Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(4-Methoxyphenyl)aminobenzoic acid

Héctor Novoa de Armas,[a]* Oswald M. Peeters,[a] Norbert M. Blaton,[a] Camiel J. De Ranter[a] and Lisbet Xuárez Marill[b]

[a]Laboratorium voor Analytische Chemie en Medicinale Fysicochemie, Faculteit Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Van Evenstraat 4, B-3000 Leuven, Belgium, and [b]Centro de Química Farmacéutica, Laboratorio de Síntesis Orgánica, 200 St. and 21 Ave. Playa., 16046 Havana, Cuba

Correspondence e-mail: hector.novoa@farm.kuleuven.ac.be

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.053
wR factor = 0.155
Data-to-parameter ratio = 7.5

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

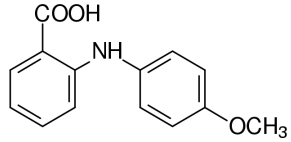
© 2001 International Union of Crystallography
Printed in Great Britain – all rights reserved

Received 8 June 2001
Accepted 21 June 2001
Online 29 June 2001

The title compound, $C_{14}H_{13}NO_3$, is a derivative of 2-aminobenzoic acid. The molecules form dimers *via* hydrogen bonding of carboxylic acid groups. The title structure has four molecules in the asymmetric unit, which is quite unusual.

Comment

2-(4-Methoxyphenyl)aminobenzoic acid, (I), is used as an intermediate in the synthesis of acridones. Fig. 1 shows the atom-numbering scheme used. An internal N—H···O hydrogen bond, with the imino N atom as donor and the carbonyl O atom as acceptor, is present. The imino group is not involved in intermolecular interactions, which is a common feature of related compounds such as fenamates (Dhanaraj & Vijayan, 1988). The carboxyl groups are, therefore, the only site for intermolecular interactions. Dimerization occurs through hydrogen bonding of carboxylic acid groups (Fig. 1).



(I)

The structure has four molecules in the asymmetric unit, which is quite unusual. There is a pseudo-centre of symmetry involving the carboxyphenyl amide groups of independent molecules, but the 4-methoxyphenyl group is rotated about N30—C31 in different directions and by different amounts for each molecule.

Experimental

The synthesis was carried out by the reaction of 2-chlorobenzoic acid with 4-methoxyaniline, in the presence of K_2CO_3, DMF and Cu powder. In the recrystallization from ethanol–water (1:1), colourless prisms of the title compound were obtained.

Crystal data

$C_{14}H_{13}NO_3$
M_r = 243.25
Monoclinic, Pc
a = 12.6506 (6) Å
b = 10.1894 (5) Å
c = 19.8565 (12) Å
β = 107.160 (5)°
V = 2445.6 (2) Å^3
Z = 8
D_x = 1.321 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 39 reflections
θ = 10.6–27.7°
μ = 0.77 mm^{-1}
T = 293 K
Plate, black
0.50 × 0.22 × 0.08 mm

Data collection

Siemens *P*4 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.699, T_{max} = 0.940
5863 measured reflections
4933 independent reflections
3152 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.053
θ_{max} = 69.1°
$h = -15 \rightarrow 1$
$k = -1 \rightarrow 12$
$l = -23 \rightarrow 24$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.155
S = 1.05
4933 reflections
658 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0808P)^2 + 0.0125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0010 (2)

Table 1
Selected geometric parameters (Å, °).

O8—C7	1.321 (11)	O68—C67	1.322 (11)
O9—C7	1.226 (10)	O69—C67	1.232 (10)
O17—C14	1.394 (10)	O77—C74	1.343 (11)
O17—C18	1.421 (11)	O77—C78	1.426 (12)
O28—C27	1.321 (11)	N10—C2	1.395 (11)
O29—C27	1.242 (10)	N10—C11	1.413 (11)
O37—C34	1.348 (12)	N30—C31	1.425 (11)
O37—C38	1.417 (10)	N30—C22	1.371 (11)
O48—C47	1.322 (10)	N50—C42	1.368 (11)
O49—C47	1.229 (10)	N50—C51	1.410 (12)
O57—C58	1.411 (10)	N70—C62	1.371 (11)
O57—C54	1.396 (10)	N70—C71	1.410 (11)
C14—O17—C18	117.8 (6)	N30—C31—C36	117.2 (6)
C34—O37—C38	118.0 (7)	N30—C31—C32	123.7 (7)
C54—O57—C58	118.0 (7)	O37—C34—C35	116.4 (8)
C74—O77—C78	116.6 (8)	O37—C34—C33	125.0 (8)
C2—N10—C11	127.4 (7)	N50—C42—C41	122.0 (7)
C22—N30—C31	127.5 (6)	N50—C42—C43	122.2 (8)
C42—N50—C51	125.9 (7)	O48—C47—C41	114.0 (7)
C62—N70—C71	128.5 (6)	O49—C47—C41	125.8 (8)
N10—C2—C3	123.0 (8)	O48—C47—O49	120.2 (7)
N10—C2—C1	119.5 (6)	N50—C51—C52	122.0 (7)
O9—C7—C1	125.7 (8)	N50—C51—C56	119.3 (6)
O8—C7—O9	120.4 (7)	O57—C54—C55	115.6 (7)
O8—C7—C1	113.9 (7)	O57—C54—C53	122.8 (7)
N10—C11—C16	126.7 (7)	N70—C62—C63	121.2 (8)
N10—C11—C12	114.7 (7)	N70—C62—C61	119.8 (6)
O17—C14—C13	123.3 (7)	O69—C67—C61	123.6 (8)
O17—C14—C15	116.7 (6)	O68—C67—C61	114.2 (7)
N30—C22—C23	120.6 (8)	O68—C67—O69	122.2 (7)
N30—C22—C21	119.7 (7)	N70—C71—C72	122.7 (7)
O28—C27—C21	115.5 (7)	N70—C71—C76	119.2 (7)
O29—C27—C21	122.9 (8)	O77—C74—C75	115.2 (8)
O28—C27—O29	121.5 (7)	O77—C74—C73	126.3 (8)

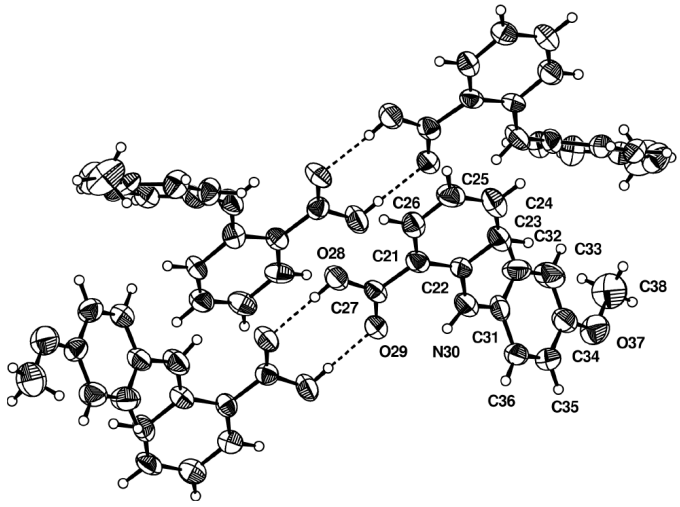


Figure 1
Plot of (I) showing the atomic numbering scheme. Displacement ellipsoids are drawn at 50% probability level for non-H atoms.

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8···O69^{i}	0.82	1.80	2.612 (8)	172
N10—H10···O9	0.86	1.97	2.662 (9)	137
O28—H28···O49^{ii}	0.82	1.82	2.644 (8)	178
N30—H30···O29	0.86	2.05	2.669 (9)	128
O48—H48···O29^{i}	0.82	1.79	2.608 (8)	174
N50—H50···O49	0.86	2.03	2.673 (9)	131
O68—H68···O9^{ii}	0.82	1.85	2.666 (8)	176
N70—H70···O69	0.86	2.01	2.673 (9)	133
C26—H26···O28	0.93	2.31	2.678 (9)	103
C46—H46···O48	0.93	2.39	2.714 (9)	100
C66—H66···O68	0.93	2.29	2.662 (9)	103

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

The H atoms were calculated geometrically and included in the refinement, but were constrained to ride on their parent atoms and with $U_{iso} = 1.2U_{eq}$ of their parent atoms.

Data collection, cell refinement and data reduction: *XSCANS* (Siemens, 1996); structure solution: *SIR*92 (Altomare *et al.*, 1994); structure refinement: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *PARST* (Nardelli, 1991) and *PLATON* (Spek, 1990).

HNDA wants to thank the KULeuven (Belgium), for support through IRO Scholarships.

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bergerhoff, G. (1996). *DIAMOND*. Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany.
Dhanaraj, V & Vijayan, M. (1988). *Acta Cryst.* B**44**, 406–412.
Nardelli, M. (1991). *PARSTCIF*. University of Parma, Italy.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Siemens (1996). *XSCANS*. Version 2.2. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Spek, A. L. (1990). *Acta Cryst.* A**46**, C-34.