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4-Amino-3-methylbenzoic acid–1,2-bis(4-pyridyl)ethane (1/1)

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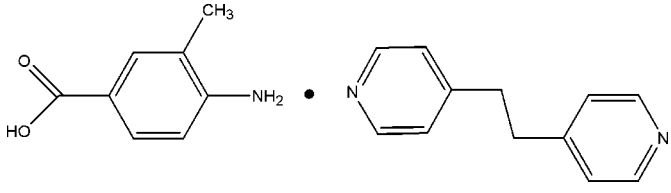
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.082; data-to-parameter ratio = 18.4.

In the crystal structure of the title 1:1 adduct, $C_{12}H_{12}N_2\cdot C_8H_9NO_2$, the 4-amino-3-methylbenzoic acid molecules and 1,2-bis(4-pyridyl)ethane molecules are linked by intermolecular O—H···N, N—H···O and N—H···N hydrogen bonds, forming a two-dimensional supramolecular network parallel to (001). In the 1,2-bis(4-pyridyl)ethane molecule, the two pyridine rings are twisted to each other by a dihedral angle of 12.12 (8)°. The non-H atoms of the 4-amino-3-methylbenzoic acid molecule are almost coplanar, the maximum atomic deviation being 0.029 (1) Å. Weak C—H···π interactions are present in the crystal structure.

Related literature

For related structures, see: Bowes *et al.* (2003); Ferguson *et al.* (1999); Shen & Lush (2010). For hydrogen-bond motifs, see: Etter *et al.* (1990).



Experimental

Crystal data

$C_{12}H_{12}N_2\cdot C_8H_9NO_2$
M_r = 335.40
Monoclinic, $P2_1/c$
a = 8.0695 (3) Å
b = 13.0677 (5) Å
c = 17.6138 (10) Å
β = 99.501 (5)°
V = 1831.89 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 297 K
0.60 × 0.18 × 0.12 mm

Data collection

Oxford Diffraction Gemini-S CCD diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.919, T_{max} = 1.000
8821 measured reflections
4277 independent reflections
1870 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.082
S = 1.03
4277 reflections
232 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

Cg is the centroid of the C2–C7 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N2	0.821 (9)	1.826 (11)	2.6407 (18)	171.6 (15)
N1—H1B···O2^{i}	0.860 (11)	2.113 (12)	2.951 (2)	164.5 (14)
N1—H1C···N3^{ii}	0.860 (7)	2.288 (9)	3.084 (2)	153.8 (14)
C12—H12A···Cg^{iii}	0.93	2.76	3.540 (2)	141

Symmetry codes: (i) $x-1, y, z$; (ii) $x-2, y+1, z$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

This work was supported financially by Yuanpei University, Taiwan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5156).

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supplementary materials

Acta Cryst. (2011). E**67**, o652 [**doi:10.1107/S1600536811005381**]

4-Amino-3-methylbenzoic acid-1,2-bis(4-pyridyl)ethane (1/1)

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Comment

The 1,2-bis(4-pyridyl)ethane is a versatile building block for the purposes of crystal engineering. Each of the pyridyl N atoms acts as a hydrogen bond acceptor, forming linear hydrogen associations (Ferguson *et al.*, 1999). Other structures related with 1,2-bis(4-pyridyl)ethane and Lewis acid were reported by Bowes *et al.* (2003) and Shen & Lush (2010). We present here the crystal structure of the 4-amino-3-methybenzoic acid and 1,2-bis(4-pyridyl)ethane 1:1 adduct.

The structure of the title compound comprises 4-amino-3-methybenzoic acid molecule and 1,2-bis(4-pyridyl)ethane molecule, with no proton transfer. In the structure, the molecules associate 4-amino-3-methybenzoic acid and 1,2-bis(4-pyridyl)ethane *via* carboxylic and pyridine group O—H···N [O···N 2.640 (18) Å] $C^2_2(19)$ (Etter *et al.*, 1990), forming linear hydrogen bonding parallel to [0 0 1], further connect a two dimensional network *via* amine and carboxylic N—H···O and N—H···N [2.951 (2) and 3.084 (2) Å], respectively. Furthermore, C—H···π ring stacking interaction is present in the structure. The distance between C12—H(12 A)···*Cg*3 ^{iii}(C2—C7) is 3.540 (2) Å [symmetry code: (iii) = 1-*X*,-1/2+*Y*,3/2-*Z*].

Experimental

The 4-amino-3-methybenzoic acid (151 mg, 1 mmol) and 1,2-bis(4-pyridyl)ethane (184 mg, 1 mmol) were dissolved in 20 ml methanol, the solution was refluxed for 30 min. The filtered solution was transferred to a 25 ml tube, at room temperature colorless crystals were formed after several days (yield 59.12%).

Refinement

Amino H atoms were located in a difference Fourier map and were refined with the distance constraints of N—H = 0.860±0.001 Å. Other H atoms were positioned geometrically with C—H = 0.93-0.97 Å, and refined using a riding model, U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for the others.

Figures

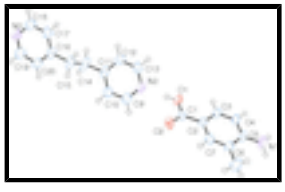

Fig. 1. View of the title compound. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

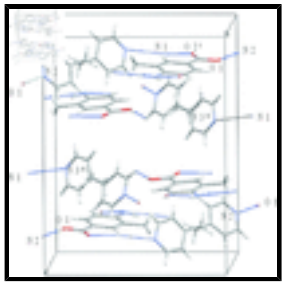

Fig. 2. The molecular packing for the title compound. Hydrogen bonds are shown as dashed lines.

4-Amino-3-methylbenzoic acid–1,2-bis(4-pyridyl)ethane (1/1)

Crystal data

$C_{12}H_{12}N_2 \cdot C_8H_9NO_2$	$F(000) = 712$
$M_r = 335.40$	$D_x = 1.216$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2506 reflections
$a = 8.0695$ (3) Å	$\theta = 3.0$–$29.0°$
$b = 13.0677$ (5) Å	$\mu = 0.08$ mm^{-1}
$c = 17.6138$ (10) Å	$T = 297$ K
$\beta = 99.501$ (5)°	Parallelepiped, colorless
$V = 1831.89$ (15) Å^3	0.60 × 0.18 × 0.12 mm
$Z = 4$	

Data collection

Oxford Diffraction Gemini-S CCD diffractometer	4277 independent reflections
Radiation source: fine-focus sealed tube	1870 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.025$
ω scans	$\theta_{max} = 29.1°$, $\theta_{min} = 3.0°$
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)	$h = -10 \rightarrow 10$
$T_{min} = 0.919$, $T_{max} = 1.000$	$k = -17 \rightarrow 16$
8821 measured reflections	$l = -24 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.044$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.082$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.025P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
4277 reflections	$(\Delta/\sigma)_{max} < 0.001$

232 parameters	$\Delta\rho_{max} = 0.15$ e Å^{-3}
3 restraints	$\Delta\rho_{min} = -0.22$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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}
N2	0.63037 (17)	0.47008 (10)	0.62737 (9)	0.0552 (6)
N3	1.58754 (19)	0.08351 (11)	0.60868 (10)	0.0692 (7)
C9	0.7078 (2)	0.47692 (12)	0.56699 (11)	0.0553 (7)
C10	0.8385 (2)	0.41502 (12)	0.55562 (10)	0.0521 (7)
C11	0.8957 (2)	0.34059 (12)	0.60903 (11)	0.0482 (7)
C12	0.8172 (2)	0.33448 (13)	0.67191 (11)	0.0650 (8)
C13	0.6872 (2)	0.39953 (15)	0.67901 (11)	0.0683 (8)
C14	1.0359 (2)	0.26912 (12)	0.59857 (12)	0.0705 (8)
C15	1.2064 (2)	0.30811 (12)	0.62896 (11)	0.0660 (7)
C16	1.3425 (2)	0.23093 (12)	0.62204 (11)	0.0506 (7)
C17	1.4071 (2)	0.16866 (14)	0.68217 (11)	0.0639 (8)
C18	1.5274 (2)	0.09729 (14)	0.67281 (12)	0.0710 (8)
C19	1.5251 (2)	0.14425 (15)	0.55151 (12)	0.0808 (9)
C20	1.4039 (2)	0.21762 (13)	0.55528 (11)	0.0686 (8)
O1	0.34436 (14)	0.56570 (8)	0.63298 (7)	0.0542 (5)
O2	0.47629 (14)	0.71109 (8)	0.61635 (7)	0.0664 (5)
N1	−0.25914 (19)	0.86901 (13)	0.64324 (10)	0.0628 (7)
C1	0.34970 (19)	0.66628 (12)	0.62564 (9)	0.0399 (4)
C2	0.18870 (19)	0.71739 (11)	0.63001 (9)	0.0399 (4)
C3	0.04752 (18)	0.66405 (11)	0.64278 (9)	0.0427 (6)
C4	−0.09994 (19)	0.71458 (11)	0.64585 (9)	0.0451 (6)
C5	−0.11212 (19)	0.82069 (12)	0.63671 (9)	0.0421 (6)
C6	0.0301 (2)	0.87564 (11)	0.62414 (9)	0.0465 (6)
C7	0.17592 (19)	0.82300 (11)	0.62061 (9)	0.0461 (6)
C8	0.0217 (2)	0.99081 (11)	0.61582 (12)	0.0818 (9)
H9A	0.67140	0.52660	0.53020	0.0660*
H10A	0.88840	0.42320	0.51200	0.0620*
H12A	0.85190	0.28610	0.71000	0.0780*
H13A	0.63640	0.39370	0.72250	0.0820*
H14A	1.01960	0.20490	0.62390	0.0850*

H14B	1.02920	0.25500	0.54410	0.0850*
H15A	1.21180	0.32640	0.68270	0.0790*
H15B	1.22680	0.36960	0.60110	0.0790*
H17A	1.36980	0.17460	0.72920	0.0770*
H18A	1.56900	0.05610	0.71470	0.0850*
H19A	1.56560	0.13720	0.50530	0.0970*
H20A	1.36450	0.25770	0.51250	0.0820*
H1A	0.4380 (9)	0.5416 (12)	0.6323 (10)	0.082 (7)*
H1B	−0.3449 (12)	0.8295 (10)	0.6418 (10)	0.075 (7)*
H1C	−0.2717 (19)	0.9312 (4)	0.6273 (8)	0.055 (6)*
H3A	0.05290	0.59340	0.64930	0.0510*
H4A	−0.19370	0.67760	0.65420	0.0540*
H7A	0.26980	0.85930	0.61160	0.0550*
H8A	0.12810	1.01620	0.60650	0.1230*
H8B	−0.00420	1.02060	0.66230	0.1230*
H8C	−0.06420	1.00870	0.57340	0.1230*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N2	0.0437 (9)	0.0556 (9)	0.0657 (11)	0.0178 (7)	0.0069 (9)	0.0008 (8)
N3	0.0678 (11)	0.0797 (11)	0.0613 (12)	0.0363 (9)	0.0146 (9)	0.0079 (10)
C9	0.0509 (12)	0.0498 (10)	0.0631 (14)	0.0097 (9)	0.0032 (10)	0.0069 (10)
C10	0.0460 (11)	0.0559 (11)	0.0560 (13)	0.0066 (9)	0.0135 (9)	−0.0026 (10)
C11	0.0385 (10)	0.0426 (11)	0.0617 (13)	0.0093 (8)	0.0030 (10)	−0.0118 (10)
C12	0.0609 (13)	0.0670 (12)	0.0668 (14)	0.0282 (10)	0.0097 (11)	0.0173 (11)
C13	0.0588 (13)	0.0887 (14)	0.0608 (14)	0.0230 (11)	0.0196 (10)	0.0105 (12)
C14	0.0474 (12)	0.0566 (11)	0.1053 (17)	0.0179 (10)	0.0062 (11)	−0.0171 (11)
C15	0.0442 (11)	0.0605 (11)	0.0922 (16)	0.0139 (10)	0.0082 (11)	−0.0143 (11)
C16	0.0388 (11)	0.0516 (11)	0.0611 (14)	0.0114 (9)	0.0077 (10)	−0.0091 (10)
C17	0.0597 (13)	0.0812 (13)	0.0535 (14)	0.0216 (11)	0.0173 (10)	−0.0002 (11)
C18	0.0713 (14)	0.0834 (15)	0.0572 (15)	0.0318 (11)	0.0071 (12)	0.0163 (11)
C19	0.0877 (16)	0.1022 (16)	0.0580 (15)	0.0442 (14)	0.0285 (12)	0.0109 (13)
C20	0.0699 (14)	0.0747 (13)	0.0617 (15)	0.0361 (11)	0.0127 (11)	0.0150 (11)
O1	0.0387 (8)	0.0491 (7)	0.0761 (9)	0.0153 (6)	0.0130 (7)	−0.0007 (6)
O2	0.0306 (7)	0.0689 (8)	0.1025 (10)	−0.0004 (6)	0.0192 (7)	0.0135 (7)
N1	0.0418 (10)	0.0476 (10)	0.1012 (14)	0.0112 (9)	0.0184 (10)	−0.0012 (10)
C1	0.0324 (7)	0.0430 (7)	0.0442 (7)	0.0040 (5)	0.0058 (5)	−0.0032 (6)
C2	0.0324 (7)	0.0430 (7)	0.0442 (7)	0.0040 (5)	0.0058 (5)	−0.0032 (6)
C3	0.0354 (10)	0.0332 (8)	0.0604 (12)	0.0031 (8)	0.0109 (8)	−0.0035 (8)
C4	0.0313 (10)	0.0403 (10)	0.0651 (13)	−0.0011 (8)	0.0123 (8)	−0.0038 (8)
C5	0.0316 (9)	0.0430 (10)	0.0519 (12)	0.0085 (8)	0.0072 (8)	−0.0072 (9)
C6	0.0411 (11)	0.0378 (9)	0.0606 (13)	0.0039 (9)	0.0088 (9)	−0.0002 (9)
C7	0.0354 (10)	0.0444 (10)	0.0594 (12)	−0.0042 (8)	0.0109 (9)	0.0003 (9)
C8	0.0647 (14)	0.0445 (11)	0.138 (2)	0.0047 (9)	0.0217 (13)	0.0091 (11)

Geometric parameters (Å, °)

O1—C1	1.3221 (19)	C13—H13A	0.9300

O2—C1	1.2118 (19)	C14—H14A	0.9700
O1—H1A	0.821 (9)	C14—H14B	0.9700
N2—C13	1.323 (2)	C15—H15B	0.9700
N2—C9	1.322 (2)	C15—H15A	0.9700
N3—C18	1.313 (3)	C17—H17A	0.9300
N3—C19	1.315 (3)	C18—H18A	0.9300
N1—C5	1.366 (2)	C19—H19A	0.9300
N1—H1C	0.860 (7)	C20—H20A	0.9300
N1—H1B	0.860 (11)	C1—C2	1.474 (2)
C9—C10	1.370 (2)	C2—C3	1.385 (2)
C10—C11	1.379 (2)	C2—C7	1.392 (2)
C11—C12	1.366 (3)	C3—C4	1.370 (2)
C11—C14	1.502 (2)	C4—C5	1.398 (2)
C12—C13	1.372 (2)	C5—C6	1.402 (2)
C14—C15	1.482 (2)	C6—C7	1.373 (2)
C15—C16	1.511 (2)	C6—C8	1.513 (2)
C16—C17	1.369 (3)	C3—H3A	0.9300
C16—C20	1.360 (3)	C4—H4A	0.9300
C17—C18	1.376 (2)	C7—H7A	0.9300
C19—C20	1.379 (2)	C8—H8A	0.9600
C9—H9A	0.9300	C8—H8B	0.9600
C10—H10A	0.9300	C8—H8C	0.9600
C12—H12A	0.9300		
C1—O1—H1A	109.6 (10)	H15A—C15—H15B	108.00
C9—N2—C13	116.35 (14)	C14—C15—H15A	109.00
C18—N3—C19	115.24 (16)	C16—C17—H17A	120.00
H1B—N1—H1C	120.4 (14)	C18—C17—H17A	120.00
C5—N1—H1B	115.2 (8)	N3—C18—H18A	118.00
C5—N1—H1C	117.8 (10)	C17—C18—H18A	118.00
N2—C9—C10	123.71 (16)	C20—C19—H19A	118.00
C9—C10—C11	119.73 (16)	N3—C19—H19A	118.00
C10—C11—C12	116.53 (15)	C16—C20—H20A	120.00
C10—C11—C14	121.95 (16)	C19—C20—H20A	120.00
C12—C11—C14	121.52 (16)	O2—C1—C2	123.92 (14)
C11—C12—C13	120.11 (17)	O1—C1—O2	122.37 (14)
N2—C13—C12	123.55 (17)	O1—C1—C2	113.71 (13)
C11—C14—C15	114.53 (14)	C1—C2—C7	119.45 (14)
C14—C15—C16	112.66 (14)	C3—C2—C7	118.13 (14)
C15—C16—C17	121.57 (16)	C1—C2—C3	122.42 (13)
C15—C16—C20	121.90 (16)	C2—C3—C4	120.46 (14)
C17—C16—C20	116.51 (16)	C3—C4—C5	121.25 (14)
C16—C17—C18	119.77 (17)	N1—C5—C4	119.65 (15)
N3—C18—C17	124.36 (18)	N1—C5—C6	121.45 (15)
N3—C19—C20	124.59 (18)	C4—C5—C6	118.85 (14)
C16—C20—C19	119.53 (17)	C5—C6—C8	120.01 (14)
C10—C9—H9A	118.00	C7—C6—C8	121.27 (14)
N2—C9—H9A	118.00	C5—C6—C7	118.72 (14)
C9—C10—H10A	120.00	C2—C7—C6	122.58 (14)
C11—C10—H10A	120.00	C2—C3—H3A	120.00

C11—C12—H12A	120.00	C4—C3—H3A	120.00
C13—C12—H12A	120.00	C3—C4—H4A	119.00
C12—C13—H13A	118.00	C5—C4—H4A	119.00
N2—C13—H13A	118.00	C2—C7—H7A	119.00
C11—C14—H14A	109.00	C6—C7—H7A	119.00
C11—C14—H14B	109.00	C6—C8—H8A	109.00
H14A—C14—H14B	108.00	C6—C8—H8B	109.00
C15—C14—H14A	109.00	C6—C8—H8C	109.00
C15—C14—H14B	109.00	H8A—C8—H8B	109.00
C16—C15—H15A	109.00	H8A—C8—H8C	110.00
C14—C15—H15B	109.00	H8B—C8—H8C	110.00
C16—C15—H15B	109.00		
C13—N2—C9—C10	0.9 (3)	C16—C17—C18—N3	0.0 (3)
C9—N2—C13—C12	−1.0 (3)	N3—C19—C20—C16	0.6 (3)
C19—N3—C18—C17	0.4 (3)	O1—C1—C2—C3	1.7 (2)
C18—N3—C19—C20	−0.7 (3)	O1—C1—C2—C7	−177.92 (14)
N2—C9—C10—C11	0.0 (3)	O2—C1—C2—C3	−178.20 (16)
C9—C10—C11—C12	−0.9 (2)	O2—C1—C2—C7	2.2 (2)
C9—C10—C11—C14	178.60 (16)	C1—C2—C3—C4	−179.52 (15)
C10—C11—C12—C13	0.8 (3)	C7—C2—C3—C4	0.1 (2)
C14—C11—C12—C13	−178.66 (16)	C1—C2—C7—C6	−179.85 (15)
C10—C11—C14—C15	87.8 (2)	C3—C2—C7—C6	0.5 (2)
C12—C11—C14—C15	−92.8 (2)	C2—C3—C4—C5	−0.4 (2)
C11—C12—C13—N2	0.1 (3)	C3—C4—C5—N1	−177.34 (16)
C11—C14—C15—C16	176.12 (16)	C3—C4—C5—C6	0.0 (2)
C14—C15—C16—C17	−96.3 (2)	N1—C5—C6—C7	177.88 (16)
C14—C15—C16—C20	81.9 (2)	N1—C5—C6—C8	−1.3 (2)
C15—C16—C17—C18	178.08 (16)	C4—C5—C6—C7	0.6 (2)
C20—C16—C17—C18	−0.1 (2)	C4—C5—C6—C8	−178.64 (15)
C15—C16—C20—C19	−178.34 (16)	C5—C6—C7—C2	−0.9 (2)
C17—C16—C20—C19	−0.1 (2)	C8—C6—C7—C2	178.32 (16)

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···N2	0.821 (9)	1.826 (11)	2.6407 (18)	171.6 (15)
N1—H1B···O2^{i}	0.860 (11)	2.113 (12)	2.951 (2)	164.5 (14)
N1—H1C···N3^{ii}	0.860 (7)	2.288 (9)	3.084 (2)	153.8 (14)
C12—H12A···Cg^{iii}	0.93	2.76	3.540 (2)	141

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*−2, *y*+1, *z*; (iii) −*x*+1, *y*−1/2, −*z*+3/2.

Fig. 1

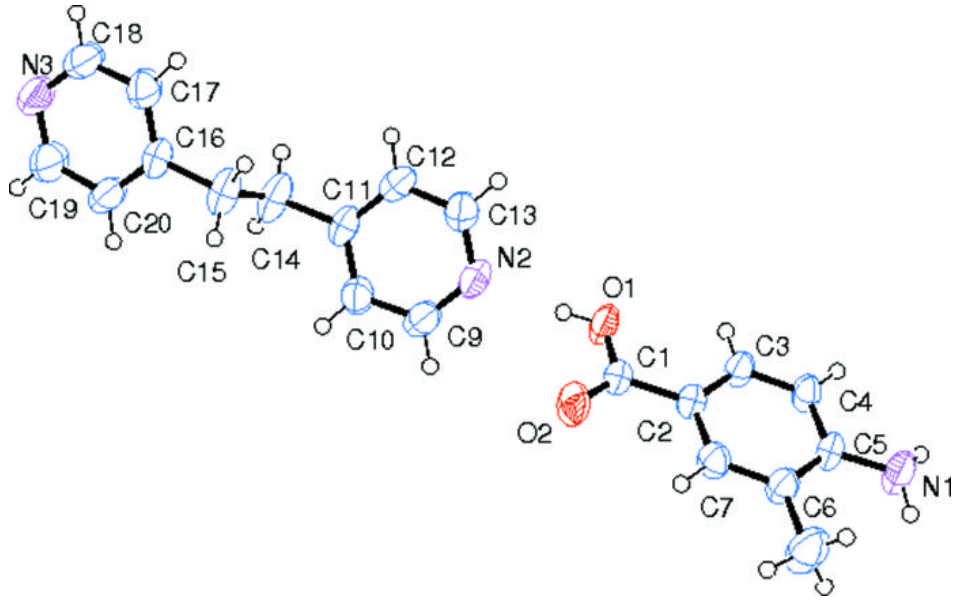
C18
N3
C17
C16
C19
C20
C15
C14
C11
C12
C13
N2
C10
C9
O1
C1
C3
C4
O2
C2
C5
N1
C7
C6

Fig. 2