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5-(Pyridin-4-yl)isophthalic acid

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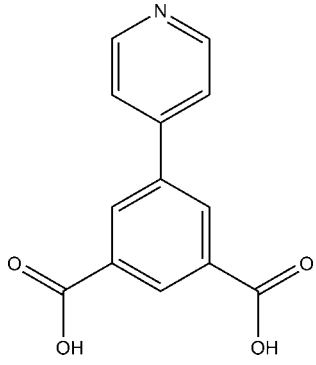
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.107; data-to-parameter ratio = 6.1.

In the title compound, $C_{13}H_9NO_4$, the two carboxylic groups and the benzene ring are approximately co-planar with a maximum atomic deviation 0.175 (4) Å, while the pyridine ring is oriented at a dihedral angle of 31.07 (18)° with respect to the benzene ring. In the crystal, molecules are linked by O—H···O, O—H···N and weak C—H···O hydrogen bonds, forming a three-dimensional supramolecular framework.

Related literature

For background to carboxylic acids as supramolecular synthons, see: Desiraju (1995); Thalladi *et al.* (1996).



Experimental

Crystal data

$C_{13}H_9NO_4$ M_r = 243.21
Orthorhombic, *Fdd*2
a = 15.5362 (16) Å
b = 37.371 (3) Å
c = 7.1716 (9) Å
V = 4163.9 (8) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.988
4224 measured reflections
1004 independent reflections
879 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.04
1004 reflections
164 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2A···N1^{i}	0.82	1.78	2.558 (3)	157
O3—H3A···O2^{ii}	0.82	1.91	2.620 (3)	144
C10—H10···O1^{iii}	0.93	2.57	3.491 (4)	172

Symmetry codes: (i) $-x+\frac{7}{4}, y+\frac{1}{4}, z-\frac{1}{4}$; (ii) $x-\frac{1}{2}, y, z+\frac{1}{2}$; (iii) $x+\frac{1}{4}, -y+\frac{1}{4}, z+\frac{1}{4}$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5043).

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supporting information

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5-(Pyridin-4-yl)isophthalic acid

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S1. Comment

Carboxylic acid is an interesting supramolecular synthon, widely used to construct supramolecular array with one to three different dimensions *via* hydrogen bonds (Desiraju, 1995; Thalladi *et al.*, 1996). In order to explore this area, the structure of the title compound, 5-(pyridin-4-yl)isophthalic acid, is reported herein.

As shown in Fig.1, the two carboxylic groups and the phenyl ring system in the title compound are almost planar with the maximum deviation 0.175Å for atom O_2 in the carboxylic group. However, the pyridine ring and the phenyl ring is not coplanar, with the dihedral angle 31.07°. This may be due to intermolecular O—H···N hydrogen-bonding interactions.

In the crystal structure, the dicarboxylic acid molecules are linked by intermolecular O—H···N, O—H···O and C—H···O hydrogen bonding interactions into a three-dimensional framework (Fig. 2).

S2. Experimental

The commercially available title compound, 5-(pyridin-4-yl)isophthalic acid, was recrystallized from an aqueous solution.

S3. Refinement

All H atoms were positioned geometrically and constrained to ride on their parent atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O). As no significant anomalous scatterings, Friedel pairs were merged.

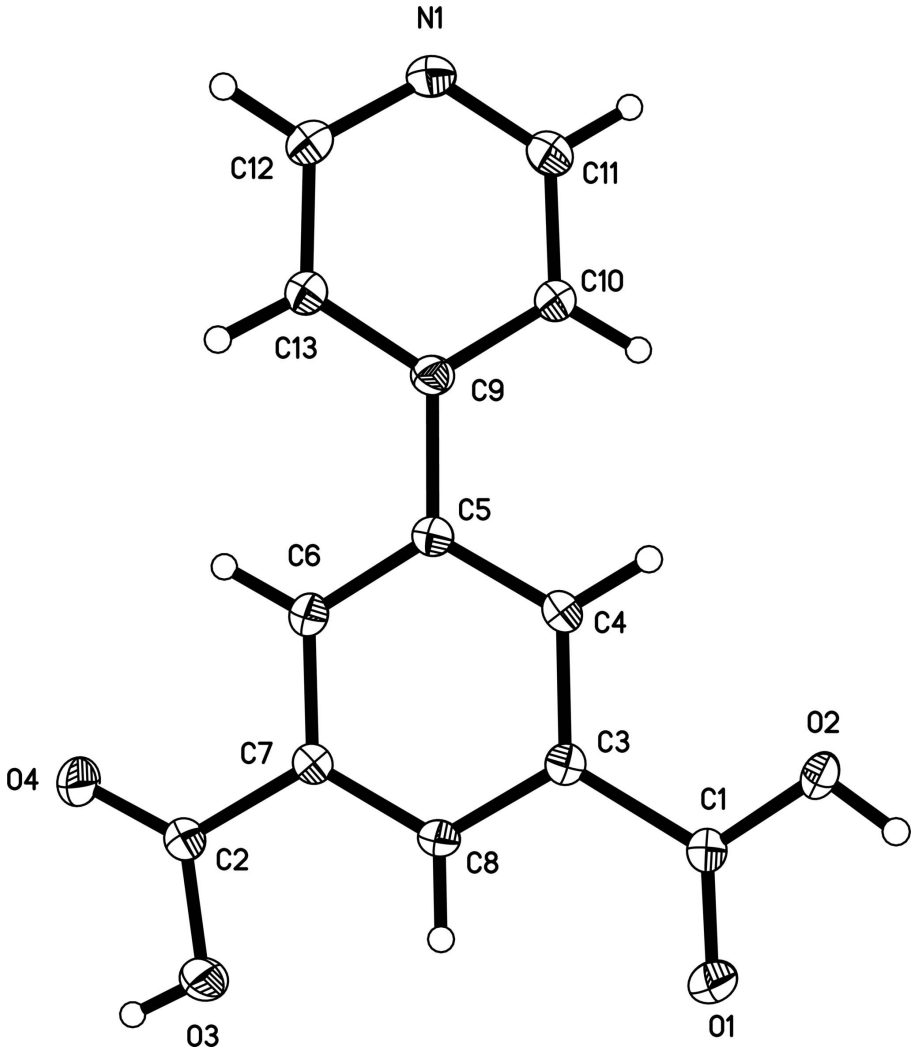

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

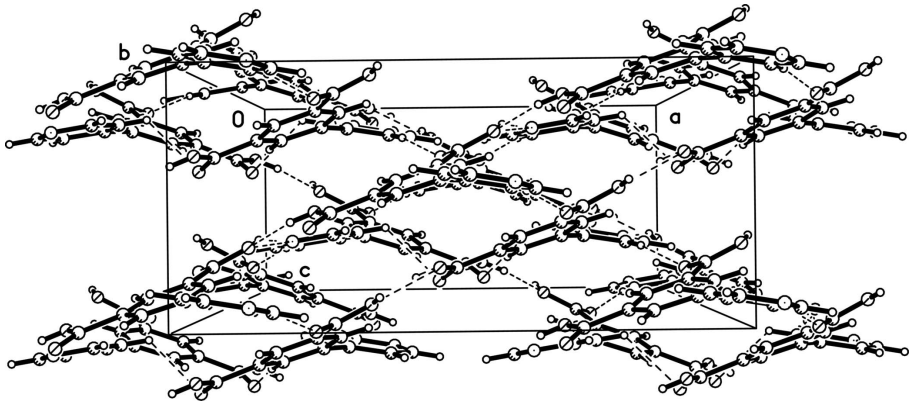

Figure 2

The packing diagram of the title compound.

5-(Pyridin-4-yl)isophthalic acid

Crystal data

$C_{13}H_9NO_4$
$M_r = 243.21$
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
$a = 15.5362$ (16) Å
$b = 37.371$ (3) Å
$c = 7.1716$ (9) Å
$V = 4163.9$ (8) Å^3
$Z = 16$
$F(000) = 2016$
$D_x = 1.552$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1601 reflections
$\theta = 2.8$–$26.5°$
$\mu = 0.12$ mm^{-1}
$T = 296$ K
Block, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.966$, $T_{max} = 0.988$
4224 measured reflections
1004 independent reflections
879 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
$h = -18\rightarrow8$
$k = -44\rightarrow38$
$l = -8\rightarrow8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.107$
$S = 1.04$
1004 reflections
164 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0701P)^2 + 2.9125P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0010 (3)

Special details

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.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.70913 (15)	0.16593 (6)	0.0729 (5)	0.0455 (7)
O2	0.81725 (15)	0.13320 (6)	−0.0349 (5)	0.0401 (7)
H2A	0.8354	0.1528	−0.0678	0.060*

O3	0.45574 (15)	0.10618 (6)	0.3114 (4)	0.0450 (8)
H3A	0.4068	0.1054	0.3541	0.068*
O4	0.45297 (14)	0.04779 (6)	0.3757 (4)	0.0451 (8)
N1	0.85168 (17)	−0.05737 (7)	0.1930 (5)	0.0351 (7)
C1	0.74454 (19)	0.13706 (8)	0.0469 (5)	0.0290 (8)
C2	0.4902 (2)	0.07358 (8)	0.3152 (6)	0.0294 (8)
C3	0.70358 (19)	0.10312 (8)	0.1149 (5)	0.0265 (7)
C4	0.74860 (19)	0.07115 (8)	0.1188 (5)	0.0274 (8)
H4	0.8058	0.0707	0.0807	0.033*
C5	0.70940 (18)	0.03966 (8)	0.1790 (5)	0.0257 (7)
C6	0.62393 (19)	0.04072 (8)	0.2376 (5)	0.0283 (8)
H6	0.5966	0.0198	0.2755	0.034*
C7	0.57949 (19)	0.07292 (8)	0.2395 (5)	0.0270 (8)
C8	0.6192 (2)	0.10389 (8)	0.1779 (5)	0.0268 (8)
H8	0.5891	0.1254	0.1788	0.032*
C9	0.7591 (2)	0.00577 (8)	0.1821 (5)	0.0276 (8)
C10	0.8478 (2)	0.00577 (8)	0.2122 (6)	0.0330 (9)
H10	0.8772	0.0272	0.2282	0.040*
C11	0.8915 (2)	−0.02631 (9)	0.2179 (6)	0.0374 (9)
H11	0.9505	−0.0262	0.2399	0.045*
C12	0.7669 (2)	−0.05810 (9)	0.1627 (6)	0.0361 (9)
H12	0.7397	−0.0800	0.1450	0.043*
C13	0.7191 (2)	−0.02726 (8)	0.1570 (5)	0.0319 (8)
H13	0.6601	−0.0284	0.1364	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0389 (14)	0.0232 (12)	0.074 (2)	0.0034 (10)	0.0125 (14)	0.0062 (14)
O2	0.0330 (12)	0.0211 (11)	0.0664 (18)	−0.0048 (10)	0.0166 (13)	0.0045 (11)
O3	0.0301 (12)	0.0342 (13)	0.071 (2)	0.0072 (10)	0.0199 (13)	0.0063 (14)
O4	0.0318 (13)	0.0342 (13)	0.069 (2)	−0.0040 (10)	0.0164 (13)	0.0055 (13)
N1	0.0337 (15)	0.0266 (14)	0.045 (2)	0.0059 (12)	0.0011 (14)	0.0036 (14)
C1	0.0239 (15)	0.0255 (17)	0.037 (2)	−0.0015 (13)	0.0017 (14)	0.0042 (15)
C2	0.0261 (15)	0.0287 (17)	0.033 (2)	−0.0007 (13)	0.0011 (15)	0.0030 (15)
C3	0.0240 (15)	0.0243 (15)	0.031 (2)	−0.0011 (12)	0.0009 (14)	0.0007 (14)
C4	0.0202 (15)	0.0279 (16)	0.034 (2)	0.0013 (12)	0.0025 (14)	−0.0003 (14)
C5	0.0241 (15)	0.0239 (15)	0.0289 (18)	0.0014 (12)	0.0013 (14)	0.0020 (15)
C6	0.0255 (16)	0.0251 (16)	0.034 (2)	−0.0024 (13)	0.0025 (15)	0.0008 (14)
C7	0.0238 (15)	0.0254 (16)	0.032 (2)	0.0003 (12)	−0.0006 (15)	0.0006 (14)
C8	0.0233 (15)	0.0234 (15)	0.034 (2)	0.0032 (12)	0.0020 (14)	0.0008 (15)
C9	0.0275 (16)	0.0253 (16)	0.030 (2)	0.0031 (13)	0.0064 (14)	0.0026 (15)
C10	0.0252 (15)	0.0253 (16)	0.048 (2)	−0.0004 (12)	0.0006 (16)	0.0026 (16)
C11	0.0269 (17)	0.0345 (19)	0.051 (3)	0.0037 (14)	−0.0009 (17)	0.0042 (17)
C12	0.0347 (18)	0.0246 (16)	0.049 (3)	−0.0007 (13)	0.0011 (18)	0.0024 (16)
C13	0.0277 (16)	0.0259 (15)	0.042 (2)	−0.0008 (13)	0.0018 (16)	0.0041 (15)

Geometric parameters (Å, º)

O1—C1	1.225 (4)	C5—C6	1.393 (4)
O2—C1	1.281 (4)	C5—C9	1.483 (4)
O2—H2A	0.8200	C6—C7	1.387 (4)
O3—C2	1.331 (4)	C6—H6	0.9300
O3—H3A	0.8200	C7—C8	1.384 (4)
O4—C2	1.205 (4)	C8—H8	0.9300
N1—C11	1.327 (4)	C9—C10	1.395 (4)
N1—C12	1.335 (4)	C9—C13	1.394 (5)
C1—C3	1.501 (4)	C10—C11	1.378 (5)
C2—C7	1.489 (4)	C10—H10	0.9300
C3—C4	1.385 (4)	C11—H11	0.9300
C3—C8	1.386 (4)	C12—C13	1.372 (5)
C4—C5	1.394 (4)	C12—H12	0.9300
C4—H4	0.9300	C13—H13	0.9300
C1—O2—H2A	109.5	C8—C7—C6	120.0 (3)
C2—O3—H3A	109.5	C8—C7—C2	121.2 (3)
C11—N1—C12	120.0 (3)	C6—C7—C2	118.8 (3)
O1—C1—O2	124.4 (3)	C7—C8—C3	120.6 (3)
O1—C1—C3	120.3 (3)	C7—C8—H8	119.7
O2—C1—C3	115.3 (3)	C3—C8—H8	119.7
O4—C2—O3	123.1 (3)	C10—C9—C13	117.4 (3)
O4—C2—C7	124.4 (3)	C10—C9—C5	121.1 (3)
O3—C2—C7	112.5 (3)	C13—C9—C5	121.5 (3)
C4—C3—C8	119.3 (3)	C11—C10—C9	119.4 (3)
C4—C3—C1	121.4 (3)	C11—C10—H10	120.3
C8—C3—C1	119.3 (3)	C9—C10—H10	120.3
C3—C4—C5	120.9 (3)	N1—C11—C10	121.8 (3)
C3—C4—H4	119.5	N1—C11—H11	119.1
C5—C4—H4	119.5	C10—C11—H11	119.1
C6—C5—C4	119.1 (3)	N1—C12—C13	121.5 (3)
C6—C5—C9	121.1 (3)	N1—C12—H12	119.3
C4—C5—C9	119.9 (3)	C13—C12—H12	119.3
C7—C6—C5	120.2 (3)	C12—C13—C9	119.9 (3)
C7—C6—H6	119.9	C12—C13—H13	120.0
C5—C6—H6	119.9	C9—C13—H13	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N1^{i}	0.82	1.78	2.558 (3)	157
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Symmetry codes: (i) −*x*+7/4, *y*+1/4, *z*−1/4; (ii) *x*−1/2, *y*, *z*+1/2; (iii) *x*+1/4, −*y*+1/4, *z*+1/4.