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2,2′-Bipyridine-5,5′-dicarboxylic acid

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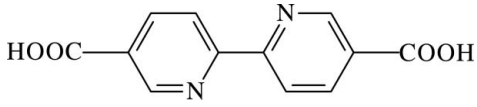
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.071; wR factor = 0.214; data-to-parameter ratio = 10.9.

The title molecule, $C_{12}H_8N_2O_4$, lies on an inversion center. In the crystal structure, intermolecular O—H···O hydrogen bonds connect molecules into one-dimensional chains along [1$\bar{1}$1].

Related literature

For synthetic applications of the title compound, see: Schokecht & Kempe (2004).



Experimental

Crystal data

$C_{12}H_8N_2O_4$
M_r = 244.20
Triclinic, $P\bar{1}$
a = 3.7384 (5) Å
b = 6.3934 (8) Å
c = 10.7786 (13) Å
α = 98.774 (2)°
β = 92.567 (1)°
γ = 90.000 (1)°
V = 254.34 (6) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 K
0.15 × 0.11 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.990
1343 measured reflections
893 independent reflections
657 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.214
S = 1.14
893 reflections
82 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.82	2.625 (3)	168

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009); 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: LH2868).

References

Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Schokecht, B. & Kempe, R. (2004). Z. Anorg. Allg. Chem. 630, 1377-1379.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2009). E**65**, o2081 [doi:10.1107/S1600536809030207]

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S1. Comment

2,2′-bipyridine-5,5′-dicarboxylate acid is a potential multi-dentate ligand with a versatile coordination mode, which has been used in self-assembled porous coordination synthesis (Schokecht & Kempe, 2004). The crystals of the title compound were obtained unintentionally as the harvested product of the hydrothermal reaction of 2,2′-bipyridine-5,5′-dicarboxylate acid, Eu_2O_3 and 1,10-phenanthroline.

The molecular structure of the title compound is shown in Fig. 1. In the crystal structure, intermolecular O—H···O hydrogen bonds connect molecules into one-dimensional chains along [1 -1 1] (Fig. 2).

S2. Experimental

Yellow needle-like crystals of the title compound were obtained by hydrothermal reaction of 2,2′-bipyridine-5,5′-dicarboxylate acid (0.04884 g), 1,10-phenanthroline (0.0360 g), Eu_2O_3 (0.0702 g) and deionized water (15 ml) in a 23 ml teflon-lined reaction vesset at 433 K for 120 h, followed by slow cooling to room temperature.

S3. Refinement

All H atoms were placed in calculated positions and included in a riding-model approximation, with C—H = 0.93 Å, O-H = 0.82Å and U_{iso}(H)= 1.2U_{eq}(C) or 1.5U_{eq}(O).

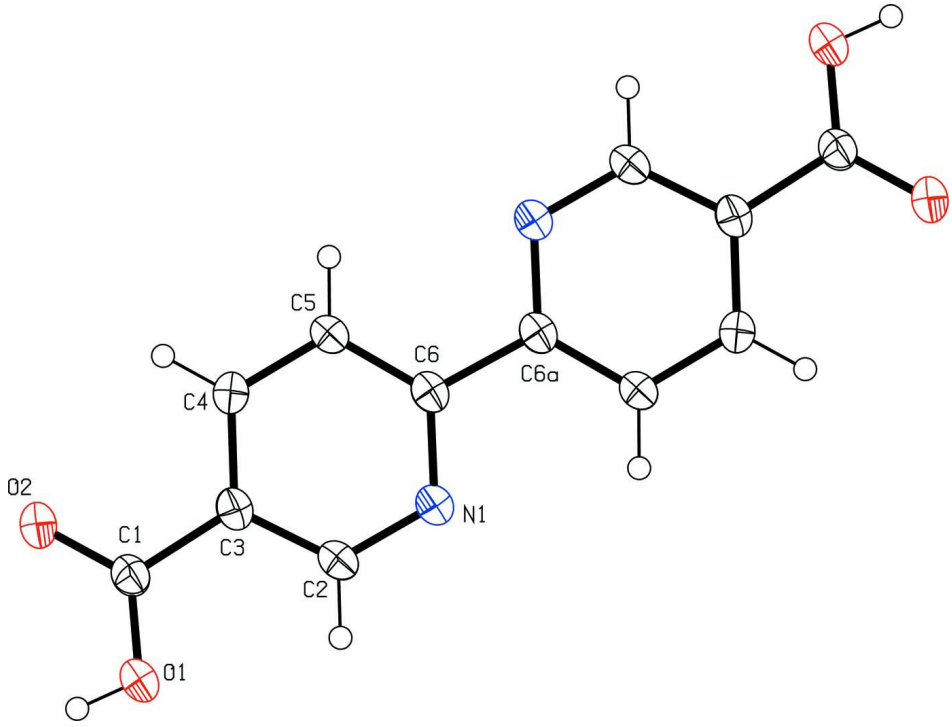

Figure 1

The molecular structure of the title compound shown with 30% probabilty ellipsoids [symmetry code: (a) -x, -y+1, -z+1].

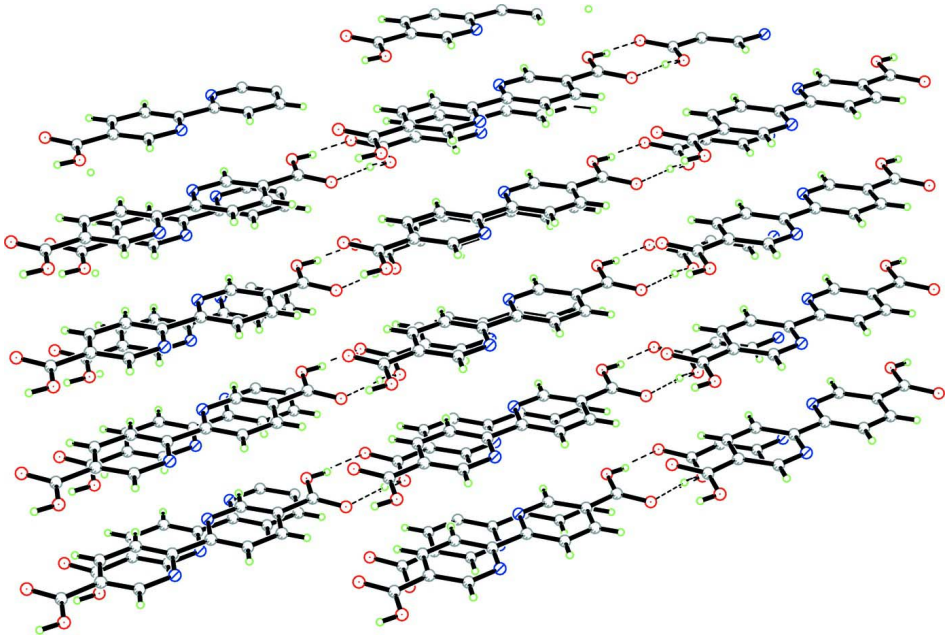

Figure 2

Part of the crystal structure of the title compound with hydrogen bonds shown as dashed lines. The one-dimensional hydrogen-bonded chains propagate along [1-11].

2,2′-Bipyridine-5,5′-dicarboxylic acid

Crystal data

$C_{12}H_8N_2O_4$
$M_r = 244.20$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 3.7384$ (5) Å
$b = 6.3934$ (8) Å
$c = 10.7786$ (13) Å
$\alpha = 98.774$ (2)°
$\beta = 92.567$ (1)°
$\gamma = 90.000$ (1)°
$V = 254.34$ (6) Å^3
$Z = 1$
$F(000) = 126$
$D_x = 1.594$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 528 reflections
$\theta = 3.2$–$27.6°$
$\mu = 0.12$ mm^{-1}
$T = 298$ K
Needle, yellow
0.15 × 0.11 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.982$, $T_{max} = 0.990$
1343 measured reflections
893 independent reflections
657 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -4 \rightarrow 4$
$k = -7 \rightarrow 7$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.214$
$S = 1.14$
893 reflections
82 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
$w = 1/[\sigma^2(F_o^2) + (0.1116P)^2 + 0.1159P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-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}
N1	0.1979 (7)	0.2556 (4)	0.5341 (2)	0.0351 (8)
O1	0.5129 (7)	−0.0316 (4)	0.8383 (2)	0.0492 (8)
H1	0.5614	−0.0788	0.9036	0.074*

O2	0.2843 (7)	0.2274 (4)	0.9736 (2)	0.0536 (9)
C1	0.3541 (8)	0.1439 (5)	0.8636 (3)	0.0334 (8)
C2	0.2905 (8)	0.1631 (5)	0.6337 (3)	0.0347 (9)
H2	0.3922	0.0293	0.6197	0.042*
C3	0.2438 (7)	0.2552 (5)	0.7571 (3)	0.0307 (9)
C4	0.0964 (8)	0.4566 (5)	0.7784 (3)	0.0353 (9)
H4	0.0640	0.5238	0.8598	0.042*
C5	−0.0008 (8)	0.5548 (5)	0.6768 (3)	0.0332 (8)
H5	−0.1009	0.6892	0.6890	0.040*
C6	0.0520 (8)	0.4512 (5)	0.5562 (3)	0.0295 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0443 (16)	0.0333 (15)	0.0284 (15)	0.0064 (12)	−0.0011 (12)	0.0079 (12)
O1	0.0724 (18)	0.0463 (16)	0.0308 (14)	0.0208 (13)	−0.0006 (12)	0.0129 (11)
O2	0.083 (2)	0.0525 (17)	0.0267 (14)	0.0231 (14)	0.0056 (12)	0.0108 (11)
C1	0.0347 (17)	0.0366 (18)	0.0297 (17)	0.0043 (14)	−0.0014 (13)	0.0088 (14)
C2	0.0390 (18)	0.0339 (18)	0.0329 (18)	0.0076 (14)	−0.0009 (13)	0.0108 (14)
C3	0.0309 (16)	0.0350 (19)	0.0271 (18)	0.0003 (14)	−0.0020 (13)	0.0083 (14)
C4	0.0446 (19)	0.0375 (19)	0.0240 (16)	0.0068 (15)	0.0024 (13)	0.0047 (13)
C5	0.0393 (18)	0.0321 (17)	0.0296 (17)	0.0078 (14)	0.0009 (13)	0.0092 (14)
C6	0.0288 (15)	0.0318 (18)	0.0289 (17)	−0.0009 (13)	−0.0021 (12)	0.0088 (14)

Geometric parameters (Å, º)

N1—C2	1.335 (4)	C2—H2	0.9300
N1—C6	1.357 (4)	C3—C4	1.391 (4)
O1—C1	1.267 (4)	C4—C5	1.378 (4)
O1—H1	0.8200	C4—H4	0.9300
O2—C1	1.263 (4)	C5—C6	1.388 (4)
C1—C3	1.484 (4)	C5—H5	0.9300
C2—C3	1.388 (4)	C6—C6^{i}	1.482 (6)
C2—N1—C6	117.4 (3)	C4—C3—C1	120.8 (3)
C1—O1—H1	109.5	C5—C4—C3	118.9 (3)
O2—C1—O1	123.7 (3)	C5—C4—H4	120.5
O2—C1—C3	118.7 (3)	C3—C4—H4	120.5
O1—C1—C3	117.6 (3)	C4—C5—C6	119.3 (3)
N1—C2—C3	123.8 (3)	C4—C5—H5	120.3
N1—C2—H2	118.1	C6—C5—H5	120.3
C3—C2—H2	118.1	N1—C6—C5	122.4 (3)
C2—C3—C4	118.2 (3)	N1—C6—C6^{i}	116.1 (3)
C2—C3—C1	121.0 (3)	C5—C6—C6^{i}	121.5 (4)
C6—N1—C2—C3	0.4 (5)	C2—C3—C4—C5	0.8 (5)
N1—C2—C3—C4	−0.9 (5)	C1—C3—C4—C5	179.7 (3)
N1—C2—C3—C1	−179.8 (3)	C3—C4—C5—C6	−0.3 (5)

O2—C1—C3—C2	−175.3 (3)	C2—N1—C6—C5	0.2 (5)
O1—C1—C3—C2	4.4 (5)	C2—N1—C6—C6^{i}	−179.3 (3)
O2—C1—C3—C4	5.9 (5)	C4—C5—C6—N1	−0.2 (5)
O1—C1—C3—C4	−174.4 (3)	C4—C5—C6—C6^{i}	179.2 (3)

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{ii}	0.82	1.82	2.625 (3)	168

Symmetry code: (ii) −*x*+1, −*y*, −*z*+2.