Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

N,*N*′-Diphenyloxalamide

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Received 24 April 2006
Accepted 1 May 2006

Key indicators

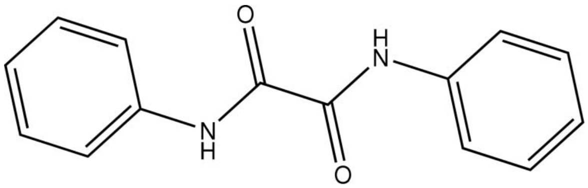
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.103
Data-to-parameter ratio = 13.7

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

The molecule of the title compound, $C_{14}H_{12}N_2O_2$, lies on a crystallographically imposed center of symmetry at the mid-point of the C—C bond of the oxalamide unit. Molecules are linked into ribbons along the *a* axis by N—H···O hydrogen bonds.

Comment

N,*N*′-Diphenyloxalamide and its derivatives have been widely applied in a number of materials as anti-oxidants, ultraviolet absorbents and/or metal ion passivators (Feng *et al.*, 1997). We report here the synthesis and structure of *N*,*N*′-diphenyloxalamide, (I) (Fig. 1 and Table 1).



(I)

The title compound has a crystallographically imposed center of symmetry at the mid-point of the C—C bond of the oxalamide unit. The bond lengths in the oxalamide unit show intermediate values due to π conjugation effects arising from the presence of the two C═O double bonds. All other bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The molecule deviates somewhat from planarity, with the two O atoms twisted to opposite sides of the molecular plane, with a maximum deviation for O1 from the mean plane through C1–C7/N1 of 0.254 (4) Å. Intramolecular hydrogen bonds (C5—H5···O1) form six-membered rings between the phenyl rings and the carbonyl O atoms. In the crystal structure, molecules are linked into ribbons along the *a* axis (Fig. 2) by inversion-related intermolecular N—H···O hydrogen bonds (Table 2).

Experimental

To a solution of aniline (16.6 g, 0.2 mol) in benzene (90 ml) was added dropwise a solution of oxalyl chloride (6.4 g, 0.05 mol) in benzene (30 ml), and the mixture was stirred at 343 K for 6 h. After cooling to room temperature, 50 ml water was added and the organic phase was washed three times with water to give a white solid. The title compound was obtained after drying at room temperature for 48 h. Colorless single crystals suitable for X-ray diffraction were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution over a period of 6 h.

doi:10.1107/S1600536806015972

Crystal data

$C_{14}H_{12}N_2O_2$
$M_r = 240.26$
Monoclinic, $P2_1/c$
$a = 5.3207\ (7)$ Å
$b = 5.3723\ (7)$ Å
$c = 20.5227\ (19)$ Å
$\beta = 101.437\ (3)^\circ$
$V = 574.98\ (12)$ Å^3

$Z = 2$
$D_x = 1.388$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
Block, colorless
0.43 × 0.21 × 0.20 mm

Data collection

Siemens SMART 1000 CCD area detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.960$, $T_{\max} = 0.981$

3076 measured reflections
1133 independent reflections
1039 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.019$
$\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.103$
$S = 1.08$
1133 reflections
83 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.089P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.203 (17)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.2209 (14)	N1—C6	1.4182 (15)
N1—C7	1.3366 (16)	C7—C7$^{\rm i}$	1.543 (2)
C7—N1—C6	127.27 (10)	O1—C7—C7$^{\rm i}$	121.16 (13)
O1—C7—N1	126.95 (11)	N1—C7—C7$^{\rm i}$	111.89 (12)

Symmetry code: (i) $-x+2, -y-2, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1$^{\rm ii}$	0.86	2.38	3.161 (1)	152
N1—H1B···O1$^{\rm i}$	0.86	2.26	2.680 (1)	110
C5—H5A···O1	0.93	2.39	2.925 (2)	116

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

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}(C,N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

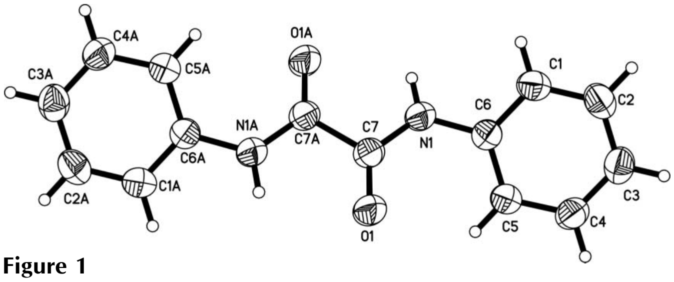


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Atoms labelled with the suffix 'A' are related to the other atoms by the symmetry code $(2-x, -2-y, -z)$, corresponding to (i) in Table 1.

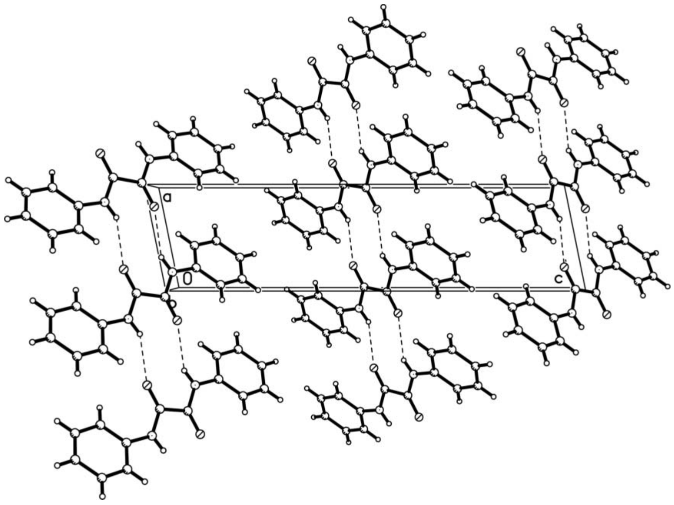


Figure 2
A view down the b axis, showing the ribbons generated by hydrogen bonds (indicated by dashed lines).

This project was supported by the Special Project of Qingdao for Leadership of Science and Technology (No. 05–2-JC-80) and the Outstanding Young-Adult Scientific Research Encouraging Foundation of Shandong Province (No. 2005BS04007).

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