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4,4′-Bipyridine–2,4-dihydroxybenzoic acid (1/1)

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.056
wR factor = 0.155
Data-to-parameter ratio = 16.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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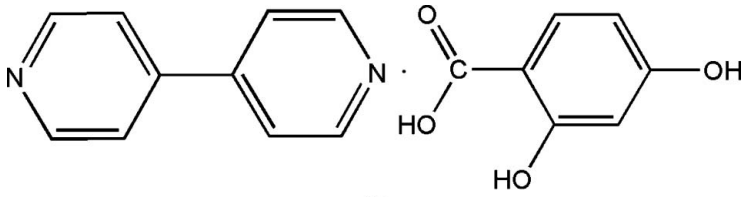
The title compound, $C_{10}H_8N_2\cdot C_7H_6O_4$, consists of 4,4′-bipyridine and 2,4-dihydroxybenzoic acid molecules, which are linked *via* O–H···N hydrogen bonds, forming infinite one-dimensional chains. Adjacent chains are further linked into a two-dimensional structure by C—H···π interactions.

Comment

The reliability of hydrogen bonds has been widely applied to organize one-, two- and three-dimensional networks. Moreover, hydrogen-bonded networks are organized according to their dimensionality and shape (Beatty, 2003). We report here the structure of the title compound, (I).



(I)

Compound (I) consists of 4,4′-bipyridine and 2,4-dihydroxybenzoic acid molecules (Fig. 1). Atoms O2 and O4 of 2,4-dihydroxybenzoic acid acts as hydrogen-bond donors to atoms N1 and N2 of 4,4′-bipyridine (Table 1), generating an infinite one-dimensional chain along the [40$\bar{1}$] direction (Fig. 2). There is also an intramolecular O—H···O hydrogen bond in 2,4-dihydroxybenzoic acid, leading to an *S*(6) ring. In addition, adjacent chains are linked into a two-dimensional framework by C—H···π interactions with an H15···*Cg*1(x, $\frac{3}{2}-y$, $z+\frac{1}{2}$) distance of 2.73 Å (Fig. 3; *Cg*1 is the centroid of the C1–C6 ring).

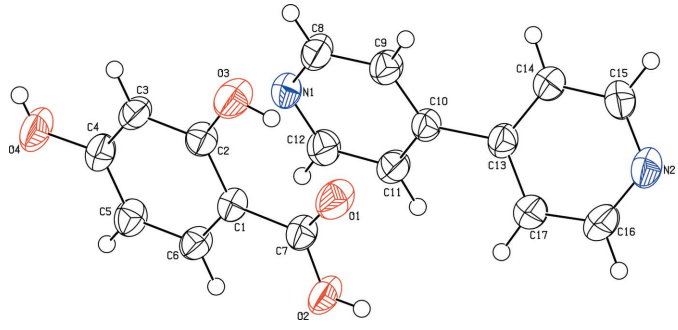


Figure 1
The asymmetric unit of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

All reagents were commercially available and of analytical grade. An ethanol solution (3 ml) of 4,4′-bipyridine (0.156 g, 1 mmol) was added dropwise to a vigorously stirred solution of 2,4-dihydroxybenzoic acid (0.31 g, 2.0 mmol) in 10 ml distilled water. The solution was then stirred for 15 min at 343 K and filtered. On slow evaporation of the filtrate for 3 d, crystals of (I) appeared and were selected. The crystal shape and IR spectrum confirmed that they were not the starting materials. We expected to prepare a bipyridinium dihydroxybenzoate salt. However, the obtained compound was, in fact, a co-crystal of the neutral molecules.

Crystal data

$C_{10}H_8N_2{\cdot}C_7H_6O_4$
M_r = 310.30
Monoclinic, $P2_1/c$
a = 6.6085 (8) Å
b = 10.7724 (12) Å
c = 20.809 (2) Å
β = 95.942 (2)°
V = 1473.4 (3) Å^3
Z = 4
D_x = 1.399 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
Plate, colorless
0.32 × 0.20 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
12686 measured reflections
3528 independent reflections
2537 reflections with $I > 2\sigma(I)$
R_{int} = 0.109
θ_{max} = 28.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.155
S = 1.00
3528 reflections
211 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0824P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.41 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—H2···N1^{i}	0.82	1.82	2.6298 (15)	172
O3—H3A···O1	0.82	1.88	2.6003 (16)	146
O4—H4···N2^{ii}	0.82	1.98	2.7622 (19)	160
C15—H15···$Cg1^{iii}$	0.93	2.73	3.3328 (19)	124

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

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

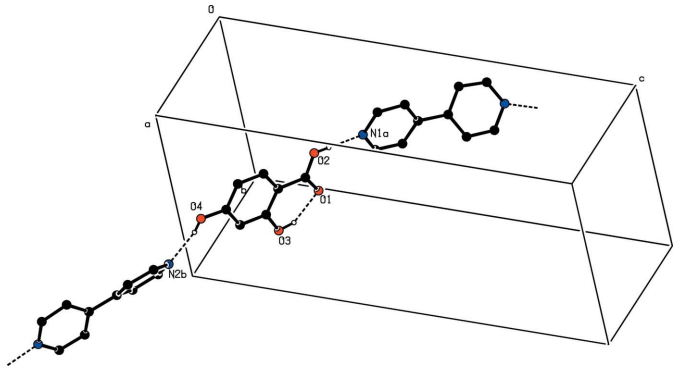


Figure 2
Part of the crystal structure of (I), showing the formation of a chain along the [40$\bar{1}$] direction. H atoms have been omitted unless involved in hydrogen bonds (dashed lines). [Symmetry codes: (*a*) $x-1, y, z$; (*b*) $1+x, \frac{3}{2}-y, z-\frac{1}{2}$.]

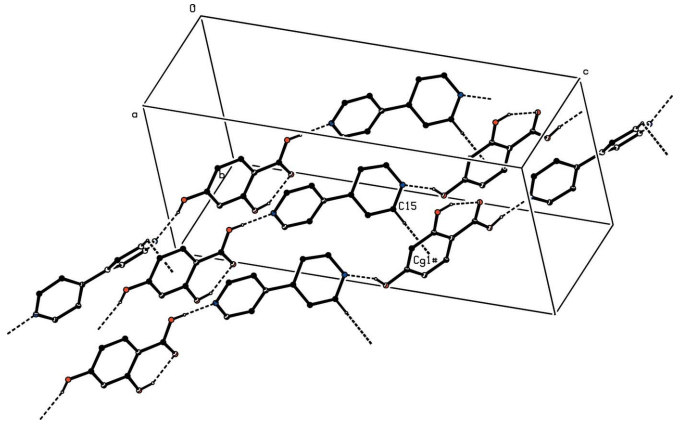


Figure 3
A part of the crystal structure of (I), showing the formation of a sheet by the C—H···π interactions between adjacent chains. H atoms have been omitted unless involved in hydrogen bonds (dashed lines). [Symmetry code: (#) $x, \frac{3}{2}-y, \frac{1}{2}+z$.]

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