Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(4-Chlorophenyl)-2-nitrobenzamide

Aamer Saeed,[a] Shahid Hussain[a] and Michael Bolte[b]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad, Pakistan, and [b]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany
Correspondence e-mail: aamersaeed@yahoo.com

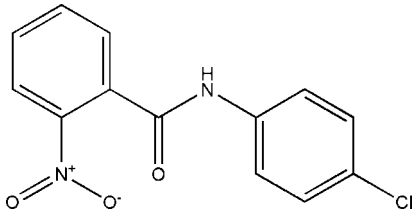
Received 25 October 2007; accepted 4 November 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.090; data-to-parameter ratio = 12.4.

In the title compound, $C_{13}H_9ClN_2O_3$, the dihedral angle between the two aromatic rings is 82.71 (6)°. The nitro group is twisted by 40.6 (2)° from the plane of its attached benzene ring. The packing is stabilized by an N—H···O hydrogen bond.

Related literature

For background, see: Makino *et al.* (2003); Igawa *et al.* (1999).



Experimental

Crystal data

$C_{13}H_9ClN_2O_3$
M_r = 276.67
Orthorhombic, *Fdd*2
a = 23.8527 (15) Å
b = 40.936 (3) Å
c = 5.0780 (4) Å
V = 4958.3 (6) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 173 (2) K
0.33 × 0.12 × 0.11 mm

Data collection

STOE IPDS II two-circle-diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.904, T_{max} = 0.956
10236 measured reflections
2181 independent reflections
2083 reflections with $I > 2\sigma(I)$
R_{int} = 0.071

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.090
S = 1.04
2181 reflections
176 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 955 Friedel pairs
Flack parameter: 0.00 (6)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88 (3)	2.05 (3)	2.874 (2)	157 (2)

Symmetry code: (i) $x, y, z+1$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

AS gratefully acknowledges a research grant from the Quaid-I-Azam University, Islamabad, Pakistan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2615).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Igawa, H., Nishimura, M., Okada, K. & Nakamura, T. (1999). Japan Patent 11 171 848.
Makino, S., Nakanishi, E. & Tsuji, T. (2003). *Bull. Kor. Chem. Soc.* **24**, 389–392.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Germany.

supplementary materials

Acta Cryst. (2007). E**63**, o4615 [**doi:10.1107/S1600536807055742**]

N-(4-Chlorophenyl)-2-nitrobenzamide

A. Saeed, S. Hussain and M. Bolte

Comment

The benzanilide core is present in compounds with such a wide range of biological activities that it has been called a privileged structure (*e.g.* Makino *et al.*, 2003; Igawa *et al.*, 1999). As part of our studies in this area, the synthesis and structure of the title compound, (I), is now presented.

The geometric parameters for (I) are in the usual ranges. The dihedral angle between the two aromatic rings is 82.71 (6)°. The nitro group is twisted by 40.6 (2)° from the plane of the phenyl ring to which it is attached (Fig. 1). The crystal packing is stabilized by an N—H···O hydrogen bond (Table 1), leading to C(4) chains propagating in [001].

Experimental

A mixture of 4-chloroaniline (10.0 g, 65.7 mmol), 2-nitrobenzoyl chloride (10 ml, 86.9 mmol) and pyridine (20 ml) was left at 298 K for 15 h. Water (100 ml) was then added, and the resulting precipitate was collected. Recrystallization from benzene gave 12.6 g (75%) of (I) as yellow needles: mp 368–369 K, 1H NMR ($CDCl_3$) δ 7.23–8.30 (m, 8H, Ar—Hs), 11.36 (br s, 1H, NH).

Refinement

All H atoms were located in a difference map. Those bonded to C were relocated in idealized positions (C—H = 0.95 Å) and refined as riding with U_{iso}(H) = 1.2 U_{eq}(C). The H atom bonded to N was freely refined.

Figures

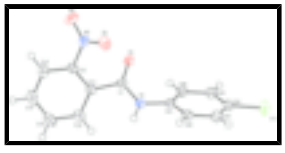


Fig. 1. The molecular structure of (I) with displacement ellipsoids for the non-hydrogen atoms at the 50% probability level.

N-(4-Chlorophenyl)-2-nitrobenzamide

Crystal data

$C_{13}H_9ClN_2O_3$	F_{000} = 2272
M_r = 276.67	D_x = 1.483 Mg m^{-3}
Orthorhombic, *Fdd*2	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: F 2 -2d	Cell parameters from 9190 reflections
a = 23.8527 (15) Å	θ = 2.8–25.2°

b = 40.936 (3) Å	μ = 0.31 mm^{-1}
c = 5.0780 (4) Å	T = 173 (2) K
V = 4958.3 (6) Å^3	Needle, colourless
Z = 16	0.33 × 0.12 × 0.11 mm

Data collection

STOE IPDS II two-circle-diffractometer	2181 independent reflections
Radiation source: fine-focus sealed tube	2083 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.071
T = 173(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -26\rightarrow28$
T_{min} = 0.904, T_{max} = 0.956	$k = -40\rightarrow48$
10236 measured reflections	$l = -6\rightarrow6$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.090	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.16 e Å^{-3}
2181 reflections	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
176 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 955 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.00 (6)
Secondary atom site location: difference Fourier map	

Special details

Experimental. ;

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.67478 (2)	0.239794 (13)	0.39083 (13)	0.03892 (17)
C1	0.41096 (8)	0.18013 (4)	0.1564 (4)	0.0221 (4)
O1	0.42715 (6)	0.18287 (4)	−0.0713 (3)	0.0355 (4)
N1	0.44331 (7)	0.18661 (4)	0.3687 (3)	0.0215 (3)
H1	0.4295 (10)	0.1826 (6)	0.526 (6)	0.026 (6)*
N2	0.35978 (7)	0.12292 (4)	−0.0872 (4)	0.0269 (4)
O2	0.40437 (7)	0.11395 (4)	0.0044 (4)	0.0413 (4)
O3	0.34094 (7)	0.11341 (5)	−0.2990 (4)	0.0481 (5)
C11	0.35158 (8)	0.17038 (5)	0.2139 (3)	0.0222 (4)
C12	0.32552 (8)	0.14551 (5)	0.0699 (4)	0.0220 (4)
C13	0.26869 (9)	0.13956 (5)	0.0811 (4)	0.0296 (5)
H13	0.2520	0.1232	−0.0258	0.036*
C14	0.23644 (9)	0.15811 (6)	0.2528 (5)	0.0360 (5)
H14	0.1973	0.1542	0.2658	0.043*
C15	0.26085 (9)	0.18207 (6)	0.4040 (6)	0.0401 (5)
H15	0.2385	0.1944	0.5228	0.048*
C16	0.31833 (9)	0.18851 (5)	0.3848 (5)	0.0320 (5)
H16	0.3347	0.2053	0.4886	0.038*
C21	0.49942 (7)	0.19862 (4)	0.3606 (4)	0.0197 (4)
C22	0.53631 (8)	0.18872 (5)	0.5573 (4)	0.0240 (4)
H22	0.5244	0.1735	0.6867	0.029*
C23	0.59041 (9)	0.20106 (5)	0.5651 (4)	0.0267 (4)
H23	0.6157	0.1943	0.6990	0.032*
C24	0.60706 (8)	0.22331 (4)	0.3755 (4)	0.0251 (4)
C25	0.57105 (8)	0.23332 (5)	0.1771 (4)	0.0260 (4)
H25	0.5833	0.2485	0.0476	0.031*
C26	0.51674 (8)	0.22091 (4)	0.1699 (4)	0.0230 (4)
H26	0.4916	0.2276	0.0354	0.028*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0231 (3)	0.0424 (3)	0.0512 (3)	−0.0075 (2)	−0.0017 (2)	0.0032 (3)
C1	0.0232 (9)	0.0261 (9)	0.0170 (9)	−0.0025 (7)	0.0021 (8)	−0.0016 (8)
O1	0.0297 (8)	0.0608 (10)	0.0161 (8)	−0.0190 (7)	0.0022 (6)	−0.0030 (7)
N1	0.0236 (8)	0.0275 (8)	0.0134 (8)	−0.0042 (6)	0.0022 (7)	0.0016 (7)
N2	0.0248 (8)	0.0264 (8)	0.0296 (9)	−0.0019 (7)	−0.0011 (8)	−0.0049 (7)
O2	0.0273 (9)	0.0520 (10)	0.0445 (10)	0.0115 (7)	−0.0022 (7)	−0.0088 (8)
O3	0.0438 (10)	0.0580 (10)	0.0424 (10)	−0.0010 (8)	−0.0110 (8)	−0.0273 (8)
C11	0.0236 (10)	0.0245 (9)	0.0185 (10)	−0.0012 (7)	0.0005 (7)	0.0015 (7)
C12	0.0230 (10)	0.0232 (8)	0.0198 (9)	0.0006 (7)	0.0011 (8)	0.0013 (7)
C13	0.0220 (10)	0.0316 (10)	0.0352 (12)	−0.0020 (7)	−0.0041 (9)	0.0046 (9)
C14	0.0201 (10)	0.0446 (12)	0.0432 (13)	0.0004 (9)	0.0032 (9)	0.0062 (10)
C15	0.0303 (11)	0.0447 (12)	0.0453 (14)	0.0078 (10)	0.0136 (11)	−0.0048 (11)

C16	0.0320 (11)	0.0348 (10)	0.0294 (11)	−0.0002 (8)	0.0055 (9)	−0.0071 (10)
C21	0.0223 (9)	0.0194 (8)	0.0173 (8)	−0.0013 (7)	−0.0001 (7)	−0.0028 (7)
C22	0.0270 (10)	0.0256 (8)	0.0196 (9)	0.0012 (8)	0.0014 (7)	0.0030 (7)
C23	0.0240 (10)	0.0310 (10)	0.0252 (10)	0.0043 (8)	−0.0037 (8)	0.0010 (8)
C24	0.0205 (9)	0.0251 (9)	0.0298 (11)	−0.0016 (7)	0.0029 (8)	−0.0055 (8)
C25	0.0295 (10)	0.0233 (8)	0.0252 (11)	−0.0040 (7)	0.0036 (8)	0.0009 (8)
C26	0.0272 (9)	0.0233 (8)	0.0185 (9)	−0.0026 (7)	−0.0001 (8)	−0.0001 (7)

Geometric parameters (Å, °)

Cl1—C24	1.7522 (19)	C14—H14	0.9500
C1—O1	1.224 (3)	C15—C16	1.400 (3)
C1—N1	1.352 (3)	C15—H15	0.9500
C1—C11	1.500 (3)	C16—H16	0.9500
N1—C21	1.426 (2)	C21—C22	1.392 (3)
N1—H1	0.88 (3)	C21—C26	1.393 (3)
N2—O2	1.218 (2)	C22—C23	1.386 (3)
N2—O3	1.229 (3)	C22—H22	0.9500
N2—C12	1.469 (3)	C23—C24	1.384 (3)
C11—C16	1.390 (3)	C23—H23	0.9500
C11—C12	1.399 (3)	C24—C25	1.386 (3)
C12—C13	1.379 (3)	C25—C26	1.392 (3)
C13—C14	1.389 (3)	C25—H25	0.9500
C13—H13	0.9500	C26—H26	0.9500
C14—C15	1.375 (4)		
O1—C1—N1	123.72 (17)	C16—C15—H15	119.7
O1—C1—C11	120.40 (17)	C11—C16—C15	120.1 (2)
N1—C1—C11	115.83 (17)	C11—C16—H16	119.9
C1—N1—C21	125.47 (16)	C15—C16—H16	119.9
C1—N1—H1	118.3 (16)	C22—C21—C26	120.14 (16)
C21—N1—H1	116.2 (16)	C22—C21—N1	118.19 (16)
O2—N2—O3	123.93 (19)	C26—C21—N1	121.59 (17)
O2—N2—C12	117.93 (17)	C23—C22—C21	120.22 (17)
O3—N2—C12	118.10 (17)	C23—C22—H22	119.9
C16—C11—C12	117.46 (18)	C21—C22—H22	119.9
C16—C11—C1	121.20 (18)	C24—C23—C22	119.14 (18)
C12—C11—C1	120.75 (17)	C24—C23—H23	120.4
C13—C12—C11	122.96 (18)	C22—C23—H23	120.4
C13—C12—N2	117.26 (17)	C23—C24—C25	121.51 (17)
C11—C12—N2	119.64 (16)	C23—C24—Cl1	119.15 (16)
C12—C13—C14	118.3 (2)	C25—C24—Cl1	119.33 (15)
C12—C13—H13	120.9	C24—C25—C26	119.21 (18)
C14—C13—H13	120.9	C24—C25—H25	120.4
C15—C14—C13	120.4 (2)	C26—C25—H25	120.4
C15—C14—H14	119.8	C25—C26—C21	119.78 (18)
C13—C14—H14	119.8	C25—C26—H26	120.1
C14—C15—C16	120.7 (2)	C21—C26—H26	120.1
C14—C15—H15	119.7		
O1—C1—N1—C21	2.6 (3)	C13—C14—C15—C16	1.0 (4)

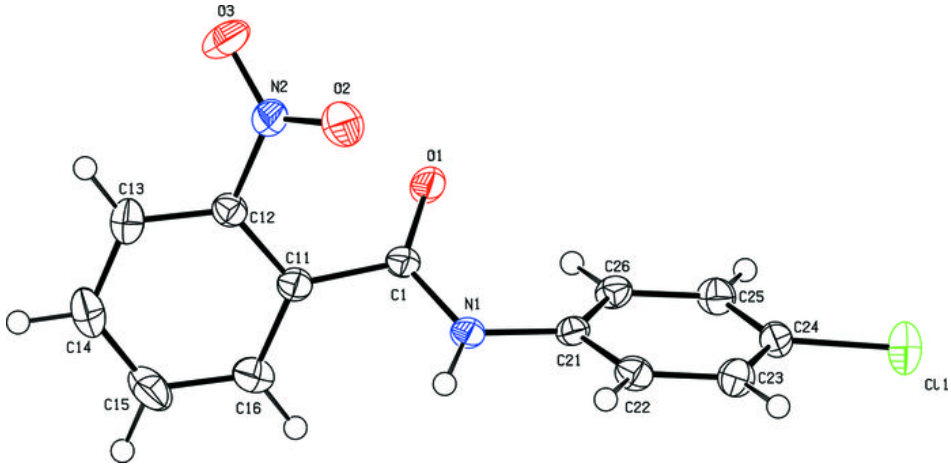
C11—C1—N1—C21	−175.00 (16)	C12—C11—C16—C15	−1.3 (3)
O1—C1—C11—C16	−128.4 (2)	C1—C11—C16—C15	170.0 (2)
N1—C1—C11—C16	49.3 (3)	C14—C15—C16—C11	−0.8 (4)
O1—C1—C11—C12	42.6 (3)	C1—N1—C21—C22	−147.03 (19)
N1—C1—C11—C12	−139.74 (19)	C1—N1—C21—C26	36.1 (3)
C16—C11—C12—C13	3.3 (3)	C26—C21—C22—C23	0.2 (3)
C1—C11—C12—C13	−168.00 (18)	N1—C21—C22—C23	−176.74 (17)
C16—C11—C12—N2	−172.14 (18)	C21—C22—C23—C24	0.1 (3)
C1—C11—C12—N2	16.5 (3)	C22—C23—C24—C25	−0.5 (3)
O2—N2—C12—C13	−137.1 (2)	C22—C23—C24—Cl1	178.17 (15)
O3—N2—C12—C13	40.6 (3)	C23—C24—C25—C26	0.6 (3)
O2—N2—C12—C11	38.6 (3)	Cl1—C24—C25—C26	−178.13 (14)
O3—N2—C12—C11	−143.7 (2)	C24—C25—C26—C21	−0.2 (3)
C11—C12—C13—C14	−3.1 (3)	C22—C21—C26—C25	−0.1 (3)
N2—C12—C13—C14	172.42 (18)	N1—C21—C26—C25	176.67 (17)
C12—C13—C14—C15	0.9 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88 (3)	2.05 (3)	2.874 (2)	157 (2)

Symmetry codes: (i) *x*, *y*, *z*+1.

Fig. 1


O3
N2
O2
O1
C13
C12
C11
C1
N1
C26
C25
C24
C14
C21
C23
CL1
C15
C16
C22