Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Hydrogen-bonded 1,2-bis(4-pyridyl)-ethylene and maleic acid

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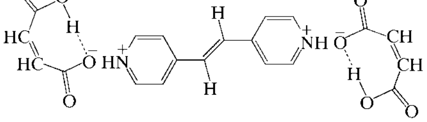
Received 23 April 2002
Accepted 19 September 2002
Online 22 October 2002

The title compound (systematic name: 4,4′-ethylenedipyridinium dimaleate), $C_{12}H_{12}N_2^{2+}\cdot 2C_4H_3O_4^{-}$, is a 1:2 adduct of 1,2-bis(4-pyridyl)ethylene (BPE) and maleic acid (MA). The interaction between the two components in the molecular complex is due to intermolecular hydrogen bonding *via* an $N^+—H\cdots O^-$ hydrogen bond.

Comment

There is growing interest in the construction of supramolecular assemblies with hydrogen bonds as the building blocks (Aakeroy & Seddon, 1993; Fredericks & Hamilton, 1996). An example is the cocrystal of 4,4′-bipyridine with maleic acid (MA), which forms a hydrogen-bonded adduct in a 1:2 molar ratio from acetone, adopting a herring-bone pattern (Chatterjee *et al.*, 1998). In this paper, we report the structural variation arising in such a complex due to the replacement of 4,4′-bipyridine with 1,2-bis(4-pyridyl)ethylene (BPE), to give the title salt, (I).



(I)

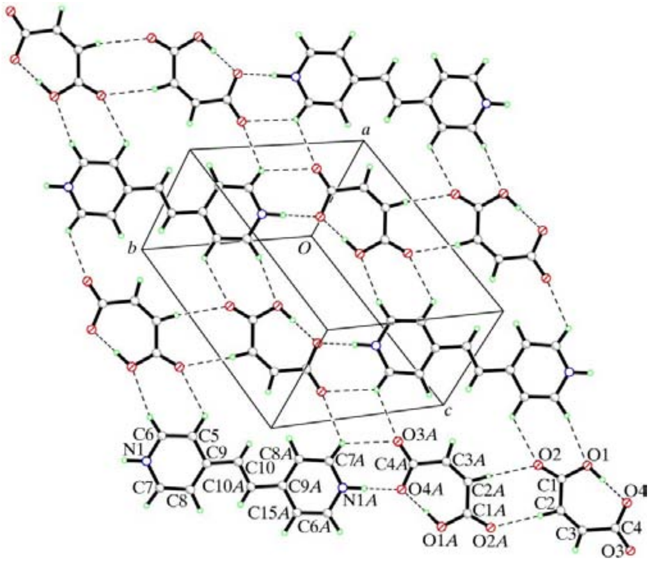


Figure 1
A packing diagram for (I).

Compound (I) forms a planar two-dimensional hydrogen-bonded network structure, but the 1:2 molar ratio between the constituents is still maintained (Fig. 2). An important feature of this complex structure is that H-atom transfer from MA to BPE results in the formation of an ionic $N^+—H\cdots O^-$ hydrogen bond. Both BPE and MA are individually planar, but with a dihedral angle of 12.1 (5)° between them.

A typical molecular arrangement in each sheet of (I) is shown in Fig. 1 and the hydrogen bonds are listed in Table 1. In each sheet, there are hydrogen bonds between BPE and MA, as well as between adjacent MA molecules, forming linear chains. While BPE and MA interact with each other *via* $N^+—H\cdots O^-$ hydrogen bonds [$H\cdots O$ = 1.70 (5) Å], adjacent MA molecules interact through $C—H\cdots O$ hydrogen bonds [$H\cdots O$ = 2.55 (4) Å]. In addition, adjacent chains are held together by $C—H\cdots O$ [$H\cdots O$ = 2.50 (3) and 2.60 (4) Å] hydrogen bonds.

Examination of the structure of (I) with *PLATON* (Spek, 1990) showed that there were no solvent-accessible voids in the crystal lattice.

Experimental

BPE was prepared following the procedure described by Yam *et al.* (1998). MA and other reagents were obtained from commercial suppliers and used without further purification. BPE and MA (in a 1:2 molar ratio) were mixed in an 8:3 (*v*/*v*) solution of acetone

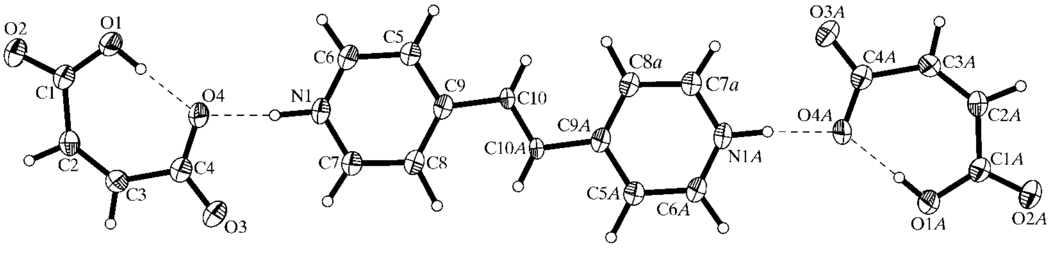


Figure 2
A view of the structure of (I), showing the atom-numbering scheme and 35% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

and ethanol, and heated until they dissolved completely. The resulting solution was evaporated slowly at room temperature for 3 d. After most of the solvent had evaporated, red crystals of (I) were obtained.

Crystal data

$C_{12}H_{12}N_2^{2+}\cdot 2C_4H_3O_4^-$
$M_r = 414.36$
Triclinic, $P\overline{1}$
$a = 5.7148$ (9) Å
$b = 8.6568$ (8) Å
$c = 10.6906$ (11) Å
$\alpha = 108.623$ (9)°
$\beta = 99.878$ (15)°
$\gamma = 105.561$ (13)°
$V = 463.26$ (10) $Å^3$

$Z = 1$
$D_x = 1.485$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 2.1$–25.0°
$\mu = 0.12$ mm^{-1}
$T = 293$ (2) K
Block, red
0.60 × 0.32 × 0.22 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: empirical (*SHELXTL*; Bruker, 1997)
$T_{min} = 0.931$, $T_{max} = 0.975$
2127 measured reflections
1600 independent reflections
1104 reflections with $I > 2\sigma(I)$

$R_{int} = 0.023$
$\theta_{max} = 25°$
$h = -1 \rightarrow 6$
$k = -9 \rightarrow 9$
$l = -12 \rightarrow 12$
3 standard reflections every 97 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.066$
$wR(F^2) = 0.188$
$S = 1.05$
1600 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0975P)^2 + 0.2216P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.72$ e $Å^{-3}$
$\Delta\rho_{min} = -0.42$ e $Å^{-3}$

With one exception, all H-atom positions were found from the difference Fourier map and all their parameters were freely refined. The exception was the single H atom bonded to atom C10, which was treated using a riding model, with a C—H distance of 0.93 Å and an isotropic displacement parameter of 0.08 $Å^2$. The highest peak was located 0.64 Å from atom C10 and the deepest hole 0.27 Å from atom H10.

Data collection: *P4 Diffractometer Control Program* (Siemens, 1994); cell refinement: *P4 Diffractometer Control Program* and *XSCANS* (Siemens, 1994); data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Table 1
Hydrogen-bonding and short-contact geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O3^{i}	0.98 (4)	2.55 (4)	3.174 (5)	122 (3)
C8—H8A···O3^{i}	1.04 (5)	2.59 (5)	3.234 (5)	120 (3)
C2—H2A···O2^{ii}	0.95 (4)	2.55 (4)	3.412 (5)	152 (3)
C6—H6A···O1^{iii}	1.00 (4)	2.43 (4)	3.404 (5)	166 (3)
C6—H6A···O2^{iii}	1.00 (4)	2.60 (4)	3.179 (5)	117 (3)
C5—H5A···O2^{iii}	1.06 (4)	2.50 (3)	3.169 (5)	120 (2)
N1—H1A···O4	0.97 (5)	1.70 (5)	2.673 (4)	179 (4)
N1—H1A···O3	0.97 (5)	2.61 (5)	3.245 (4)	123 (4)
O1—H···O4	0.94 (5)	1.53 (5)	2.475 (4)	180 (5)
C7—H7A···O3	0.98 (4)	2.52 (4)	3.218 (5)	128 (3)

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

The authors gratefully acknowledge financial support from the National Natural Science Foundation of China (grant No. 29992590-5) and the Major State Basic Research Development Programme (grant No. G2000078102).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1187). Services for accessing these data are described at the back of the journal.

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