

**(E)-1-[4-(4-Chlorobenzoyloxy)benzylidene]-  
2-(2,4-dinitrophenyl)hydrazine****Jun Shi†**

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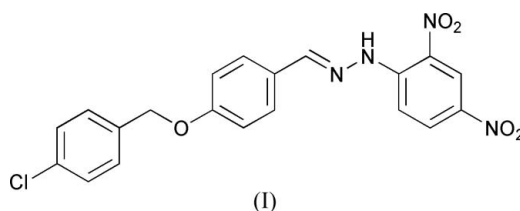
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**Key indicators**Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.040  
 $wR$  factor = 0.107  
Data-to-parameter ratio = 12.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The molecule of the title compound,  $\text{C}_{20}\text{H}_{15}\text{ClN}_4\text{O}_5$ , is not planar; the dinitrophenylhydrazine system makes dihedral angles of  $57.46$  (5) and  $5.77$  (12) $^\circ$  with the terminal benzene ring and the central benzene ring, respectively. An intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond helps to establish the molecular conformation.

**Comment**

Metal complexes involving Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986). Research in this area has been stimulated by biological modelling applications, catalysis, design of molecular magnets and materials chemistry (Larson & Pecoraro, 1991). Consequently, a large number of Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics, such as models to mimic hydrolase in the hydrolysis of *p*-nitrophenyl picolinate (Li *et al.*, 2005).



In the present study, we report the synthesis and molecular structure of the dinitrophenylhydrazine Schiff base derivative, (I) (Fig. 1). The dinitrophenylhydrazine system (atoms C15–C20/O2–O5/N1–N4) is essentially planar, with an r.m.s deviation for fitted atoms of 0.034 Å. This plane makes dihedral angles of  $57.46$  (5) and  $5.77$  (12) $^\circ$  with the terminal benzene ring (C1–C6) and the central benzene ring (C8–C13), respectively. The dihedral angle between the terminal benzene and the central benzene rings is  $56.10$  (8) $^\circ$ . All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The  $\text{O2}-\text{N3}-\text{C20}-\text{C19}$ ,  $\text{O3}-\text{N3}-\text{C20}-\text{C15}$ ,  $\text{O5}-\text{N4}-\text{C18}-\text{C19}$  and  $\text{O4}-\text{N3}-\text{C18}-\text{C17}$  torsion angles are  $-179.7$  (2),  $-178.1$  (2),  $175.8$  (2) and  $175.6$  (2) $^\circ$ , respectively, confirming the coplanarity of the two nitro groups ( $\text{O2}/\text{N3}/\text{O3}$  and  $\text{O4}/\text{N4}/\text{O5}$ ) and their attached aromatic ring (C15–C20).

An intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond (Table 1) helps to stabilize the conformation of the molecule (Fig. 2).

**Experimental**

An anhydrous ethanol solution (50 ml) of 4-(4-chlorobenzoyloxy)benzaldehyde (2.47 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 1-(2,4-dinitrophenyl)hydrazine (1.98 g,

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10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a red precipitate. The product was isolated, recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 88% yield. Red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution.

Crystal data

$C_{20}H_{15}ClN_4O_5$   $V = 946.7(4) \text{ \AA}^3$   
 $M_r = 426.81$   $Z = 2$   
 Triclinic,  $P\bar{1}$   $D_x = 1.497 \text{ Mg m}^{-3}$   
 $a = 7.0914(16) \text{ \AA}$  Mo  $K\alpha$  radiation  $\mu = 0.25 \text{ mm}^{-1}$   
 $b = 11.975(3) \text{ \AA}$   $T = 294(2) \text{ K}$   
 $c = 12.121(3) \text{ \AA}$  Block, red  
 $\alpha = 69.858(4)^\circ$   $0.26 \times 0.20 \times 0.10 \text{ mm}$   
 $\beta = 78.456(4)^\circ$   
 $\gamma = 85.193(4)^\circ$

Data collection

Bruker SMART APEX CCD area-detector diffractometer 4841 measured reflections  
 3332 independent reflections  
 $\varphi$  and  $\omega$  scans 2131 reflections with  $I > 2\sigma(I)$   
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  $R_{int} = 0.020$   
 $\theta_{max} = 25.0^\circ$   
 $T_{min} = 0.921$ ,  $T_{max} = 0.976$

Refinement

Refinement on  $F^2$   $w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 0.08P]$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$  where  $P = (F_o^2 + 2F_c^2)/3$   
 $wR(F^2) = 0.107$   $(\Delta/\sigma)_{max} = 0.004$   
 $S = 1.03$   $\Delta\rho_{max} = 0.18 \text{ e \AA}^{-3}$   
 3332 reflections  $\Delta\rho_{min} = -0.22 \text{ e \AA}^{-3}$   
 271 parameters  
 H-atom parameters constrained

Table 1

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H2 \cdots O2$	0.86	2.01	2.621(2)	128

The H atoms were positioned geometrically and constrained to ride on their parent atoms, with  $Csp^2-H = 0.93 \text{ \AA}$ , methylene  $C-H = 0.97 \text{ \AA}$ ,  $N-H = 0.86 \text{ \AA}$  and  $U_{iso}(H) = 1.2U_{eq}(C,N)$

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

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

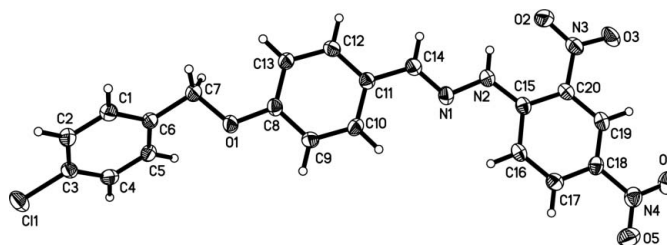


Figure 1 The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

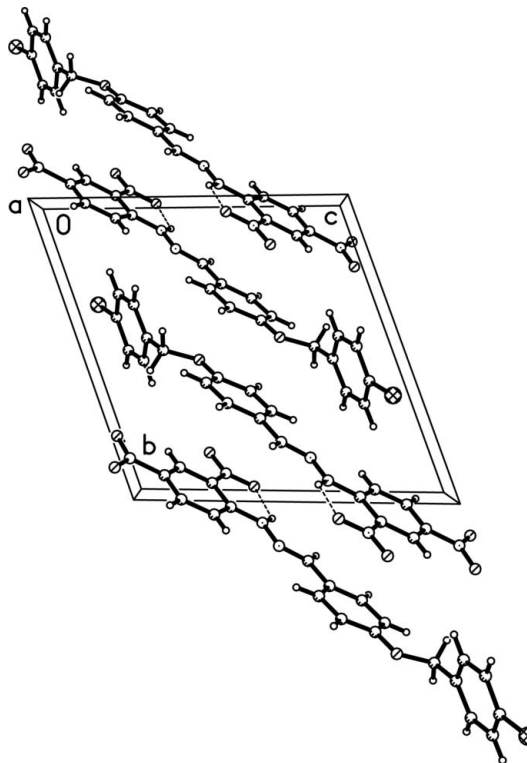


Figure 2 Packing diagram for (I), with hydrogen bonds shown as dashed lines.

Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.  
 Larson, E. J. & Pecoraro, V. L. (1991). *J. Am. Chem. Soc.* **113**, 3810–3818.  
 Li, J.-Z., Xu, B., Li, S.-X., Zeng, W. & Qin, S.-Y. (2005). *Transition Met. Chem.* **30**, 669–676.  
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997a). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997b). *SHELXTL97*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.