Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N,*N*′-Bis(4-chlorobenzylidene)hydrazine

Peng-Wu Zheng,[a]* Wei Wang[b] and Xue-Min Duan[a]

[a]School of Pharmacy, Jiangxi Science and Technology Normal University, Nanchang 330013, People's Republic of China, and [b]Department of Chemical Engineering, Anshan University of Science and Technology, Anshan 114002, People's Republic of China

Correspondence e-mail: zhengpw@sohu.com

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.101
Data-to-parameter ratio = 15.6

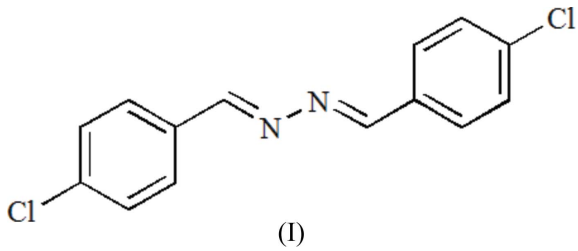
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 August 2005
Accepted 17 August 2005
Online 20 August 2005

The title compound, $C_{14}H_{10}Cl_2N_2$, possesses a crystallographically imposed center of symmetry at the mid-point of the N—N bond and assumes a planar structure.

Comment

Thus far a number of azine compounds containing both a diimine linkage and an N—N bond have been investigated in terms of their crystallography and coordination chemistry (Kundu *et al.*, 2005; Kesslen & Euler, 1999; Armstrong *et al.*, 1998; Xu *et al.*, 1997). We report here the crystal structure of the title compound, (I), in which the two 4-chlorobenzylidene units are directly linked, without a spacer unit, through the imine N atoms.



(I)

In the solid state, the molecule of (I) possesses a crystallographically imposed center of symmetry at the mid-point of the N—N bond. The C═N—N═C linkage is planar. The N—N bond [1.414 (3) Å] is slightly longer than in related azine compounds (Xu *et al.*, 2005; Liu *et al.*, 2004; Şengül *et al.*, 2004). The C═N—N angle [112.6 (2)°] is significantly smaller than the ideal sp^2 value of 120°, as a consequence of repulsion between the nitrogen lone pairs and the adjacent C═N bond. The whole molecule is essentially planar, the r.m.s deviation being 0.020 (2) Å.

Experimental

The title compound was synthesized by the reaction of 4-chlorobenzaldehyde with hydrazine hydrate in refluxing ethanol (Liu *et al.*, 2004). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a cyclohexane solution.

Crystal data

$C_{14}H_{10}Cl_2N_2$
M_r = 277.14
Monoclinic, $P2_1/c$
a = 3.9585 (10) Å
b = 6.9894 (17) Å
c = 23.150 (6) Å
β = 90.416 (4)°
V = 640.5 (3) Å^3
Z = 2
D_x = 1.437 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1257 reflections
θ = 3.0–25.3°
μ = 0.49 mm^{-1}
T = 294 (2) K
Block, colorless
0.26 × 0.20 × 0.14 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.824, T_{max} = 0.934
3387 measured reflections
1281 independent reflections
944 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.3°
$h = -3 \rightarrow 4$
$k = -8 \rightarrow 7$
$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.05
1281 reflections
82 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0392P)^2 + 0.2929P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C5	1.742 (2)	N1—N1^{i}	1.414 (3)
N1—C1	1.269 (3)		
C1—N1—N1^{i}	112.6 (2)	N1—C1—C2	121.8 (2)
N1^{i}—N1—C1—C2	−179.9 (2)	N1—C1—C2—C3	4.7 (3)
N1—C1—C2—C7	−176.1 (2)		

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

All H atoms were positioned geometrically and refined as riding, with C—H distances of 0.93 Å and with U_{iso}(H) = 1.2U_{eq}(C).

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

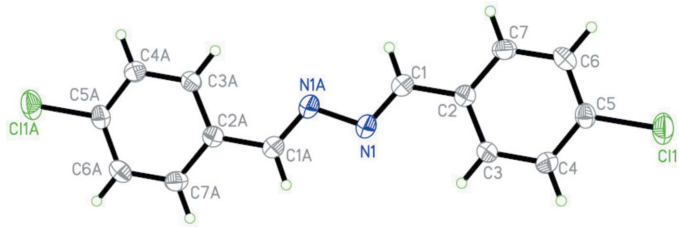


Figure 1
View of the molecule of (I), with displacement ellipsoids drawn at the 30% probability level. The suffix A corresponds to symmetry code (i) in Table 1.

The authors gratefully acknowledge financial support from the Foundation for Excellent Young Teachers of Jiangxi Science and Technology Normal University.

References

Armstrong, J. A., Barnes, J. C. & Weakley, T. J. R. (1998). *Acta Cryst.* C**54**, 1923–1925.
Bruker (1997). *SMART*, *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Kesslen, E. C. & Euler, W. B. (1999). *Chem. Mater.* **11**, 336–340.
Kundu, N., Chatterjee, P. B., Chaudhury, M. & Tiekink, E. R. T. (2005). *Acta Cryst.* E**61**, m1583–m1585.
Liu, S. L., Chen, Y., Dai, J. F. & Liu, H. W. (2004). *Chin. J. Synth. Chem.* **12**, 219–221.
Şengül, A., Karadayi, N. & Büyükgüngör, O. (2004). *Acta Cryst.* C**60**, o507–o508.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Xu, L.-Z., Xu, H.-Z., Yang, S.-H., Li, C.-L & Zhou, K. (2005). *Acta Cryst.* E**61**, o31–o32.
Xu, Z., Thompson, L. K. & Miller, D. O. (1997). *Inorg. Chem.* **36**, 3985–3995.