Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-(2-Aminophenyl)-2-anilinobenzamide

Kun Huang, Feng Huang and Da-Bin Qin*

School of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, People's Republic of China
Correspondence e-mail: qindabincwnu@yahoo.com.cn

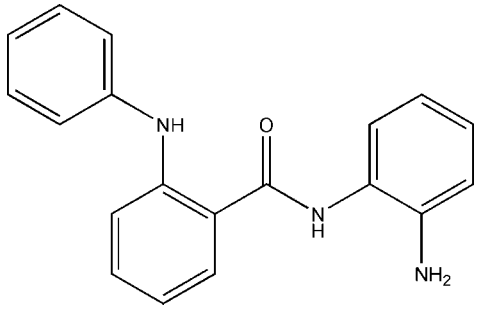
Received 16 March 2009; accepted 6 April 2009

Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.072; data-to-parameter ratio = 8.2.

In the title compound, $C_{19}H_{17}N_3O$, the planes of the aromatic substituents attached to the benzamide moiety are almost perpendicular to one another, making a dihedral angle of 88.16 (7)°. The observed conformation of the molecule is produced by an intramolecular N—H···O hydrogen bond.

Related literature

For the synthesis, see: Martín *et al.* (2006); Charton *et al.* (2006). For related structures, see: Yusof *et al.* (2003); Du *et al.* (2009).



Experimental

Crystal data

$C_{19}H_{17}N_3O$
M_r = 303.36
Monoclinic, Cc
a = 6.707 (3) Å
b = 25.95 (1) Å
c = 9.480 (5) Å
β = 103.398 (7)°
V = 1605.0 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 93 K
0.40 × 0.27 × 0.10 mm

Data collection

Rigaku Spider diffractometer
Absorption correction: none
6515 measured reflections
1844 independent reflections
1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.072
S = 1.00
1844 reflections
224 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1	0.88 (3)	1.96 (3)	2.714 (3)	142 (2)

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the Scientific Research Fund Projects of China West Normal University (grant No. 06B003) and the Youth Fund Projects of Sichuan Educational Department (grant No. 2006B039).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2107).

References

Charton, J., Mizzi, S. G., Fontaine, M. A. D., Foufelle, F., Hainault, I., Espiard, J. G. B., Caignard, D. H. & Sergheraert, C. (2006). *Bioorg. Med. Chem.* **14**, 4490–4518.
Du, P., Jiang, X. K. & Li, Z. T. (2009). *Tetrahedron Lett.* **50**, 316–319.
Martín, A., Mesa, M., Docampo, M. L., Gómez, V. & Pellón, R. F. (2006). *Synth. Commun.* **36**, 271–277.
Rigaku/MSC (2004). *RAPID-AUTO*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yusof, M. S. M., Yamin, B. M. & Shamsuddin, M. (2003). *Acta Cryst.* E**59**, o810–o811.

supporting information

Acta Cryst. (2009). E**65**, o1108 [doi:10.1107/S1600536809013014]

N-(2-Aminophenyl)-2-anilinobenzamide

Kun Huang, Feng Huang and Da-Bin Qin

S1. Comment

Nowadays many researchers are intrested in the synthesis of new insecticides. Benzamide or its derivatives or analogs are used in the pharmaceutical industry for this purpose. We herein report the crystal structure of the title compound.

Bond lengths and angles in the title molecule (Fig. 1) are within normal ranges. The planes of the aromatic substituents attached to the benzamide moiety (C7—C12 and C14—C19) are almost perpendicular to one another, with a dihedral angle of 88.16 (7)° whereas the dihedral angle between C7—C12 and C1—C6 measures to 47.28 (9)°. The planes between C7—C12 and the amide moiety C12/C13/N2/O1 enclose an angle of 63.06 (8)°.

S2. Experimental

The title compound was prepared according to the reported procedure of Martín *et al.* (2006). and Charton *et al.* (2006). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from dichloromethane.

S3. Refinement

H atoms were placed in calculated positions with N—H = 0.88–0.93 Å and C—H = 0.95 Å and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C,*N*). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

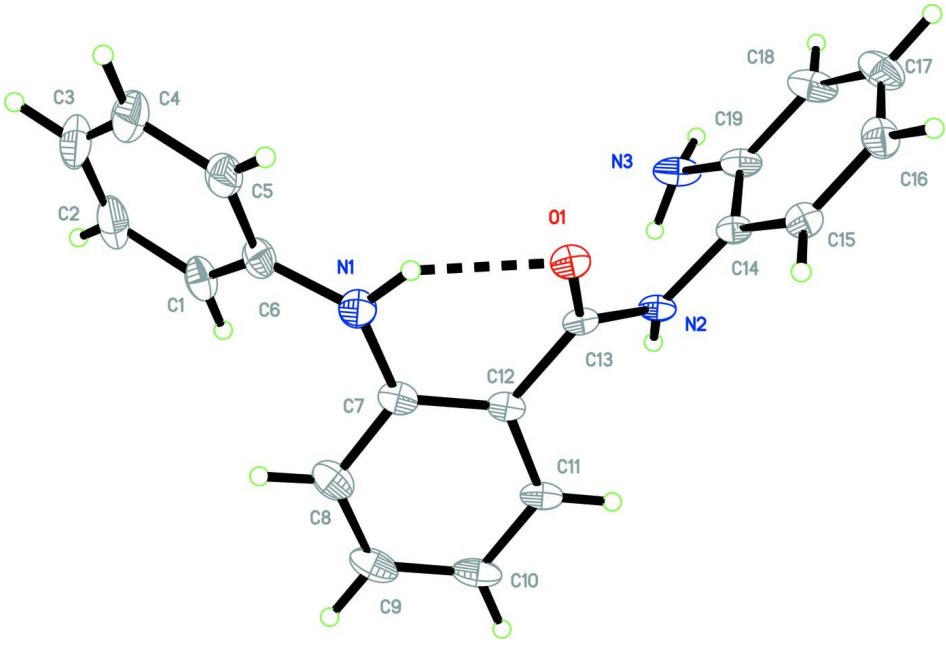


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering.

N-(2-Aminophenyl)-2-anilinobenzamide

Crystal data

$C_{19}H_{17}N_3O$
$M_r = 303.36$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 6.707\ (3)$ Å
$b = 25.95\ (1)$ Å
$c = 9.480\ (5)$ Å
$\beta = 103.398\ (7)°$
$V = 1605.0\ (14)$ Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.255$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2858 reflections
$\theta = 3.1–27.5°$
$\mu = 0.08$ mm^{-1}
$T = 93$ K
Platelet, colorless
0.40 × 0.27 × 0.10 mm

Data collection

Rigaku Spider diffractometer
Radiation source: Rotating Anode
Graphite monochromator
ω scans
6515 measured reflections
1844 independent reflections
1695 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow8$
$k = -33\rightarrow31$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.072$
$S = 1.00$
1844 reflections
224 parameters
2 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H atoms treated by a mixture of independent and constrained refinement	$\Delta\rho_{max} = 0.14$ e Å^{-3}
	$\Delta\rho_{min} = -0.15$ e Å^{-3}

Special details

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.4009 (2)	0.47225 (5)	0.56166 (13)	0.0295 (3)
N2	0.3896 (2)	0.51617 (6)	0.35407 (16)	0.0257 (3)
N1	0.4426 (3)	0.36962 (7)	0.52152 (19)	0.0368 (4)
N3	0.0087 (3)	0.53595 (9)	0.16236 (19)	0.0418 (5)
H3A	0.106 (4)	0.5228 (9)	0.121 (3)	0.053 (7)*
H3B	−0.103 (4)	0.5495 (10)	0.097 (3)	0.063 (8)*
C1	0.3021 (4)	0.28921 (8)	0.3998 (2)	0.0435 (6)
H1	0.3647	0.2955	0.3212	0.052*
C2	0.1803 (4)	0.24613 (9)	0.3980 (3)	0.0600 (7)
H2	0.1605	0.2230	0.3183	0.072*
C3	0.0878 (5)	0.23638 (10)	0.5100 (4)	0.0725 (9)
H3	0.0028	0.2070	0.5080	0.087*
C4	0.1209 (5)	0.27031 (10)	0.6262 (4)	0.0674 (8)
H4	0.0588	0.2638	0.7049	0.081*
C5	0.2422 (4)	0.31325 (9)	0.6295 (3)	0.0470 (6)
H5	0.2633	0.3360	0.7100	0.056*
C6	0.3335 (3)	0.32336 (8)	0.5156 (2)	0.0366 (5)
C7	0.5729 (3)	0.38514 (8)	0.4348 (2)	0.0326 (5)
C8	0.7016 (3)	0.34982 (9)	0.3887 (2)	0.0425 (5)
H8	0.6954	0.3144	0.4127	0.051*
C9	0.8377 (4)	0.36594 (10)	0.3087 (2)	0.0475 (6)
H9	0.9231	0.3413	0.2773	0.057*
C10	0.8519 (3)	0.41732 (10)	0.2733 (2)	0.0429 (6)
H10	0.9467	0.4281	0.2187	0.052*
C11	0.7264 (3)	0.45261 (9)	0.3184 (2)	0.0331 (5)
H11	0.7366	0.4880	0.2952	0.040*
C12	0.5841 (3)	0.43752 (8)	0.39754 (18)	0.0271 (4)
C13	0.4524 (3)	0.47661 (7)	0.44460 (18)	0.0245 (4)
C14	0.2603 (3)	0.55640 (7)	0.38352 (19)	0.0272 (4)

C15	0.3209 (3)	0.58570 (8)	0.5089 (2)	0.0324 (4)
H15	0.4505	0.5797	0.5728	0.039*
C16	0.1931 (4)	0.62359 (9)	0.5410 (2)	0.0420 (5)
H16	0.2341	0.6435	0.6269	0.050*
C17	0.0059 (4)	0.63226 (10)	0.4473 (2)	0.0492 (6)
H17	−0.0831	0.6579	0.4697	0.059*
C18	−0.0532 (4)	0.60405 (10)	0.3216 (2)	0.0468 (6)
H18	−0.1821	0.6108	0.2577	0.056*
C19	0.0727 (3)	0.56574 (8)	0.2863 (2)	0.0339 (5)
H1N	0.400 (4)	0.3966 (10)	0.563 (3)	0.053 (7)*
H2N	0.414 (3)	0.5148 (7)	0.269 (2)	0.030 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0355 (7)	0.0417 (8)	0.0137 (6)	−0.0010 (6)	0.0106 (5)	−0.0004 (5)
N2	0.0232 (8)	0.0413 (9)	0.0144 (7)	0.0023 (7)	0.0076 (6)	0.0006 (7)
N1	0.0459 (11)	0.0375 (10)	0.0305 (9)	−0.0001 (8)	0.0162 (8)	−0.0020 (8)
N3	0.0251 (9)	0.0777 (15)	0.0209 (9)	0.0039 (9)	0.0022 (8)	−0.0025 (9)
C1	0.0528 (14)	0.0313 (11)	0.0418 (13)	0.0092 (10)	0.0019 (11)	0.0049 (10)
C2	0.0694 (18)	0.0288 (12)	0.0729 (18)	0.0060 (11)	−0.0017 (16)	0.0033 (12)
C3	0.078 (2)	0.0320 (14)	0.107 (3)	−0.0012 (13)	0.0214 (19)	0.0199 (16)
C4	0.084 (2)	0.0450 (15)	0.081 (2)	0.0042 (14)	0.0353 (17)	0.0261 (15)
C5	0.0580 (15)	0.0393 (12)	0.0475 (14)	0.0108 (11)	0.0199 (12)	0.0167 (11)
C6	0.0423 (13)	0.0324 (11)	0.0330 (11)	0.0081 (9)	0.0043 (9)	0.0101 (9)
C7	0.0315 (11)	0.0456 (13)	0.0207 (10)	0.0045 (9)	0.0058 (8)	−0.0018 (9)
C8	0.0457 (13)	0.0486 (13)	0.0325 (12)	0.0126 (10)	0.0076 (10)	−0.0025 (10)
C9	0.0411 (13)	0.0673 (17)	0.0364 (13)	0.0193 (12)	0.0137 (11)	−0.0061 (11)
C10	0.0275 (11)	0.0734 (17)	0.0294 (12)	0.0091 (10)	0.0098 (9)	−0.0053 (11)
C11	0.0226 (9)	0.0560 (13)	0.0207 (10)	0.0036 (9)	0.0050 (8)	−0.0017 (9)
C12	0.0239 (9)	0.0413 (11)	0.0151 (9)	0.0032 (8)	0.0025 (7)	−0.0017 (8)
C13	0.0198 (9)	0.0383 (11)	0.0153 (9)	−0.0034 (8)	0.0037 (7)	−0.0020 (8)
C14	0.0263 (10)	0.0371 (10)	0.0193 (9)	0.0006 (8)	0.0079 (8)	0.0041 (8)
C15	0.0366 (11)	0.0403 (11)	0.0211 (10)	−0.0017 (9)	0.0082 (8)	0.0019 (9)
C16	0.0592 (15)	0.0385 (12)	0.0340 (11)	0.0015 (10)	0.0225 (11)	0.0003 (10)
C17	0.0615 (16)	0.0546 (15)	0.0392 (14)	0.0227 (12)	0.0274 (13)	0.0120 (11)
C18	0.0390 (13)	0.0721 (16)	0.0319 (12)	0.0204 (12)	0.0132 (10)	0.0145 (11)
C19	0.0287 (11)	0.0548 (13)	0.0196 (9)	0.0035 (9)	0.0085 (8)	0.0064 (9)

Geometric parameters (Å, º)

O1—C13	1.241 (2)	C7—C8	1.397 (3)
N2—C13	1.342 (2)	C7—C12	1.411 (3)
N2—C14	1.425 (2)	C8—C9	1.380 (3)
N2—H2N	0.86 (2)	C8—H8	0.9500
N1—C7	1.391 (3)	C9—C10	1.384 (4)
N1—C6	1.400 (3)	C9—H9	0.9500
N1—H1N	0.88 (3)	C10—C11	1.377 (3)

N3—C19	1.389 (3)	C10—H10	0.9500
N3—H3A	0.90 (3)	C11—C12	1.400 (3)
N3—H3B	0.93 (3)	C11—H11	0.9500
C1—C2	1.382 (4)	C12—C13	1.480 (2)
C1—C6	1.389 (3)	C14—C15	1.390 (3)
C1—H1	0.9500	C14—C19	1.398 (3)
C2—C3	1.372 (4)	C15—C16	1.384 (3)
C2—H2	0.9500	C15—H15	0.9500
C3—C4	1.387 (4)	C16—C17	1.378 (3)
C3—H3	0.9500	C16—H16	0.9500
C4—C5	1.376 (4)	C17—C18	1.376 (4)
C4—H4	0.9500	C17—H17	0.9500
C5—C6	1.383 (3)	C18—C19	1.394 (3)
C5—H5	0.9500	C18—H18	0.9500

C13—N2—C14	123.37 (15)	C8—C9—C10	121.1 (2)
C13—N2—H2N	118.0 (13)	C8—C9—H9	119.4
C14—N2—H2N	118.0 (13)	C10—C9—H9	119.4
C7—N1—C6	128.24 (19)	C11—C10—C9	119.0 (2)
C7—N1—H1N	110.2 (17)	C11—C10—H10	120.5
C6—N1—H1N	118.5 (17)	C9—C10—H10	120.5
C19—N3—H3A	117.9 (16)	C10—C11—C12	121.5 (2)
C19—N3—H3B	113.5 (16)	C10—C11—H11	119.3
H3A—N3—H3B	114 (2)	C12—C11—H11	119.3
C2—C1—C6	120.4 (2)	C11—C12—C7	119.10 (18)
C2—C1—H1	119.8	C11—C12—C13	119.91 (18)
C6—C1—H1	119.8	C7—C12—C13	120.96 (17)
C3—C2—C1	120.8 (3)	O1—C13—N2	122.03 (17)
C3—C2—H2	119.6	O1—C13—C12	121.07 (17)
C1—C2—H2	119.6	N2—C13—C12	116.89 (15)
C2—C3—C4	118.7 (3)	C15—C14—C19	120.58 (18)
C2—C3—H3	120.7	C15—C14—N2	119.84 (17)
C4—C3—H3	120.7	C19—C14—N2	119.57 (17)
C5—C4—C3	121.1 (3)	C16—C15—C14	120.2 (2)
C5—C4—H4	119.4	C16—C15—H15	119.9
C3—C4—H4	119.4	C14—C15—H15	119.9
C4—C5—C6	120.1 (3)	C17—C16—C15	119.5 (2)
C4—C5—H5	119.9	C17—C16—H16	120.2
C6—C5—H5	119.9	C15—C16—H16	120.2
C5—C6—C1	118.9 (2)	C18—C17—C16	120.5 (2)
C5—C6—N1	116.9 (2)	C18—C17—H17	119.8
C1—C6—N1	124.09 (19)	C16—C17—H17	119.8
N1—C7—C8	120.88 (19)	C17—C18—C19	121.2 (2)
N1—C7—C12	120.29 (18)	C17—C18—H18	119.4
C8—C7—C12	118.77 (19)	C19—C18—H18	119.4
C9—C8—C7	120.6 (2)	N3—C19—C18	120.96 (19)
C9—C8—H8	119.7	N3—C19—C14	121.04 (19)
C7—C8—H8	119.7	C18—C19—C14	117.92 (19)

C6—C1—C2—C3	0.2 (4)	N1—C7—C12—C13	−2.4 (3)
C1—C2—C3—C4	−0.8 (4)	C8—C7—C12—C13	−179.51 (17)
C2—C3—C4—C5	0.6 (4)	C14—N2—C13—O1	0.2 (3)
C3—C4—C5—C6	0.1 (4)	C14—N2—C13—C12	179.19 (17)
C4—C5—C6—C1	−0.7 (4)	C11—C12—C13—O1	−145.63 (18)
C4—C5—C6—N1	175.5 (2)	C7—C12—C13—O1	32.5 (3)
C2—C1—C6—C5	0.5 (3)	C11—C12—C13—N2	35.3 (2)
C2—C1—C6—N1	−175.4 (2)	C7—C12—C13—N2	−146.50 (18)
C7—N1—C6—C5	169.1 (2)	C13—N2—C14—C15	57.6 (2)
C7—N1—C6—C1	−14.9 (3)	C13—N2—C14—C19	−121.91 (19)
C6—N1—C7—C8	−37.1 (3)	C19—C14—C15—C16	1.8 (3)
C6—N1—C7—C12	145.9 (2)	N2—C14—C15—C16	−177.67 (18)
N1—C7—C8—C9	−176.8 (2)	C14—C15—C16—C17	−0.4 (3)
C12—C7—C8—C9	0.2 (3)	C15—C16—C17—C18	−0.9 (3)
C7—C8—C9—C10	0.7 (3)	C16—C17—C18—C19	0.7 (3)
C8—C9—C10—C11	−0.5 (3)	C17—C18—C19—N3	177.3 (2)
C9—C10—C11—C12	−0.7 (3)	C17—C18—C19—C14	0.7 (3)
C10—C11—C12—C7	1.6 (3)	C15—C14—C19—N3	−178.58 (18)
C10—C11—C12—C13	179.76 (18)	N2—C14—C19—N3	0.9 (3)
N1—C7—C12—C11	175.75 (17)	C15—C14—C19—C18	−2.0 (3)
C8—C7—C12—C11	−1.3 (3)	N2—C14—C19—C18	177.54 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1	0.88 (3)	1.96 (3)	2.714 (3)	142 (2)