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3-(4-Pyridyl)benzoic acid

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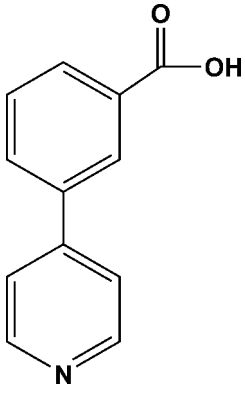
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.135; data-to-parameter ratio = 17.3.

The molecule of the title compound, $C_{12}H_9NO_2$, is not planar, the benzene and pyridine rings making a dihedral angle of 32.14 (7)°. The carboxy group is slightly twisted with respect to the benzene ring by 11.95 (10)°. In the crystal structure, intermolecular O—H···N hydrogen bonds link neighboring molecules into infinite chains along the c axis.

Related literature

For coordination polymers with pyridine carboxylate, see: Lu & Luck (2003); Luo *et al.* (2007).



Experimental

Crystal data

$C_{12}H_9NO_2$
M_r = 199.20
Orthorhombic, *Pbca*
a = 13.839 (3) Å
b = 7.013 (7) Å
c = 19.469 (10) Å
V = 1890 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 K
0.33 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.958, T_{max} = 0.979
11481 measured reflections
2365 independent reflections
1480 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.135
S = 1.03
2365 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1^{i}	0.82	1.83	2.6526 (18)	178

Symmetry code: (i) $x, -y-\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2447).

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supporting information

Acta Cryst. (2009). E**65**, o1239 [doi:10.1107/S1600536809015530]

3-(4-Pyridyl)benzoic acid

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S1. Comment

As part of an ongoing investigation into coordination polymer with pyridine carboxylate (Lu *et al.*, 2003; Luo *et al.*, 2007), the crystal structure of the title compound is presented here.

The molecule of the title compound, $C_{12}H_9NO_2$, is not planar, the phenyl and the pyridine rings make a dihedral angle of 32.14 (7)° (Fig. 1). The acetic group is slightly twisted with respect to the phenyl ring by 11.95 (10)°. In the crystal structure, intermolecular O—H···N hydrogen bonds link neighboring molecules into infinite chains along the c axis (Table 1, Fig. 2).

S2. Experimental

Commercially available 3-Pyrid-4-ylbenzoic acid was further purified by repeated recrystallization anhydrous ethanol from. Single crystals suitable for X-ray analysis were grown by slow evaporation of an anhydrous ethanol solution at room temperature.

S3. Refinement

All H atoms attached to C atoms and O atom were fixed geometrically and treated as riding with C—H = 0.93 Å and O—H = 0.82 Å with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(O)$.

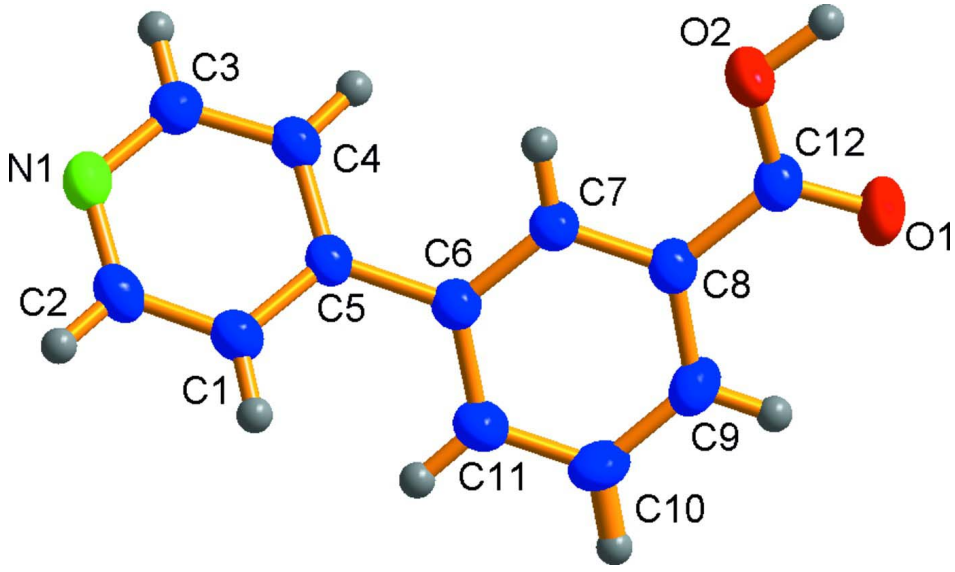

Figure 1

Molecular structure of the title compound with the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probalility level. H atoms are represented as small spheres of arbitrary radii.

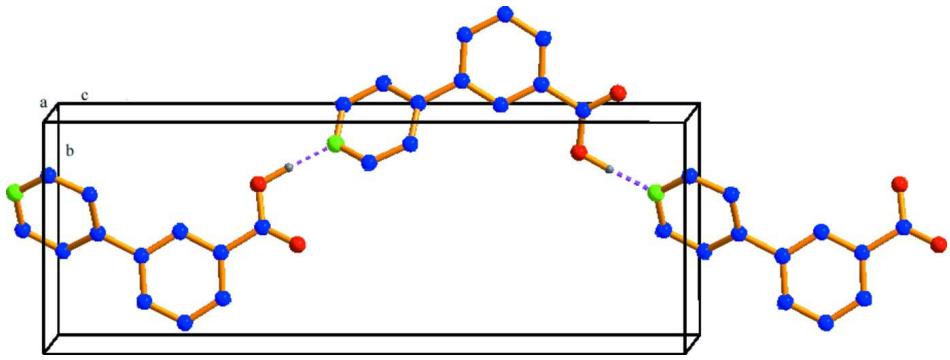

Figure 2

Partial packing view showing the formation of infinite chain through the O-H···N hydrogen bondings. H bonds are shown as dashed lines. H atoms not involved in hydrogen bondings have been omitted for clarity.

3-(4-Pyridyl)benzoic acid

Crystal data

$C_{12}H_9NO_2$
$M_r = 199.20$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.839$ (3) Å
$b = 7.013$ (7) Å
$c = 19.469$ (10) Å
$V = 1890$ (2) Å^3
$Z = 8$
$F(000) = 832$
$D_x = 1.400$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 1695 reflections
$\theta = 2.6$–$24.3°$
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Block, colorless
0.33 × 0.25 × 0.20 mm

Data collection

Bruker APEX2 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.958$, $T_{max} = 0.979$
11481 measured reflections
2365 independent reflections
1480 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 28.5°$, $\theta_{min} = 2.1°$
$h = -12 \rightarrow 18$
$k = -9 \rightarrow 8$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.135$
$S = 1.03$
2365 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.2238P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.40429 (11)	0.07701 (18)	0.11778 (6)	0.0584 (4)
O2	0.36926 (10)	−0.18026 (17)	0.17987 (6)	0.0522 (4)
H2	0.3707	−0.2322	0.1422	0.078*
N1	0.37092 (10)	−0.1441 (2)	0.55920 (6)	0.0404 (4)
C1	0.32413 (12)	0.1110 (2)	0.48533 (8)	0.0394 (4)
H1	0.2910	0.2254	0.4801	0.047*
C2	0.32519 (12)	0.0204 (2)	0.54811 (8)	0.0409 (4)
H2A	0.2924	0.0767	0.5845	0.049*
C3	0.41717 (12)	−0.2214 (2)	0.50565 (8)	0.0412 (4)
H3	0.4495	−0.3362	0.5123	0.049*
C4	0.41965 (13)	−0.1406 (2)	0.44148 (8)	0.0384 (4)
H4	0.4527	−0.2007	0.4059	0.046*
C5	0.37253 (11)	0.0313 (2)	0.42988 (7)	0.0333 (4)
C6	0.37464 (11)	0.1281 (2)	0.36208 (7)	0.0351 (4)
C7	0.37848 (12)	0.0237 (2)	0.30137 (8)	0.0367 (4)
H7	0.3784	−0.1088	0.3034	0.044*
C8	0.38238 (11)	0.1135 (2)	0.23794 (8)	0.0370 (4)
C9	0.38217 (13)	0.3104 (2)	0.23504 (9)	0.0449 (4)
H9	0.3859	0.3718	0.1928	0.054*
C10	0.37647 (14)	0.4159 (2)	0.29454 (9)	0.0517 (5)
H10	0.3752	0.5484	0.2922	0.062*
C11	0.37260 (13)	0.3262 (2)	0.35748 (9)	0.0449 (4)
H11	0.3686	0.3989	0.3973	0.054*
C12	0.38692 (12)	0.0033 (2)	0.17260 (8)	0.0405 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0891 (11)	0.0554 (8)	0.0308 (7)	−0.0103 (7)	0.0039 (6)	0.0069 (6)
O2	0.0824 (10)	0.0435 (7)	0.0306 (6)	−0.0105 (7)	0.0057 (6)	−0.0034 (5)
N1	0.0462 (9)	0.0433 (8)	0.0316 (7)	−0.0036 (6)	−0.0016 (6)	0.0014 (6)
C1	0.0434 (10)	0.0387 (9)	0.0361 (9)	0.0052 (7)	0.0005 (7)	−0.0049 (7)
C2	0.0436 (10)	0.0468 (10)	0.0322 (9)	−0.0013 (8)	0.0036 (7)	−0.0073 (7)
C3	0.0483 (10)	0.0375 (8)	0.0377 (9)	0.0036 (8)	−0.0022 (7)	0.0007 (7)
C4	0.0460 (10)	0.0373 (9)	0.0319 (8)	0.0016 (7)	0.0039 (7)	−0.0037 (7)
C5	0.0374 (8)	0.0340 (8)	0.0285 (8)	−0.0034 (7)	−0.0011 (6)	−0.0023 (6)

C6	0.0381 (9)	0.0342 (8)	0.0330 (8)	−0.0005 (7)	0.0009 (7)	0.0000 (6)
C7	0.0452 (9)	0.0319 (8)	0.0330 (8)	−0.0011 (7)	0.0011 (7)	0.0008 (6)
C8	0.0406 (9)	0.0385 (9)	0.0320 (8)	−0.0026 (7)	−0.0008 (7)	0.0013 (6)
C9	0.0567 (11)	0.0409 (10)	0.0370 (9)	−0.0037 (8)	−0.0058 (8)	0.0095 (7)
C10	0.0732 (14)	0.0300 (9)	0.0519 (11)	0.0004 (9)	−0.0051 (9)	0.0038 (8)
C11	0.0590 (11)	0.0359 (9)	0.0399 (9)	0.0018 (8)	−0.0004 (8)	−0.0047 (7)
C12	0.0468 (10)	0.0423 (10)	0.0324 (9)	−0.0017 (7)	−0.0010 (7)	0.0035 (7)

Geometric parameters (Å, º)

O1—C12	1.2102 (18)	C5—C6	1.485 (2)
O2—C12	1.318 (2)	C6—C7	1.391 (2)
O2—H2	0.8200	C6—C11	1.393 (2)
N1—C2	1.333 (2)	C7—C8	1.387 (2)
N1—C3	1.338 (2)	C7—H7	0.9300
C1—C2	1.378 (2)	C8—C9	1.382 (2)
C1—C5	1.388 (2)	C8—C12	1.490 (2)
C1—H1	0.9300	C9—C10	1.377 (2)
C2—H2A	0.9300	C9—H9	0.9300
C3—C4	1.372 (2)	C10—C11	1.379 (2)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.389 (2)	C11—H11	0.9300
C4—H4	0.9300		
C12—O2—H2	109.5	C11—C6—C5	120.85 (13)
C2—N1—C3	116.83 (14)	C8—C7—C6	121.25 (15)
C2—C1—C5	119.96 (15)	C8—C7—H7	119.4
C2—C1—H1	120.0	C6—C7—H7	119.4
C5—C1—H1	120.0	C9—C8—C7	119.33 (15)
N1—C2—C1	123.21 (15)	C9—C8—C12	118.92 (14)
N1—C2—H2A	118.4	C7—C8—C12	121.75 (15)
C1—C2—H2A	118.4	C10—C9—C8	120.19 (15)
N1—C3—C4	123.66 (16)	C10—C9—H9	119.9
N1—C3—H3	118.2	C8—C9—H9	119.9
C4—C3—H3	118.2	C9—C10—C11	120.32 (16)
C3—C4—C5	119.64 (15)	C9—C10—H10	119.8
C3—C4—H4	120.2	C11—C10—H10	119.8
C5—C4—H4	120.2	C10—C11—C6	120.77 (15)
C1—C5—C4	116.70 (14)	C10—C11—H11	119.6
C1—C5—C6	121.14 (14)	C6—C11—H11	119.6
C4—C5—C6	122.15 (14)	O1—C12—O2	123.30 (16)
C7—C6—C11	118.12 (14)	O1—C12—C8	122.67 (16)
C7—C6—C5	121.03 (14)	O2—C12—C8	114.03 (14)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O2—H2···N1^{i}	0.82	1.83	2.6526 (18)	178

Symmetry code: (i) x, $-y-1/2$, $z-1/2$.