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4,4′-Bipyridine–*trans*,*trans*-hexa-2,4-dienedioic acid (1/1)

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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 = 0.116; data-to-parameter ratio = 14.6.

The title cocrystal, $C_{10}H_8N_2 \cdot C_6H_6O_4$, crystallizes with half-molecules of 4,4′-bipyridine and *trans*,*trans*-hexa-2,4-dienedioic acid in the asymmetric unit, as each is located about a crystallographic inversion center. The bipyridine molecule is planar from symmetry. In the dicarboxylic acid molecule, the O—C—C—C torsion angle is −13.0 (2)°. In the crystal, O—H⋯N and C—H⋯O hydrogen bonds generate a three-dimensional network.

Related literature

For cocrystals of carboxylic acid and pyridine, see: Bhogala & Nangia (2003); Hou *et al.* (2008); Jiang & Hou (2012). For background to the applications of cocrystals, see: Bhogala & Nangia (2003); Gao *et al.* (2004); Hori *et al.* (2009); Weyna *et al.* (2009).

Experimental

Crystal data

$C_{10}H_8N_2 \cdot C_6H_6O_4$
M_r = 298.29
Triclinic, $P\overline{1}$
a = 5.8481 (5) Å
b = 7.6348 (6) Å
c = 8.4677 (7) Å
α = 91.837 (5)°
β = 92.584 (5)°
γ = 111.907 (4)°
V = 349.93 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.40 × 0.26 × 0.24 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.976
5973 measured reflections
1517 independent reflections
1336 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.04
1517 reflections
104 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1⋯N1	1.06 (2)	1.58 (2)	2.6148 (14)	164 (2)
C2—H2⋯O2^{i}	0.95	2.65	3.5130 (15)	151
C3—H3⋯O2^{ii}	0.95	2.58	3.4457 (16)	152
C4—H4⋯O1^{iii}	0.95	2.58	3.4848 (17)	160
C8—H8⋯O2^{iv}	0.95	2.56	3.3555 (17)	141

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1998); 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: SJ5219).

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supplementary materials

Acta Cryst. (2012). E**68**, o1201 [doi:10.1107/S1600536812012391]

4,4′-Bipyridine–*trans,trans*-hexa-2,4-dienedioic acid (1/1)

Suk-Hee Moon and Ki-Min Park

Comment

Considerable effort has been devoted to form co-crystals made up of two or more components because of their potential applications in pharmaceutical chemisty (Weyna *et al.*, 2009), supramolecular chemistry (Bhogala & Nangia, 2003; Gao *et al.*, 2004) and materials chemistry (Hori *et al.*, 2009). In particular, numerous studies have focused on hydrogen bonding between carboxylic acid and pyridine molecules (Bhogala & Nangia, 2003; Hou *et al.*, 2008; Jiang & Hou, 2012). We report here the structure of a co-crystal of *trans*, *trans*-hexa-2,4-dienedioic acid with 4,4′-bipyridine in the solid state.

The title compound is shown in Fig. 1. The asymmetric unit contains half-molecules of 4,4′-bipyridine and *trans*,*trans*-1,3 -butadiene-1,4-dicarboxylic acid each located on crystallographic inversion centers. Both components are planar by symmetry and tilted by 32.02 (7)° with respect to each other.

In the crystal, the dicarboxylic acid molecules are arranged side by side by intermolecular C—H···O hydrogen bonds between the dicarboxylic acid molecules, leading to the formation of a one dimensional chain. Moreover, intermolecular O—H···N and C—H···O hydrogen bonds between dicarboxylic acid and 4,4′-bipyridine molecules generate a three-dimensional network (Fig. 2, Table 1).

Experimental

A mixture of stoichiometric amounts of *trans*, *trans*-hexa-2,4-dienedioic acid and 4,4′-bipyridine in DMF (in a 1:1 volume ratio) was heated until the two components dissolved and was then kept at room temperature. Upon slow evaporation of the solvent, *X*–ray quality single crystals were obtained.

Refinement

The carboxyl-H atom was located in a difference Fourier map and refined isotropically. Csp^2 H atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

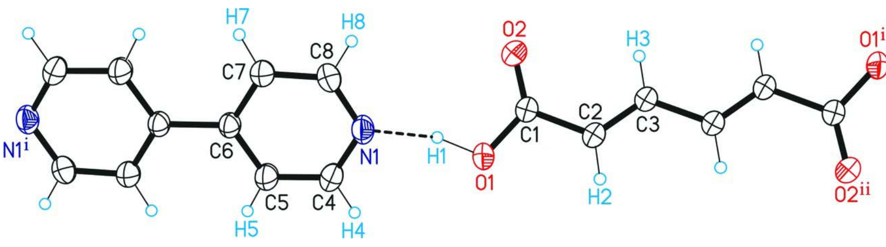

Figure 1

The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. (Symmetry codes: i) -*x* + 1, -*y* + 1, -*z* + 1; ii) -*x*, -*y* + 3, -*z*.)

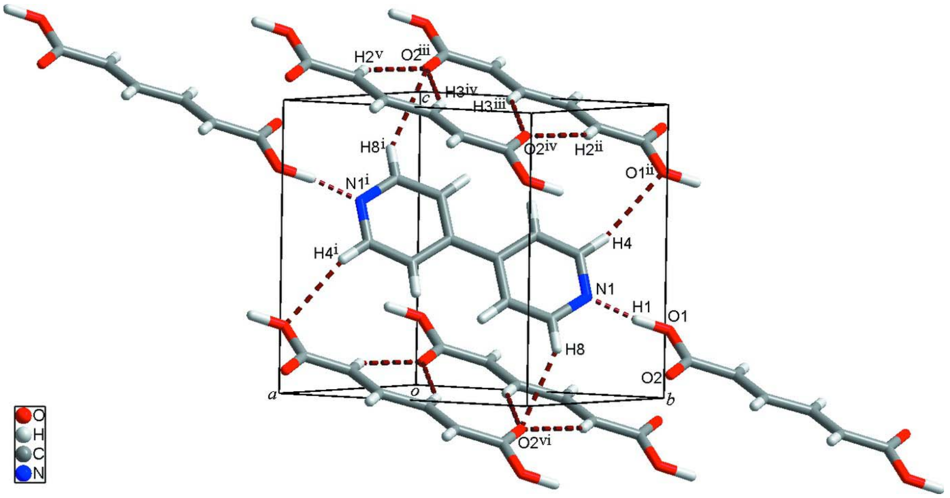

Figure 2

Crystal packing of the title compound with intermolecular O—H···N and C—H···O hydrogen bonds shown as dashed lines. (Symmetry codes: i) -*x* + 1, -*y* + 1, -*z* + 1; ii) -*x*, -*y* + 2, -*z* + 1; iii) *x*, *y* - 1, *z* + 1; iv) -*x* + 1, -*y* + 2, -*z* + 1; v) *x* + 1, *y* + 1, *z* + 1; vi) -*x* + 1, -*y* + 2, -*z*.)

4,4′-Bipyridine–*trans*,*trans*-hexa-2,4-dienedioic acid (1/1)

Crystal data

$C_{10}H_8N_2{\cdot}C_6H_6O_4$
$M_r = 298.29$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.8481\ (5)$ Å
$b = 7.6348\ (6)$ Å
$c = 8.4677\ (7)$ Å
$\alpha = 91.837\ (5)°$
$\beta = 92.584\ (5)°$
$\gamma = 111.907\ (4)°$
$V = 349.93\ (5)$ Å^3

$Z = 1$
$F(000) = 156$
$D_x = 1.415$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4151 reflections
$\theta = 2.4–28.4°$
$\mu = 0.10$ mm^{-1}
$T = 173$ K
Block, colourless
0.40 × 0.26 × 0.24 mm

Data collection

Bruker APEXII CCD
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator

φ and ω scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.960$, $T_{max} = 0.976$

5973 measured reflections
1517 independent reflections
1336 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.031$

$\theta_{\text{max}} = 27.0°$, $\theta_{\text{min}} = 2.4°$
$h = -7\rightarrow7$
$k = -9\rightarrow9$
$l = -10\rightarrow10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.116$
$S = 1.04$
1517 reflections
104 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0688P)^2 + 0.0753P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.24$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.25$ 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}
O1	0.05949 (18)	1.05053 (14)	0.23387 (13)	0.0414 (3)
H1	0.184 (4)	0.987 (3)	0.271 (3)	0.084 (7)*
O2	0.37461 (17)	1.23144 (14)	0.09959 (12)	0.0394 (3)
C1	0.1653 (2)	1.18769 (18)	0.13952 (14)	0.0285 (3)
C2	−0.0033 (2)	1.28402 (18)	0.09016 (15)	0.0299 (3)
H2	−0.1740	1.2262	0.1077	0.036*
C3	0.0786 (2)	1.44912 (17)	0.02208 (14)	0.0288 (3)
H3	0.2485	1.5031	0.0013	0.035*
N1	0.3031 (2)	0.85144 (15)	0.34658 (13)	0.0331 (3)
C4	0.2266 (3)	0.7745 (2)	0.48325 (17)	0.0374 (3)
H4	0.1161	0.8150	0.5389	0.045*
C5	0.3007 (3)	0.6385 (2)	0.54775 (16)	0.0350 (3)
H5	0.2419	0.5882	0.6458	0.042*
C6	0.4615 (2)	0.57572 (16)	0.46878 (14)	0.0262 (3)
C7	0.5464 (3)	0.6613 (2)	0.32875 (16)	0.0351 (3)
H7	0.6611	0.6270	0.2719	0.042*
C8	0.4627 (3)	0.79683 (19)	0.27252 (16)	0.0362 (3)
H8	0.5224	0.8532	0.1766	0.043*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0346 (5)	0.0401 (6)	0.0593 (7)	0.0222 (4)	0.0127 (5)	0.0259 (5)
O2	0.0314 (5)	0.0469 (6)	0.0488 (6)	0.0229 (4)	0.0109 (4)	0.0174 (5)
C1	0.0283 (6)	0.0293 (6)	0.0319 (6)	0.0148 (5)	0.0032 (5)	0.0056 (5)
C2	0.0260 (6)	0.0327 (7)	0.0355 (6)	0.0156 (5)	0.0037 (5)	0.0077 (5)
C3	0.0270 (6)	0.0324 (6)	0.0316 (6)	0.0156 (5)	0.0042 (5)	0.0067 (5)
N1	0.0322 (6)	0.0287 (6)	0.0407 (6)	0.0141 (5)	−0.0015 (5)	0.0074 (4)
C4	0.0397 (7)	0.0387 (7)	0.0434 (7)	0.0248 (6)	0.0073 (6)	0.0078 (6)
C5	0.0406 (7)	0.0390 (7)	0.0339 (7)	0.0234 (6)	0.0080 (5)	0.0106 (5)
C6	0.0253 (6)	0.0255 (6)	0.0291 (6)	0.0110 (5)	−0.0015 (5)	0.0030 (5)
C7	0.0372 (7)	0.0377 (7)	0.0373 (7)	0.0205 (6)	0.0084 (5)	0.0114 (6)
C8	0.0395 (7)	0.0351 (7)	0.0382 (7)	0.0176 (6)	0.0055 (6)	0.0135 (6)

Geometric parameters (Å, º)

O1—C1	1.3162 (15)	C4—C5	1.3839 (18)
O1—H1	1.06 (2)	C4—H4	0.9500
O2—C1	1.2096 (16)	C5—C6	1.3907 (17)
C1—C2	1.4873 (16)	C5—H5	0.9500
C2—C3	1.3310 (18)	C6—C7	1.3929 (18)
C2—H2	0.9500	C6—C6^{ii}	1.492 (2)
C3—C3^{i}	1.452 (2)	C7—C8	1.3872 (17)
C3—H3	0.9500	C7—H7	0.9500
N1—C8	1.3286 (17)	C8—H8	0.9500
N1—C4	1.3337 (18)		
C1—O1—H1	110.3 (13)	C5—C4—H4	118.5
O2—C1—O1	124.23 (11)	C4—C5—C6	119.86 (12)
O2—C1—C2	124.24 (11)	C4—C5—H5	120.1
O1—C1—C2	111.52 (10)	C6—C5—H5	120.1
C3—C2—C1	121.76 (12)	C5—C6—C7	116.57 (11)
C3—C2—H2	119.1	C5—C6—C6^{ii}	121.53 (14)
C1—C2—H2	119.1	C7—C6—C6^{ii}	121.90 (14)
C2—C3—C3^{i}	123.31 (15)	C8—C7—C6	119.78 (12)
C2—C3—H3	118.3	C8—C7—H7	120.1
C3^{i}—C3—H3	118.3	C6—C7—H7	120.1
C8—N1—C4	117.62 (11)	N1—C8—C7	123.05 (12)
N1—C4—C5	123.05 (12)	N1—C8—H8	118.5
N1—C4—H4	118.5	C7—C8—H8	118.5
O2—C1—C2—C3	−13.0 (2)	C4—C5—C6—C6^{ii}	−177.69 (14)
O1—C1—C2—C3	166.14 (12)	C5—C6—C7—C8	−2.2 (2)
C1—C2—C3—C3^{i}	−177.53 (14)	C6^{ii}—C6—C7—C8	177.72 (14)
C8—N1—C4—C5	−1.8 (2)	C4—N1—C8—C7	1.8 (2)
N1—C4—C5—C6	−0.3 (2)	C6—C7—C8—N1	0.2 (2)
C4—C5—C6—C7	2.3 (2)		

Symmetry codes: (i) $-x$, $-y+3$, $-z$; (ii) $-x+1$, $-y+1$, $-z+1$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	1.06 (2)	1.58 (2)	2.6148 (14)	164 (2)
C2—H2···O2^{iii}	0.95	2.65	3.5130 (15)	151
C3—H3···O2^{iv}	0.95	2.58	3.4457 (16)	152
C4—H4···O1^{v}	0.95	2.58	3.4848 (17)	160
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Symmetry codes: (iii) $x-1, y, z$; (iv) $-x+1, -y+3, -z$; (v) $-x, -y+2, -z+1$; (vi) $-x+1, -y+2, -z$.