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## 4-Aminobenzoic acid–quinoline (1/1)

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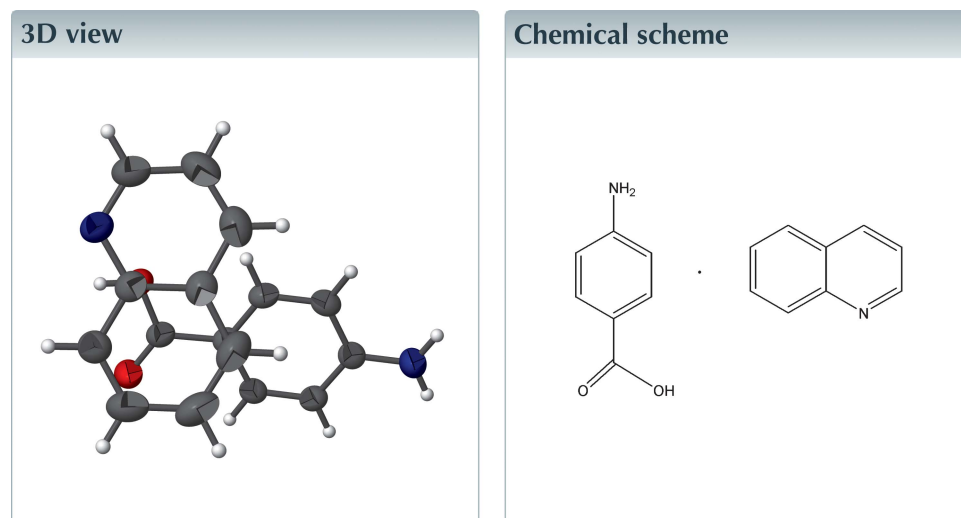
Edited by W. T. A. Harrison, University of Aberdeen, Scotland

Keywords: crystal structure; quinoline derivative; 4-aminobenzoic acid; hydrogen bonding;  $\pi$ – $\pi$  stacking.

CCDC reference: 1473449

Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

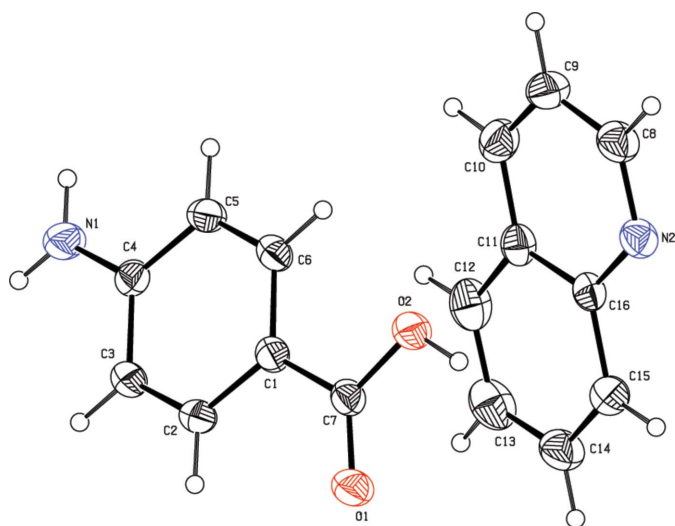
In the title 1:1 adduct,  $C_9H_7N \cdot C_7H_7NO_2$ , the carboxyl group is twisted at an angle of 5.42 (8) Å with respect to its attached benzene ring. In the crystal, the carboxylic acid molecule is linked to the quinoline molecule by an O–H...N hydrogen bond. The 4-aminobenzoic acid molecules are linked by N–H...O hydrogen bonds, forming sheets propagating in (001). Weak aromatic  $\pi$ – $\pi$  stacking [centroid-to-centroid distances = 3.758 (1) and 3.888 (1) Å] interactions also occur.



### Structure description

Quinoline derivatives are known to exhibit pharmacological activities such as anti-viral (Font *et al.*, 1997) and anti-inflammatory (Sloboda *et al.*, 1991). As part of our studies in this area, we now describe the synthesis and structure of the title adduct (Fig. 1), which contains one quinoline and one 4-aminobenzoic acid molecule in the asymmetric unit. The quinoline ring system (N1/C8–C16) is almost planar with a maximum deviation of 0.0133 (13) Å for atom N1. In the 4-aminobenzoic acid molecule, the carboxyl group is twisted at an angle of 5.42 (8) Å to the attached benzene ring. The geometric parameters are comparable with similar structures (Divya Bharathi *et al.*, 2015; Li & Chai, 2007; Song *et al.*, 2011).

In the crystal, the 4-aminobenzoic acid molecules are linked by N–H...O hydrogen bonds (Table 1), forming zigzag sheets propagating in the (001) plane (Fig. 2). The quinoline molecule accepts an O–H...N hydrogen bond (Table 1) from the 4-aminobenzoic acid molecule, and lies pendant to the (001) sheets (Fig. 2). The crystal structure is also influenced by weak  $\pi$ – $\pi$  interactions [ $Cg3 \cdots Cg2^i = 3.888$  (1) Å;  $Cg3 \cdots Cg3^i = 3.758$  (1) Å; symmetry code: (i)  $1 - x, -y, 1 - z$ ; Cg2 and Cg3 are the centroids of the (N2/C8–C11/C16) and (C11–C16) rings, respectively].



**Figure 1**  
The molecular structure, with 30% probability displacement ellipsoids for non-H atoms.

### Synthesis and crystallization

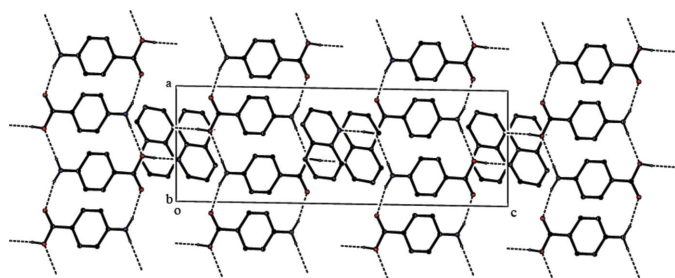
Quinoline (1.29 g) and 4-aminobenzoic acid (1.37 g) in an equimolar ratio (1:1) were mixed in acetone and the mixture was stirred for 4 h. The solution was filtered and kept at room temperature. Colourless blocks were obtained by slow evaporation.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

### Acknowledgements

The authors acknowledge the SAIF, IIT, Madras, for the data collection.



**Figure 2**  
The crystal packing of the title compound viewed along the *b* axis. The hydrogen bonds are shown as dashed lines (see Table 1), and C-bound H atoms have been omitted for clarity.

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

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H1A···O1 <sup>i</sup>	0.86	2.15	2.9855 (17)	164
N1—H1B···O2 <sup>iii</sup>	0.86	2.28	3.1355 (17)	175
O2—H2A···N2 <sup>iii</sup>	0.85 (1)	1.79 (1)	2.6364 (16)	174 (2)

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>9</sub> H <sub>7</sub> N·C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>
<i>M<sub>r</sub></i>	266.29
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>c</i>
Temperature (K)	295
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.6842 (7), 8.1013 (6), 22.0669 (16)
$\beta$ (°)	90.893 (3)
<i>V</i> (Å <sup>3</sup> )	1373.54 (19)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.09
Crystal size (mm)	0.24 × 0.20 × 0.18
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.980, 0.985
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	16394, 3616, 2427
<i>R<sub>int</sub></i>	0.025
(sin $\theta/\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.680
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.044, 0.117, 1.03
No. of reflections	3616
No. of parameters	184
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	0.21, -0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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## full crystallographic data

*IUCrData* (2016). **1**, x160604 [doi:10.1107/S2414314616006040]

## 4-Aminobenzoic acid–quinoline (1/1)

P. Sivakumar, S. Sudhahar, S. Israel and G. Chakkaravarthi

## 4-Aminobenzoic acid–quinoline (1/1)

*Crystal data*

$C_9H_7N \cdot C_7H_7NO_2$

$M_r = 266.29$

Monoclinic,  $P2_1/c$

Hall symbol:  $-P 2_1/c$

$a = 7.6842$  (7) Å

$b = 8.1013$  (6) Å

$c = 22.0669$  (16) Å

$\beta = 90.893$  (3)°

$V = 1373.54$  (19) Å<sup>3</sup>

$Z = 4$

$F(000) = 560$

$D_x = 1.288$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 4104 reflections

$\theta = 2.6$ – $25.6$ °

$\mu = 0.09$  mm<sup>-1</sup>

$T = 295$  K

Block, colourless

$0.24 \times 0.20 \times 0.18$  mm

*Data collection*

Bruker Kappa APEXII CCD  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  and  $\phi$  scan

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.980$ ,  $T_{\max} = 0.985$

16394 measured reflections

3616 independent reflections

2427 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$

$\theta_{\max} = 28.9$ °,  $\theta_{\min} = 2.7$ °

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 11$

$l = -30 \rightarrow 29$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.117$

$S = 1.03$

3616 reflections

184 parameters

1 restraint

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H atoms treated by a mixture of independent  
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.3668P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.21$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.19$  e Å<sup>-3</sup>

*Special details*

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.24265 (18)	0.44594 (17)	0.31360 (6)	0.0376 (3)
C2	0.09036 (18)	0.41448 (19)	0.28042 (6)	0.0426 (3)
H2	-0.0152	0.4538	0.2946	0.051*
C3	0.09303 (18)	0.32657 (19)	0.22717 (6)	0.0442 (3)
H3	-0.0102	0.3083	0.2057	0.053*
C4	0.24935 (19)	0.26426 (18)	0.20497 (6)	0.0402 (3)
C5	0.40228 (18)	0.29667 (18)	0.23807 (6)	0.0429 (3)
H5	0.5080	0.2571	0.2241	0.052*
C6	0.39846 (18)	0.38607 (17)	0.29087 (6)	0.0408 (3)
H6	0.5020	0.4071	0.3119	0.049*
C7	0.23461 (18)	0.53452 (18)	0.37202 (6)	0.0404 (3)
C8	0.7831 (2)	0.3218 (2)	0.46278 (8)	0.0548 (4)
H8	0.8725	0.3851	0.4796	0.066*
C9	0.8106 (2)	0.2457 (2)	0.40693 (8)	0.0594 (4)
H9	0.9157	0.2591	0.3872	0.071*
C10	0.6829 (2)	0.1524 (2)	0.38192 (7)	0.0563 (4)
H10	0.7000	0.0999	0.3450	0.068*
C11	0.5234 (2)	0.13473 (18)	0.41201 (6)	0.0445 (3)
C12	0.3816 (3)	0.0413 (2)	0.38928 (8)	0.0615 (5)
H12	0.3913	-0.0137	0.3525	0.074*
C13	0.2319 (3)	0.0311 (2)	0.42048 (9)	0.0675 (5)
H13	0.1398	-0.0316	0.4052	0.081*
C14	0.2149 (2)	0.1137 (2)	0.47528 (8)	0.0610 (5)
H14	0.1108	0.1065	0.4961	0.073*
C15	0.3476 (2)	0.2045 (2)	0.49891 (7)	0.0508 (4)
H15	0.3343	0.2586	0.5357	0.061*
C16	0.50510 (19)	0.21711 (17)	0.46791 (6)	0.0397 (3)
N1	0.25232 (17)	0.17624 (18)	0.15233 (6)	0.0558 (4)
H1A	0.1573	0.1584	0.1323	0.067*
H1B	0.3493	0.1386	0.1391	0.067*
N2	0.63746 (16)	0.30866 (15)	0.49269 (5)	0.0464 (3)
O1	0.09822 (14)	0.57684 (16)	0.39513 (5)	0.0575 (3)
O2	0.38721 (13)	0.56351 (14)	0.39791 (5)	0.0494 (3)
H2A	0.373 (2)	0.601 (2)	0.4336 (5)	0.074*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0362 (7)	0.0386 (7)	0.0381 (7)	-0.0014 (6)	-0.0026 (6)	0.0029 (6)
C2	0.0330 (7)	0.0511 (9)	0.0437 (7)	0.0013 (6)	0.0006 (6)	-0.0017 (6)

C3	0.0341 (7)	0.0558 (9)	0.0424 (7)	-0.0015 (6)	-0.0047 (6)	-0.0025 (7)
C4	0.0412 (8)	0.0427 (8)	0.0367 (7)	-0.0022 (6)	0.0017 (6)	0.0037 (6)
C5	0.0345 (7)	0.0460 (8)	0.0484 (8)	0.0029 (6)	0.0038 (6)	0.0019 (6)
C6	0.0339 (7)	0.0420 (8)	0.0462 (8)	-0.0017 (6)	-0.0056 (6)	0.0036 (6)
C7	0.0367 (8)	0.0440 (8)	0.0405 (7)	-0.0037 (6)	-0.0042 (6)	0.0032 (6)
C8	0.0449 (9)	0.0584 (10)	0.0608 (10)	-0.0089 (8)	-0.0043 (7)	0.0052 (8)
C9	0.0484 (10)	0.0710 (11)	0.0592 (10)	0.0040 (9)	0.0111 (8)	0.0126 (9)
C10	0.0646 (11)	0.0587 (10)	0.0458 (8)	0.0125 (9)	0.0051 (8)	0.0006 (7)
C11	0.0510 (9)	0.0401 (8)	0.0421 (7)	0.0041 (7)	-0.0054 (6)	0.0027 (6)
C12	0.0739 (13)	0.0531 (10)	0.0569 (10)	-0.0033 (9)	-0.0150 (9)	-0.0105 (8)
C13	0.0606 (12)	0.0613 (11)	0.0799 (12)	-0.0163 (9)	-0.0195 (10)	-0.0010 (10)
C14	0.0435 (9)	0.0697 (11)	0.0698 (11)	-0.0090 (8)	-0.0025 (8)	0.0098 (9)
C15	0.0462 (9)	0.0590 (10)	0.0472 (8)	-0.0025 (8)	0.0000 (7)	-0.0002 (7)
C16	0.0406 (8)	0.0388 (7)	0.0394 (7)	0.0010 (6)	-0.0060 (6)	0.0045 (6)
N1	0.0437 (7)	0.0776 (10)	0.0461 (7)	0.0009 (7)	0.0035 (6)	-0.0152 (7)
N2	0.0425 (7)	0.0499 (7)	0.0465 (7)	-0.0051 (6)	-0.0051 (5)	-0.0010 (6)
O1	0.0384 (6)	0.0846 (9)	0.0494 (6)	0.0027 (6)	-0.0029 (5)	-0.0158 (6)
O2	0.0383 (6)	0.0654 (7)	0.0444 (6)	-0.0057 (5)	-0.0045 (5)	-0.0092 (5)

*Geometric parameters (Å, °)*

C1—C6	1.3924 (19)	C9—H9	0.9300
C1—C2	1.3941 (19)	C10—C11	1.410 (2)
C1—C7	1.4777 (19)	C10—H10	0.9300
C2—C3	1.3745 (19)	C11—C16	1.412 (2)
C2—H2	0.9300	C11—C12	1.413 (2)
C3—C4	1.3986 (19)	C12—C13	1.352 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—N1	1.3635 (18)	C13—C14	1.390 (3)
C4—C5	1.3987 (19)	C13—H13	0.9300
C5—C6	1.373 (2)	C14—C15	1.355 (2)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—C16	1.403 (2)
C7—O1	1.2217 (17)	C15—H15	0.9300
C7—O2	1.3174 (17)	C16—N2	1.3660 (18)
C8—N2	1.3122 (19)	N1—H1A	0.8600
C8—C9	1.397 (2)	N1—H1B	0.8600
C8—H8	0.9300	O2—H2A	0.852 (9)
C9—C10	1.350 (2)		
C6—C1—C2	117.81 (13)	C9—C10—C11	119.72 (15)
C6—C1—C7	122.09 (13)	C9—C10—H10	120.1
C2—C1—C7	120.05 (13)	C11—C10—H10	120.1
C3—C2—C1	121.34 (13)	C10—C11—C16	117.59 (14)
C3—C2—H2	119.3	C10—C11—C12	123.95 (15)
C1—C2—H2	119.3	C16—C11—C12	118.47 (15)
C2—C3—C4	120.72 (13)	C13—C12—C11	120.66 (16)
C2—C3—H3	119.6	C13—C12—H12	119.7

C4—C3—H3	119.6	C11—C12—H12	119.7
N1—C4—C3	120.86 (13)	C12—C13—C14	120.35 (16)
N1—C4—C5	121.19 (13)	C12—C13—H13	119.8
C3—C4—C5	117.94 (13)	C14—C13—H13	119.8
C6—C5—C4	120.89 (13)	C15—C14—C13	121.07 (17)
C6—C5—H5	119.6	C15—C14—H14	119.5
C4—C5—H5	119.6	C13—C14—H14	119.5
C5—C6—C1	121.29 (13)	C14—C15—C16	120.09 (15)
C5—C6—H6	119.4	C14—C15—H15	120.0
C1—C6—H6	119.4	C16—C15—H15	120.0
O1—C7—O2	122.18 (13)	N2—C16—C15	119.13 (13)
O1—C7—C1	123.24 (13)	N2—C16—C11	121.51 (14)
O2—C7—C1	114.58 (12)	C15—C16—C11	119.36 (14)
N2—C8—C9	123.36 (16)	C4—N1—H1A	120.0
N2—C8—H8	118.3	C4—N1—H1B	120.0
C9—C8—H8	118.3	H1A—N1—H1B	120.0
C10—C9—C8	119.26 (16)	C8—N2—C16	118.56 (13)
C10—C9—H9	120.4	C7—O2—H2A	109.7 (13)
C8—C9—H9	120.4		
C6—C1—C2—C3	0.3 (2)	C9—C10—C11—C16	0.0 (2)
C7—C1—C2—C3	-177.33 (13)	C9—C10—C11—C12	179.34 (16)
C1—C2—C3—C4	0.7 (2)	C10—C11—C12—C13	-179.45 (16)
C2—C3—C4—N1	179.65 (14)	C16—C11—C12—C13	-0.1 (2)
C2—C3—C4—C5	-1.1 (2)	C11—C12—C13—C14	0.5 (3)
N1—C4—C5—C6	179.67 (14)	C12—C13—C14—C15	-0.6 (3)
C3—C4—C5—C6	0.4 (2)	C13—C14—C15—C16	0.3 (3)
C4—C5—C6—C1	0.7 (2)	C14—C15—C16—N2	-179.68 (15)
C2—C1—C6—C5	-1.0 (2)	C14—C15—C16—C11	0.2 (2)
C7—C1—C6—C5	176.59 (13)	C10—C11—C16—N2	-1.0 (2)
C6—C1—C7—O1	-174.12 (14)	C12—C11—C16—N2	179.57 (14)
C2—C1—C7—O1	3.5 (2)	C10—C11—C16—C15	179.15 (14)
C6—C1—C7—O2	5.29 (19)	C12—C11—C16—C15	-0.3 (2)
C2—C1—C7—O2	-177.13 (13)	C9—C8—N2—C16	-0.6 (2)
N2—C8—C9—C10	-0.5 (3)	C15—C16—N2—C8	-178.85 (14)
C8—C9—C10—C11	0.8 (3)	C11—C16—N2—C8	1.3 (2)

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1A...O1 <sup>i</sup>	0.86	2.15	2.9855 (17)	164
N1—H1B...O2 <sup>ii</sup>	0.86	2.28	3.1355 (17)	175
O2—H2A...N2 <sup>iii</sup>	0.85 (1)	1.79 (1)	2.6364 (16)	174 (2)

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