F^2$             | Primary atom site location: structure-invariant direct methods         |
| Least-squares matrix: full      | Secondary atom site location: difference Fourier map                   |
| $R[F^2 > 2\sigma(F^2)] = 0.051$ | Hydrogen site location: inferred from neighbouring sites               |
| $wR(F^2) = 0.146$               | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.03$                      | $w = 1/[\sigma^2(F_o^2) + (0.0569P)^2 + 0.5874P]$                      |
| 2931 reflections                | where $P = (F_o^2 + 2F_c^2)/3$   |
| 193 parameters                  | $(\Delta/\sigma)_{\text{max}} < 0.001$                                 |
| 1 restraint                     | $\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$                    |
|                                 | $\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$                   |

### *Special details*

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

|     | x            | y             | z            | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| C11 | 0.23505 (8)  | 0.62569 (6)   | 1.10065 (9)  | 0.0782 (3)                       |
| H2  | 0.246 (3)    | 0.265 (2)     | 1.1045 (13)  | 0.080*                           |
| N1  | 0.18950 (18) | 0.33163 (14)  | 0.9198 (2)   | 0.0444 (5)                       |
| N2  | 0.23517 (19) | 0.25548 (14)  | 1.0072 (2)   | 0.0446 (5)                       |
| N3  | 0.4488 (2)   | -0.1478 (2)   | 1.3026 (3)   | 0.0667 (7)                       |
| O1  | 0.26845 (19) | 0.15983 (13)  | 0.80373 (18) | 0.0620 (5)                       |
| O2  | 0.4173 (3)   | -0.23176 (19) | 1.2688 (3)   | 0.1126 (10)                      |
| O3  | 0.5111 (2)   | -0.12928 (18) | 1.4092 (3)   | 0.0902 (8)                       |
| C1  | 0.1488 (2)   | 0.59971 (19)  | 0.9450 (3)   | 0.0513 (6)                       |
| C2  | 0.1308 (2)   | 0.50090 (18)  | 0.8991 (3)   | 0.0452 (6)                       |
| C3  | 0.0625 (2)   | 0.4872 (2)    | 0.7698 (3)   | 0.0553 (7)                       |
| H3  | 0.0493       | 0.4227        | 0.7348       | 0.066*                           |
| C4  | 0.0149 (3)   | 0.5657 (3)    | 0.6941 (3)   | 0.0679 (8)                       |
| H4  | -0.0312      | 0.5541        | 0.6094       | 0.082*                           |
| C5  | 0.0344 (3)   | 0.6622 (2)    | 0.7416 (4)   | 0.0709 (9)                       |
| H5  | 0.0020       | 0.7154        | 0.6885       | 0.085*                           |
| C6  | 0.1015 (3)   | 0.6800 (2)    | 0.8673 (4)   | 0.0644 (8)                       |
| H6  | 0.1149       | 0.7450        | 0.8998       | 0.077*                           |
| C7  | 0.1807 (2)   | 0.41629 (18)  | 0.9816 (3)   | 0.0463 (6)                       |
| H7  | 0.2061       | 0.4247        | 1.0796       | 0.056*                           |
| C8  | 0.2731 (2)   | 0.17126 (17)  | 0.9389 (3)   | 0.0434 (6)                       |
| C9  | 0.3213 (2)   | 0.09038 (17)  | 1.0373 (2)   | 0.0392 (5)                       |
| C10 | 0.3769 (2)   | 0.10957 (18)  | 1.1718 (3)   | 0.0443 (6)                       |
| H10 | 0.3845       | 0.1751        | 1.2052       | 0.053*                           |
| C11 | 0.4216 (2)   | 0.03155 (19)  | 1.2576 (3)   | 0.0495 (6)                       |
| H11 | 0.4605       | 0.0441        | 1.3474       | 0.059*                           |
| C12 | 0.4069 (2)   | -0.06443 (19) | 1.2070 (3)   | 0.0479 (6)                       |
| C13 | 0.3536 (2)   | -0.08568 (19) | 1.0728 (3)   | 0.0558 (7)                       |
| H13 | 0.3456       | -0.1514       | 1.0404       | 0.067*                           |
| C14 | 0.3122 (2)   | -0.00768 (19) | 0.9871 (3)   | 0.0539 (7)                       |
| H14 | 0.2777       | -0.0207       | 0.8947       | 0.065*                           |

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

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$     | $U^{23}$    |
|-----|-------------|-------------|-------------|-------------|--------------|-------------|
| C11 | 0.1009 (6)  | 0.0532 (5)  | 0.0802 (6)  | -0.0085 (4) | -0.0221 (5)  | -0.0047 (4) |
| N1  | 0.0560 (12) | 0.0374 (11) | 0.0397 (11) | -0.0027 (9) | -0.0030 (9)  | 0.0046 (9)  |
| N2  | 0.0662 (13) | 0.0345 (11) | 0.0329 (11) | -0.0010 (9) | -0.0045 (9)  | -0.0007 (9) |
| N3  | 0.0637 (15) | 0.0569 (16) | 0.0792 (18) | 0.0213 (12) | -0.0113 (13) | 0.0006 (14) |

## supplementary materials

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|     |             |             |             |              |              |              |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O1  | 0.1089 (16) | 0.0463 (10) | 0.0308 (10) | -0.0018 (10) | -0.0020 (9)  | -0.0018 (8)  |
| O2  | 0.134 (2)   | 0.0514 (15) | 0.152 (3)   | 0.0189 (14)  | -0.0636 (19) | 0.0076 (15)  |
| O3  | 0.1053 (18) | 0.0902 (18) | 0.0747 (16) | 0.0349 (14)  | -0.0268 (14) | -0.0009 (13) |
| C1  | 0.0545 (14) | 0.0475 (15) | 0.0518 (15) | -0.0003 (12) | 0.0045 (12)  | 0.0070 (12)  |
| C2  | 0.0504 (13) | 0.0428 (14) | 0.0425 (14) | 0.0001 (11)  | 0.0078 (11)  | 0.0052 (11)  |
| C3  | 0.0590 (16) | 0.0573 (17) | 0.0496 (16) | 0.0051 (13)  | -0.0006 (12) | -0.0021 (13) |
| C4  | 0.0709 (19) | 0.078 (2)   | 0.0548 (17) | 0.0151 (16)  | -0.0082 (14) | 0.0057 (16)  |
| C5  | 0.081 (2)   | 0.063 (2)   | 0.068 (2)   | 0.0191 (16)  | 0.0024 (17)  | 0.0202 (16)  |
| C6  | 0.0742 (19) | 0.0443 (16) | 0.075 (2)   | 0.0044 (14)  | 0.0094 (16)  | 0.0094 (14)  |
| C7  | 0.0579 (14) | 0.0440 (14) | 0.0369 (13) | -0.0017 (11) | -0.0019 (11) | 0.0026 (11)  |
| C8  | 0.0579 (14) | 0.0369 (13) | 0.0353 (13) | -0.0113 (11) | -0.0005 (10) | 0.0003 (10)  |
| C9  | 0.0476 (12) | 0.0365 (12) | 0.0337 (12) | -0.0051 (10) | 0.0043 (10)  | -0.0016 (10) |
| C10 | 0.0510 (13) | 0.0369 (13) | 0.0450 (14) | -0.0038 (10) | -0.0014 (11) | -0.0087 (11) |
| C11 | 0.0507 (14) | 0.0530 (16) | 0.0446 (14) | 0.0034 (12)  | -0.0080 (11) | -0.0057 (12) |
| C12 | 0.0468 (13) | 0.0443 (14) | 0.0526 (15) | 0.0089 (11)  | 0.0004 (11)  | 0.0007 (12)  |
| C13 | 0.0694 (17) | 0.0355 (13) | 0.0625 (18) | 0.0044 (12)  | -0.0095 (14) | -0.0119 (12) |
| C14 | 0.0749 (18) | 0.0416 (14) | 0.0450 (14) | -0.0001 (13) | -0.0130 (13) | -0.0117 (12) |

### *Geometric parameters (Å, °)*

|           |             |             |           |
|-----------|-------------|-------------|-----------|
| C11—C1    | 1.729 (3)   | C4—H4       | 0.9300    |
| N1—C7     | 1.265 (3)   | C5—C6       | 1.373 (4) |
| N1—N2     | 1.382 (3)   | C5—H5       | 0.9300    |
| N2—C8     | 1.353 (3)   | C6—H6       | 0.9300    |
| N2—H2     | 0.891 (10)  | C7—H7       | 0.9300    |
| N3—O3     | 1.207 (3)   | C8—C9       | 1.495 (3) |
| N3—O2     | 1.216 (3)   | C9—C10      | 1.380 (3) |
| N3—C12    | 1.482 (3)   | C9—C14      | 1.390 (3) |
| O1—C8     | 1.224 (3)   | C10—C11     | 1.389 (3) |
| C1—C6     | 1.385 (4)   | C10—H10     | 0.9300    |
| C1—C2     | 1.399 (3)   | C11—C12     | 1.372 (3) |
| C2—C3     | 1.399 (3)   | C11—H11     | 0.9300    |
| C2—C7     | 1.462 (3)   | C12—C13     | 1.371 (3) |
| C3—C4     | 1.358 (4)   | C13—C14     | 1.375 (4) |
| C3—H3     | 0.9300      | C13—H13     | 0.9300    |
| C4—C5     | 1.377 (5)   | C14—H14     | 0.9300    |
| C7—N1—N2  | 116.14 (19) | N1—C7—C2    | 120.1 (2) |
| C8—N2—N1  | 118.26 (19) | N1—C7—H7    | 119.9     |
| C8—N2—H2  | 122 (2)     | C2—C7—H7    | 119.9     |
| N1—N2—H2  | 120 (2)     | O1—C8—N2    | 122.8 (2) |
| O3—N3—O2  | 123.6 (3)   | O1—C8—C9    | 120.5 (2) |
| O3—N3—C12 | 119.0 (3)   | N2—C8—C9    | 116.7 (2) |
| O2—N3—C12 | 117.4 (3)   | C10—C9—C14  | 119.4 (2) |
| C6—C1—C2  | 122.0 (3)   | C10—C9—C8   | 122.8 (2) |
| C6—C1—C11 | 117.5 (2)   | C14—C9—C8   | 117.8 (2) |
| C2—C1—C11 | 120.5 (2)   | C9—C10—C11  | 120.3 (2) |
| C1—C2—C3  | 116.5 (2)   | C9—C10—H10  | 119.8     |
| C1—C2—C7  | 121.9 (2)   | C11—C10—H10 | 119.8     |
| C3—C2—C7  | 121.6 (2)   | C12—C11—C10 | 118.5 (2) |

|          |           |             |           |
|----------|-----------|-------------|-----------|
| C4—C3—C2 | 121.7 (3) | C12—C11—H11 | 120.7     |
| C4—C3—H3 | 119.2     | C10—C11—H11 | 120.7     |
| C2—C3—H3 | 119.2     | C13—C12—C11 | 122.4 (2) |
| C3—C4—C5 | 120.6 (3) | C13—C12—N3  | 119.2 (2) |
| C3—C4—H4 | 119.7     | C11—C12—N3  | 118.4 (2) |
| C5—C4—H4 | 119.7     | C12—C13—C14 | 118.5 (2) |
| C6—C5—C4 | 120.1 (3) | C12—C13—H13 | 120.7     |
| C6—C5—H5 | 119.9     | C14—C13—H13 | 120.7     |
| C4—C5—H5 | 119.9     | C13—C14—C9  | 120.7 (2) |
| C5—C6—C1 | 119.1 (3) | C13—C14—H14 | 119.6     |
| C5—C6—H6 | 120.4     | C9—C14—H14  | 119.6     |
| C1—C6—H6 | 120.4     |             |           |

*Hydrogen-bond geometry (Å, °)*

| <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> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| N2—H2 $\cdots$ O1 <sup>i</sup> | 0.89 (1)    | 2.06 (1)            | 2.915 (3)                  | 160 (3)                       |

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

Fig. 1

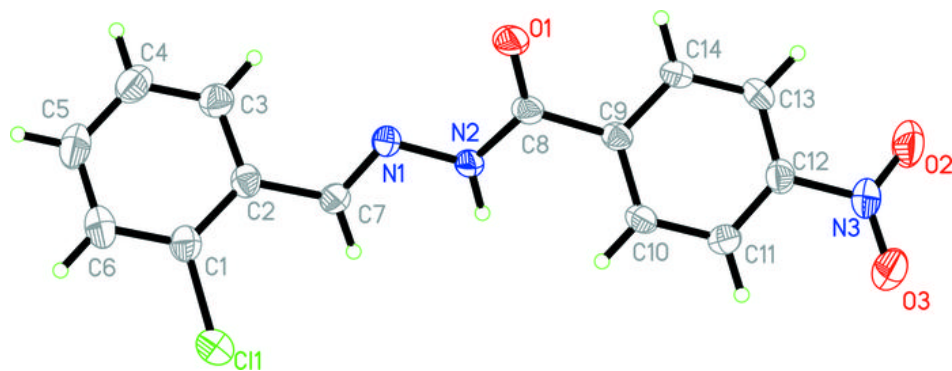




Fig. 2

