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3-(Pyridin-3-yl)propionic acid

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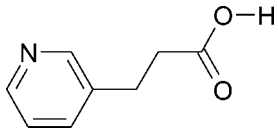
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.115; data-to-parameter ratio = 17.1.

In the crystal of the title compound, $C_8H_9NO_2$, molecules assemble to form $C(8)$ chains along the b axis by N—H···O hydrogen bonds, supported by weaker C—H···O hydrogen bonded-interactions between adjacent chains.

Related literature

For use of the title compound in coordination polymers, see: Wang *et al.* (2006). For graph-set nomenclature of hydrogen bonds, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_8H_9NO_2$
M_r = 151.16
Monoclinic, $P2_1/c$
a = 6.7157 (4) Å
b = 14.6544 (13) Å
c = 7.2993 (6) Å
β = 92.566 (5)°
V = 717.64 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.42 × 0.27 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: integration (*XPREP*; Bruker, 1999)
T_{min} = 0.967, T_{max} = 0.995
10553 measured reflections
1729 independent reflections
1341 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.02
1729 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.84	1.75	2.5868 (13)	172
C3—H3···O1^{ii}	0.95	2.47	3.3468 (15)	154
C5—H5···O2^{iii}	0.95	2.63	3.3328 (15)	131

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2372).

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Acta Cryst. (2011). E**67**, o215 [https://doi.org/10.1107/S1600536810052384]

3-(Pyridin-3-yl)propionic acid

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S1. Comment

The molecule 3-pyridinepropionic acid (I) has been used as a ligand to make coordination polymers using Ag, Cu and Zn (Wang *et al.*, 2006). The crystal structure of the molecule itself has not been reported. The solid state packing involves forming chains of molecules, generated by hydrogen bonding interactions from the carboxylic acid H to the lone pair of the pyridine N atom. The chain, described using graph set notation (Bernstein *et al.*, 1995) as C(8), is generated by the twofold screw axis inherent in the spacegroup $P2_1/c$, and runs along the crystallographic *b* axis (See Fig 2). Adjacent chains are stabilized by two C—H···O hydrogen bonds (See Table 1).

S2. Experimental

Crystals where grown by slow evaporation at ambient conditions of a methanol solution of 3-pyridinepropionic acid.

S3. Refinement

The C-bound H atoms were geometrically placed (C—H bond lengths of 0.95 (aromatic CH) and 0.99 (CH_2) Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$. The O-bound H atom were geometrically placed and refined as riding with $U_{iso}(H) = 1.5U_{eq}(O)$.

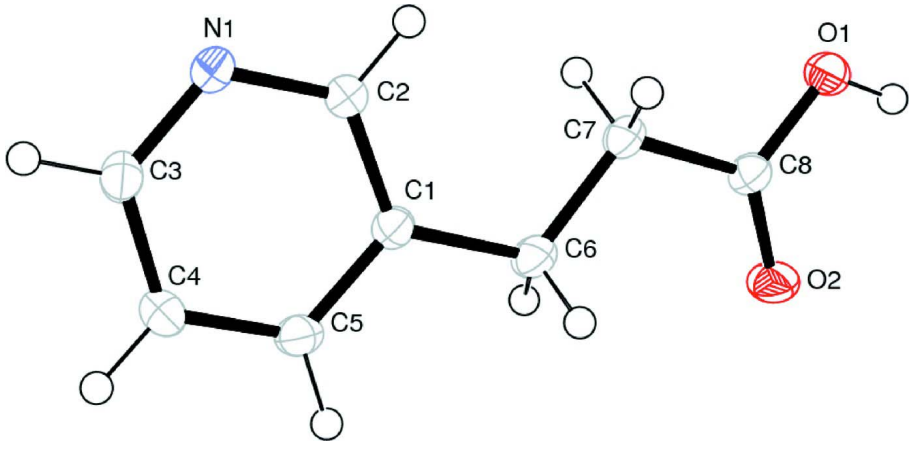

Figure 1

View of (I) (50% probability displacement ellipsoids)

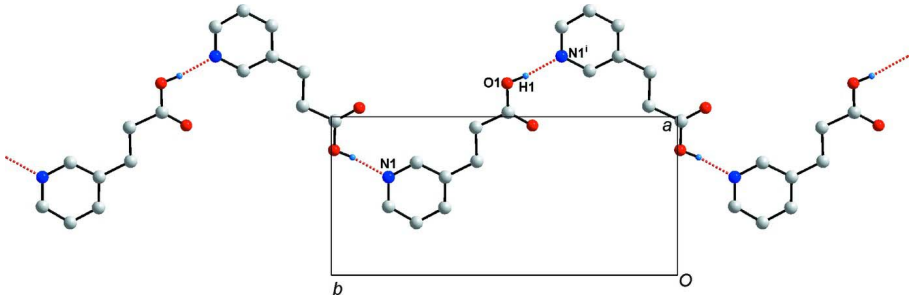

Figure 2

Hydrogen bonding C(8) chain of (I) using N—H···O hydrogen bonds (red dashed lines), generated by the twofold screw axis. Symmetry code: (i) -*x* + 2, *y* - 1/2, -*z* + 1/2.

3-(Pyridin-3-yl)propionic acid

Crystal data

$C_8H_9NO_2$
M_r = 151.16
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.7157 (4) Å
b = 14.6544 (13) Å
c = 7.2993 (6) Å
β = 92.566 (5)°
V = 717.64 (10) Å^3
Z = 4
F(000) = 320
D_x = 1.399 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 3866 reflections
θ = 0.4–30.0°
μ = 0.10 mm^{-1}
T = 173 K
Plate, colourless
0.42 × 0.27 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
2.0° *π* and *ω* scans
Absorption correction: integration (*XPREP*; Bruker, 1999)
T_{min} = 0.967, T_{max} = 0.995
10553 measured reflections
1729 independent reflections
1341 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 28°, θ_{min} = 3.0°
h = −8→7
k = −19→19
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.02
1729 reflections
101 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0616P)^2 + 0.1772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Experimental. Numerical integration absorption corrections based on indexed crystal faces were applied using the *XPREP* routine (Bruker, 1999)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.61989 (17)	0.67074 (7)	0.12796 (15)	0.0187 (3)
C2	0.71028 (18)	0.75445 (8)	0.16533 (16)	0.0198 (3)
H2	0.8419	0.755	0.2186	0.024*
C3	0.43377 (18)	0.83489 (8)	0.05545 (16)	0.0229 (3)
H3	0.3693	0.8916	0.0312	0.028*
C4	0.33224 (19)	0.75458 (8)	0.01309 (18)	0.0242 (3)
H4	0.2003	0.7561	−0.0395	0.029*
C5	0.42692 (18)	0.67253 (8)	0.04903 (16)	0.0221 (3)
H5	0.3602	0.6169	0.0198	0.026*
C6	0.71897 (18)	0.57984 (8)	0.16581 (17)	0.0236 (3)
H6A	0.7149	0.5443	0.0503	0.028*
H6B	0.6391	0.5461	0.2543	0.028*
C7	0.93261 (17)	0.58303 (8)	0.24056 (16)	0.0215 (3)
H7A	0.9366	0.6121	0.3631	0.026*
H7B	1.0116	0.6214	0.159	0.026*
C8	1.02756 (18)	0.48938 (7)	0.25664 (16)	0.0206 (3)
N1	0.61911 (15)	0.83489 (6)	0.12917 (14)	0.0212 (3)
O1	1.21073 (13)	0.49226 (6)	0.32765 (13)	0.0294 (3)
H1	1.2566	0.439	0.3362	0.044*
O2	0.94438 (13)	0.41935 (6)	0.20706 (13)	0.0315 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0190 (6)	0.0172 (6)	0.0201 (6)	0.0000 (4)	0.0022 (4)	0.0003 (4)
C2	0.0191 (6)	0.0182 (6)	0.0220 (6)	−0.0004 (4)	−0.0009 (4)	0.0008 (4)
C3	0.0229 (6)	0.0203 (6)	0.0255 (6)	0.0032 (5)	0.0000 (5)	0.0035 (4)
C4	0.0187 (6)	0.0262 (6)	0.0273 (6)	−0.0001 (5)	−0.0029 (5)	0.0026 (5)
C5	0.0214 (6)	0.0195 (6)	0.0254 (6)	−0.0038 (4)	0.0007 (5)	−0.0011 (4)
C6	0.0223 (6)	0.0152 (5)	0.0334 (7)	−0.0005 (4)	0.0004 (5)	−0.0006 (5)
C7	0.0224 (6)	0.0145 (5)	0.0276 (6)	0.0003 (4)	0.0002 (5)	0.0002 (4)
C8	0.0218 (6)	0.0173 (6)	0.0228 (6)	−0.0006 (4)	0.0017 (5)	−0.0001 (4)
N1	0.0231 (5)	0.0166 (5)	0.0238 (5)	−0.0002 (4)	−0.0004 (4)	0.0011 (4)
O1	0.0255 (5)	0.0153 (4)	0.0462 (6)	0.0024 (3)	−0.0115 (4)	−0.0022 (4)
O2	0.0256 (5)	0.0172 (4)	0.0510 (6)	−0.0014 (3)	−0.0074 (4)	−0.0048 (4)

Geometric parameters (Å, º)

C1—C2	1.3903 (16)	C5—H5	0.95
C1—C5	1.3947 (17)	C6—C7	1.5127 (16)
C1—C6	1.5090 (16)	C6—H6A	0.99
C2—N1	1.3489 (15)	C6—H6B	0.99
C2—H2	0.95	C7—C8	1.5156 (15)
C3—N1	1.3338 (16)	C7—H7A	0.99
C3—C4	1.3881 (17)	C7—H7B	0.99

C3—H3	0.95	C8—O2	1.2157 (14)
C4—C5	1.3798 (17)	C8—O1	1.3140 (15)
C4—H4	0.95	O1—H1	0.84
C2—C1—C5	117.00 (10)	C1—C6—H6A	108.2
C2—C1—C6	123.91 (10)	C7—C6—H6A	108.2
C5—C1—C6	119.09 (10)	C1—C6—H6B	108.2
N1—C2—C1	122.84 (11)	C7—C6—H6B	108.2
N1—C2—H2	118.6	H6A—C6—H6B	107.4
C1—C2—H2	118.6	C6—C7—C8	112.89 (9)
N1—C3—C4	122.01 (11)	C6—C7—H7A	109
N1—C3—H3	119	C8—C7—H7A	109
C4—C3—H3	119	C6—C7—H7B	109
C5—C4—C3	118.62 (11)	C8—C7—H7B	109
C5—C4—H4	120.7	H7A—C7—H7B	107.8
C3—C4—H4	120.7	O2—C8—O1	123.65 (10)
C4—C5—C1	120.44 (11)	O2—C8—C7	123.72 (11)
C4—C5—H5	119.8	O1—C8—C7	112.62 (9)
C1—C5—H5	119.8	C3—N1—C2	119.09 (10)
C1—C6—C7	116.24 (10)	C8—O1—H1	109.5
C5—C1—C2—N1	0.27 (18)	C5—C1—C6—C7	176.33 (10)
C6—C1—C2—N1	179.56 (11)	C1—C6—C7—C8	−174.20 (10)
N1—C3—C4—C5	0.09 (19)	C6—C7—C8—O2	3.16 (17)
C3—C4—C5—C1	0.63 (18)	C6—C7—C8—O1	−177.75 (10)
C2—C1—C5—C4	−0.79 (18)	C4—C3—N1—C2	−0.62 (18)
C6—C1—C5—C4	179.88 (10)	C1—C2—N1—C3	0.43 (18)
C2—C1—C6—C7	−2.95 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.84	1.75	2.5868 (13)	172
C3—H3···O1^{ii}	0.95	2.47	3.3468 (15)	154
C5—H5···O2^{iii}	0.95	2.63	3.3328 (15)	131

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