Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,4-Dichloro-1,4-diphenyl-2,3-diazabuta-1,3-diene

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.031
wR factor = 0.090
Data-to-parameter ratio = 13.8

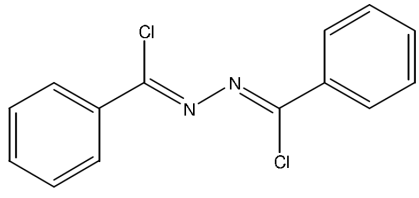
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 25 June 2002
Accepted 10 July 2002
Online 19 July 2002

The title molecule, $C_{14}H_{10}Cl_2N_2$, shows a non-planar geometry, with the two phenyl rings oriented at an angle of 58.28 (9)° to each other. The crystal structure is stabilized by van der Waals interactions.

Comment

Nitric oxide has been found to prevent the damage of cardiovascular, renal, respiratory, gastrointestinal, inflammatory, infective and other diseases (Lehman, 2000; Utepbergenov *et al.*, 1995). Extensive research is under way into the synthesis of NO donors for pharmacological evaluation. The title compound, (I), has been synthesized to monitor the stability factors, *e.g.* interactions stabilizing the structure and *E* or *Z* configuration possessed by the molecule, which might affect further transformations to lead molecules. Thus, an X-ray crystallographic study was needed to confirm the three-dimensional structure, which was not known to date. Moreover, it was possible to perform further reactions in the synthesis of NO donors to achieve pharmacologically active lead molecules. The synthetic route opens a vast number of possibilities for the generation of acyclic and cyclic nitric oxide donors and their analogs; these are frequently used in the management of cardiovascular and other disorders (Lehman, 2000; Utepbergenov *et al.*, 1995).



(I)

The title molecule shows a non-planar geometry, with the planes of the two phenyl rings forming a dihedral angle of 58.28 (9)°. The C7—N8 [1.261 (2) Å], C10—N9 [1.266 (2) Å] and N8—N9 [1.382 (2) Å] distances show normal values. In the crystal, the molecules form layer-like structures parallel to the *ac* plane. The structure is stabilized by van der Waals interactions.

Experimental

The reaction of 1,2-dibenzoylhydrazine with phosphorus pentachloride in dry benzene gave the title compound, 1,4-dichloro-1,4-diphenyl-2,3-diazabuta-1,3-diene (Pechman, 1894). Diffraction-quality crystals were grown at room temperature by slow evaporation of a solution in ethyl acetate.

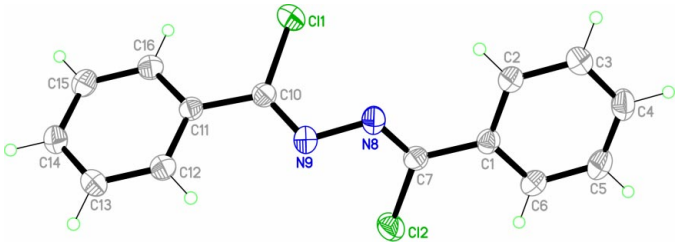


Figure 1
A view of the title compound, showing the atom-labelling scheme and 30% probability ellipsoids.

Crystal data

$C_{14}H_{10}Cl_2N_2$
$M_r = 277.14$
Monoclinic, $P2_1/n$
$a = 11.501\ (1)$ Å
$b = 7.5319\ (7)$ Å
$c = 14.958\ (2)$ Å
$\beta = 99.25\ (1)^\circ$
$V = 1278.9\ (2)$ Å^3
$Z = 4$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 39 reflections
$\theta = 4.5$–12.5°
$\mu = 0.49$ mm^{-1}
$T = 293\ (2)$ K
Block, yellow
0.40 × 0.38 × 0.15 mm

Data collection

Bruker $P4$ diffractometer
θ–2θ scans
Absorption correction: none
3023 measured reflections
2245 independent reflections
1989 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.0^\circ$
$h = -13 \rightarrow 1$
$k = -8 \rightarrow 1$
$l = -17 \rightarrow 17$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.090$
$S = 1.06$
2245 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.2899P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-NT* (Bruker, 1997); program(s) used to refine structure: *SHELXTL-NT*; molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

The authors thank the Molecular and Structural Biology Division, CDRI, Lucknow, India, and M. Zabel, X-ray unit, University of Regensburg, for X-ray services and helpful discussions.

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