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2-Carboxypyridinium maleate

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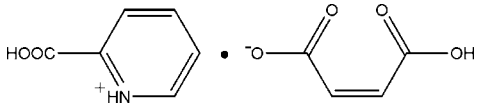
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.071; wR factor = 0.199; data-to-parameter ratio = 16.5.

In the title molecular salt, $C_6H_6NO_2^+\cdot C_4H_3O_4^-$, the 2-carboxypyridinium cation is essentially planar with a maximum deviation of 0.003 (3) Å. In the crystal, adjacent cations and anions are linked by an extensive system of weak N—H···O, O—H···O and C—H···O interactions, forming a layer parallel to the *ab* plane.

Related literature

For details of pyridine and its derivatives, see: Banerjee & Murugavel (2004); Bis *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_6H_6NO_2\cdot C_4H_3O_4$
M_r = 239.18
Monoclinic, $P2_1/c$
a = 14.6498 (9) Å
b = 10.3976 (8) Å
c = 6.9067 (5) Å
β = 100.089 (3)°
V = 1035.78 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 295 K
0.24 × 0.20 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.970, T_{max} = 0.980
9722 measured reflections
2557 independent reflections
2092 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.199
S = 1.10
2557 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	2.28	2.639 (3)	105
O5—H5A···O4	0.82	1.73	2.540 (3)	168
N1—H1···O1^{i}	0.86	2.02	2.725 (3)	139
O2—H2A···O3^{ii}	0.82	1.71	2.463 (3)	152
C2—H2···O2^{iii}	0.93	2.54	3.462 (4)	170
C3—H3···O6^{iv}	0.93	2.59	3.221 (4)	125
C5—H5···O4^{v}	0.93	2.40	3.251 (4)	152
C8—H8···O6^{vi}	0.93	2.40	3.285 (4)	158

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2380).

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2-Carboxypyridinium maleate

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S1. Comment

Pyridine and its derivatives are some of the most frequently used synthons in supramolecular chemistry based on hydrogen bonds (Banerjee & Murugavel, 2004; Bis *et al.*, 2006). We herewith report the molecular and crystal structures of the title compound, **I**, which belongs to this class of compounds.

The asymmetric unit of **I**, (Fig. 1), contains a 2–carboxypyridinium cation and a malonate anion. The bond lengths (Allen *et al.*, 1987) and angles are within the normal range. The crystal structure exhibit weak intermolecular N—H···O, O—H···O and C—H···O (Table 1 & Fig. 2) interactions.

S2. Experimental

A solution of picolinic acid (0.123 g, 1 mmol) in 10 ml ethanol was added with stirring to a solution of maleic acid (0.116 g, 1 mmol) in 10 ml of distilled water at 303 K. After some time, white precipitate was obtained, which was dissolved in ethanol and colourless block–shaped single crystals were obtained by slow evaporation of the ethanol solution.

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H, N—H = 0.86Å and U_{iso}(H) = 1.2U_{eq}(N) for amine H and O—H = 0.82Å and U_{iso}(H) = 1.5U_{eq}(O) for hydroxyl H.

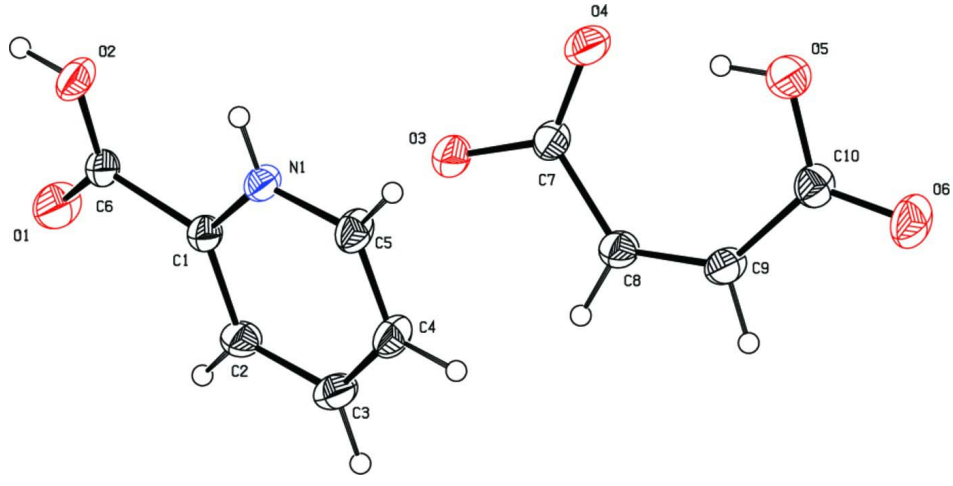

Figure 1

The molecular structure of title compound with atom labels. Displacement ellipsoids are drawn at 30% probability level. H atoms are presented as asmall spheres of arbitrary radius.

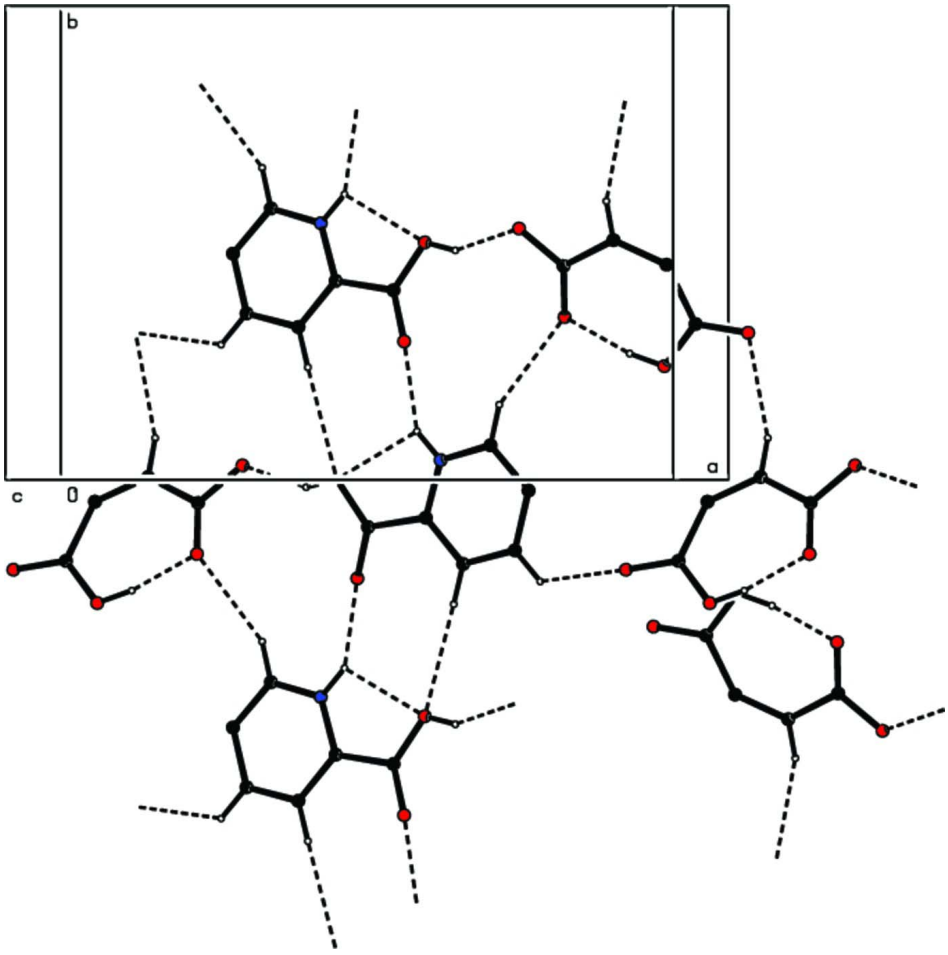

Figure 2

The packing of **I**, viewed down *c* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

2-Carboxypyridinium maleate

Crystal data

$C_6H_6NO_2{\cdot}C_4H_3O_4$
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Monoclinic, $P2_1/c$
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$c = 6.9067\ (5)$ Å
$\beta = 100.089\ (3)°$
$V = 1035.78\ (13)$ Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.534$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4245 reflections
$\theta = 2.4–28.3°$
$\mu = 0.13$ mm^{-1}
$T = 295$ K
Block, colourless
0.24 × 0.20 × 0.16 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω– and φ–scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.970$, $T_{max} = 0.980$

9722 measured reflections
2557 independent reflections
2092 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 28.3°$, $\theta_{min} = 1.4°$
$h = -19 \rightarrow 18$
$k = -13 \rightarrow 13$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.199$
$S = 1.10$
2557 reflections
155 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
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 1.8972P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.015 (3)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.57261 (18)	−0.0804 (3)	0.3125 (4)	0.0320 (6)
C2	0.6336 (2)	−0.1778 (3)	0.3751 (5)	0.0389 (7)
H2	0.6170	−0.2628	0.3454	0.047*
C3	0.7201 (2)	−0.1492 (3)	0.4825 (5)	0.0438 (7)
H3	0.7618	−0.2149	0.5261	0.053*
C4	0.7440 (2)	−0.0230 (3)	0.5246 (5)	0.0412 (7)
H4	0.8020	−0.0027	0.5963	0.049*
C5	0.6817 (2)	0.0725 (3)	0.4599 (5)	0.0401 (7)
H5	0.6971	0.1582	0.4869	0.048*
N1	0.59856 (15)	0.0413 (2)	0.3575 (4)	0.0342 (5)
H1	0.5599	0.1021	0.3187	0.041*
C6	0.47635 (19)	−0.1001 (3)	0.1946 (4)	0.0346 (6)
C7	0.79780 (19)	0.0490 (3)	0.0421 (4)	0.0354 (6)
C8	0.8827 (2)	−0.0055 (3)	0.1646 (5)	0.0373 (6)
H8	0.8762	−0.0878	0.2130	0.045*
C9	0.9664 (2)	0.0462 (3)	0.2149 (5)	0.0388 (7)
H9	1.0084	−0.0061	0.2955	0.047*
C10	1.0058 (2)	0.1714 (3)	0.1674 (5)	0.0401 (7)
O1	0.45516 (17)	−0.2082 (2)	0.1321 (4)	0.0566 (7)
O2	0.42766 (14)	0.0007 (2)	0.1721 (4)	0.0453 (6)
H2A	0.3766	−0.0161	0.1075	0.068*
O3	0.72935 (14)	−0.0300 (2)	0.0195 (4)	0.0446 (6)
O4	0.79341 (16)	0.1568 (2)	−0.0311 (4)	0.0601 (8)
O5	0.95136 (17)	0.2604 (2)	0.0741 (4)	0.0559 (7)
H5A	0.8978	0.2340	0.0523	0.084*
O6	1.08852 (16)	0.1899 (3)	0.2139 (4)	0.0580 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0282 (13)	0.0299 (13)	0.0366 (14)	−0.0020 (10)	0.0024 (10)	0.0014 (11)
C2	0.0389 (15)	0.0262 (13)	0.0493 (17)	0.0000 (11)	0.0014 (13)	0.0055 (12)
C3	0.0374 (15)	0.0392 (16)	0.0514 (18)	0.0078 (13)	−0.0014 (13)	0.0081 (14)
C4	0.0284 (13)	0.0471 (17)	0.0440 (17)	−0.0014 (12)	−0.0051 (12)	−0.0031 (13)
C5	0.0310 (14)	0.0349 (15)	0.0518 (18)	−0.0029 (11)	0.0001 (12)	−0.0068 (13)
N1	0.0270 (11)	0.0274 (11)	0.0458 (14)	0.0014 (9)	−0.0005 (10)	0.0004 (10)
C6	0.0270 (13)	0.0327 (14)	0.0417 (15)	−0.0060 (10)	−0.0003 (11)	0.0041 (11)
C7	0.0295 (13)	0.0331 (14)	0.0426 (15)	0.0006 (11)	0.0031 (11)	−0.0015 (12)
C8	0.0358 (14)	0.0296 (13)	0.0451 (16)	0.0011 (11)	0.0029 (12)	0.0029 (12)
C9	0.0352 (14)	0.0320 (14)	0.0452 (17)	0.0020 (11)	−0.0041 (12)	0.0017 (12)
C10	0.0378 (15)	0.0350 (15)	0.0459 (17)	−0.0054 (12)	0.0024 (13)	−0.0057 (13)
O1	0.0479 (13)	0.0352 (12)	0.0781 (18)	−0.0090 (10)	−0.0125 (12)	−0.0019 (12)
O2	0.0261 (10)	0.0393 (12)	0.0648 (15)	−0.0008 (9)	−0.0079 (9)	−0.0009 (10)
O3	0.0323 (10)	0.0425 (12)	0.0555 (14)	−0.0055 (9)	−0.0018 (9)	0.0043 (10)
O4	0.0395 (12)	0.0409 (13)	0.092 (2)	−0.0009 (10)	−0.0120 (12)	0.0193 (13)
O5	0.0458 (13)	0.0373 (12)	0.0786 (18)	−0.0083 (10)	−0.0054 (12)	0.0109 (12)
O6	0.0378 (12)	0.0526 (15)	0.0787 (19)	−0.0125 (11)	−0.0037 (12)	−0.0083 (13)

Geometric parameters (Å, º)

C1—N1	1.342 (4)	C6—O2	1.261 (3)
C1—C2	1.370 (4)	C7—O4	1.227 (4)
C1—C6	1.514 (4)	C7—O3	1.284 (3)
C2—C3	1.384 (4)	C7—C8	1.488 (4)
C2—H2	0.9300	C8—C9	1.328 (4)
C3—C4	1.376 (5)	C8—H8	0.9300
C3—H3	0.9300	C9—C10	1.484 (4)
C4—C5	1.369 (4)	C9—H9	0.9300
C4—H4	0.9300	C10—O6	1.213 (4)
C5—N1	1.336 (4)	C10—O5	1.315 (4)
C5—H5	0.9300	O2—H2A	0.8200
N1—H1	0.8600	O5—H5A	0.8200
C6—O1	1.224 (4)		
N1—C1—C2	118.8 (2)	O1—C6—O2	128.0 (3)
N1—C1—C6	116.8 (2)	O1—C6—C1	117.9 (3)
C2—C1—C6	124.4 (3)	O2—C6—C1	114.0 (2)
C1—C2—C3	119.7 (3)	O4—C7—O3	123.4 (3)
C1—C2—H2	120.1	O4—C7—C8	124.1 (3)
C3—C2—H2	120.1	O3—C7—C8	112.5 (3)
C4—C3—C2	119.5 (3)	C9—C8—C7	129.5 (3)
C4—C3—H3	120.2	C9—C8—H8	115.2
C2—C3—H3	120.2	C7—C8—H8	115.2
C5—C4—C3	119.5 (3)	C8—C9—C10	132.4 (3)
C5—C4—H4	120.3	C8—C9—H9	113.8

C3—C4—H4	120.3	C10—C9—H9	113.8
N1—C5—C4	119.4 (3)	O6—C10—O5	120.7 (3)
N1—C5—H5	120.3	O6—C10—C9	119.4 (3)
C4—C5—H5	120.3	O5—C10—C9	120.0 (3)
C5—N1—C1	123.1 (2)	C6—O2—H2A	109.5
C5—N1—H1	118.5	C10—O5—H5A	109.5
C1—N1—H1	118.5		
N1—C1—C2—C3	0.0 (5)	C2—C1—C6—O1	−8.5 (5)
C6—C1—C2—C3	−179.9 (3)	N1—C1—C6—O2	−7.8 (4)
C1—C2—C3—C4	−0.3 (5)	C2—C1—C6—O2	172.1 (3)
C2—C3—C4—C5	0.2 (5)	O4—C7—C8—C9	−1.2 (6)
C3—C4—C5—N1	0.2 (5)	O3—C7—C8—C9	178.2 (3)
C4—C5—N1—C1	−0.6 (5)	C7—C8—C9—C10	−1.2 (6)
C2—C1—N1—C5	0.5 (5)	C8—C9—C10—O6	−171.4 (4)
C6—C1—N1—C5	−179.7 (3)	C8—C9—C10—O5	8.0 (6)
N1—C1—C6—O1	171.6 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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O5—H5*A*···O4	0.82	1.73	2.540 (3)	168
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