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Ethylenediaminium dinicotinate

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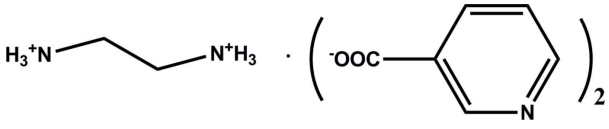
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.062; wR factor = 0.147; data-to-parameter ratio = 16.0.

In the title compound, $C_2H_{10}N_2^{2+}\cdot 2C_6H_4NO_2^-$, the cation lies on an inversion centre. The asymmetric unit is composed of one nicotinate anion and one half ethylenediaminium cation. All the amino H atoms are involved in N—H···O and N—H···N hydrogen bonds. These hydrogen bonds link the ionic units into a three-dimensional network. In addition, π–π interactions between pyridine rings [centroid–centroid distance = 3.6037 (7) Å] further stabilize the crystal structure.

Related literature

For applications of amino compounds, see: Fu *et al.* (2010); Aminabhavi *et al.* (1986).



Experimental

Crystal data

$C_2H_{10}N_2^{2+}\cdot 2C_6H_4NO_2^-$
M_r = 306.32
Monoclinic, $P2_1/c$
a = 6.2953 (13) Å
b = 16.835 (3) Å
c = 6.8288 (14) Å
β = 102.03 (3)°
V = 707.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.30 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
7181 measured reflections
1618 independent reflections
1162 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.147
S = 1.08
1618 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 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
N1—H1B···N2^{i}	0.90	2.24	2.971 (3)	138
N1—H1C···O1^{ii}	0.90	1.85	2.729 (3)	164
N1—H1A···O2	0.90	1.83	2.711 (3)	166

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: BX2355).

References

Aminabhavi, T. M., Biradar, N. S. & Patil, S. B. (1986). *Inorg. Chim. Acta*, **125**, 125–128.
Fu, D.-W., Dai, J., Ge, J.-Z., Ye, H.-Y. & Qu, Z.-R. (2010). *Inorg. Chem. Commun.* **13**, 282-285.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o1789 [doi:10.1107/S1600536811023877]

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S1. Comment

The amino derivatives have found wide range of applications in material science, such as magnetic, fluorescent and dielectric behaviors, and there has been an increased interest motif in the preparation of amino cocrystal compounds (Aminabhavi *et al.,* 1986; Fu, *et al.* 2010). We report here the crystal structure of the title compound. In the title compound, $[(C_2H_{10}N_2)(C_6H_4NO_2)_2]$, the cation lies on inversion centre. The asymmetric unit is composed of one nicotinate anion and one-half ethylenediaminium cation, (Fig.1). Both the amine N atoms of the ethylenediaminium cation are protonated. The geometric parameters are in the normal range. In the crystal structure, all the amino group H atoms are involved in N—H···O and N—H···N hydrogen bonds (Table1). These hydrogen bonds link the ionic units into a three-dimentional network. In addition, the pyridine rings π–π (centroid-to-centroid distance = 3.6037 (7) Å, symmetry code: x, 1/2-y, 1/2+z) interactions further stabilized the structure (Fig. 2).

S2. Experimental

A mixture of ethylenediamine (0.4 mmol) and nicotinic acid (0.8 mmol) were dissolved in distilled water (10 ml). Colorless block crystals suitable for X-ray analysis were obtained after 3 days.

S3. Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C— H = 0.97 Å(methylene) and C — H = 0.93 Å(aromatic) with U_{iso}(H) = 1.2U_{eq}(C). The positional parameters of the H atoms (N1) were refined freely, in the last stage of the refinement, it were restrained with the H—N = 0.90 (2) Å, with U_{iso}(H) = 1.5U_{eq}(N).

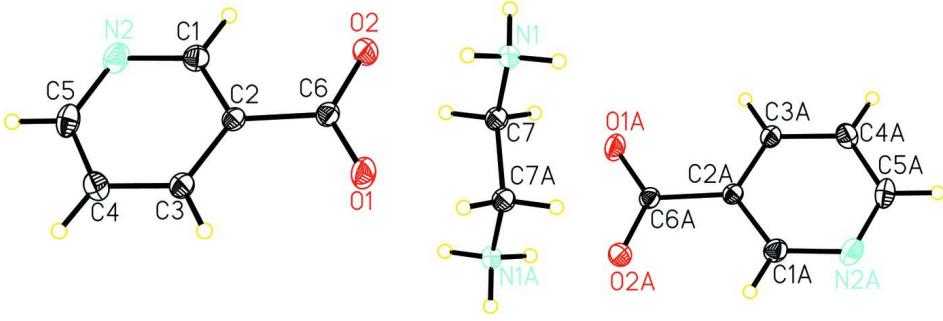

Figure 1

Molecular view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

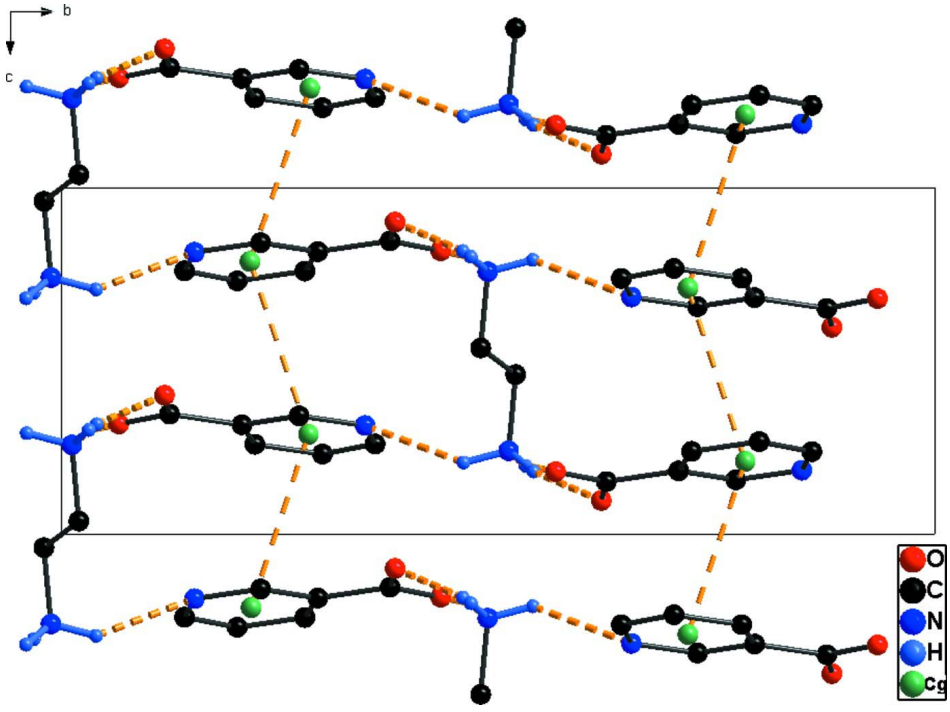

Figure 2

The crystal packing of the title compound viewed along the *c* axis showing the one-dimensionnal hydrogen bondings chain (dashed line). Hydrogen atoms not involved in hydrogen bonding have been omitted for clarity.

Ethylenediaminium dinicotinate

Crystal data

$C_2H_{10}N_2^{2+}\cdot 2C_6H_4NO_2^-$
$M_r = 306.32$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.2953\ (13)$ Å
$b = 16.835\ (3)$ Å
$c = 6.8288\ (14)$ Å
$\beta = 102.03\ (3)°$
$V = 707.8\ (3)$ Å^3
$Z = 2$
$F(000) = 324$
$D_x = 1.437$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1618 reflections
$\theta = 3.3–27.5°$
$\mu = 0.11$ mm^{-1}
$T = 298$ K
Block, colourless
0.30 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.910$, $T_{max} = 1.000$
7181 measured reflections
1618 independent reflections
1162 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -7\rightarrow 8$
$k = -21\rightarrow 21$
$l = -8\rightarrow 8$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.147$
$S = 1.08$
1618 reflections
101 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
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.4625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.032 (6)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.0882 (3)	0.56578 (10)	0.8189 (3)	0.0407 (5)
O2	0.4172 (3)	0.61799 (10)	0.9019 (3)	0.0415 (5)
C2	0.1214 (3)	0.70652 (13)	0.8166 (3)	0.0226 (5)
N1	0.6707 (3)	0.51198 (11)	0.7583 (3)	0.0284 (5)
H1A	0.5813	0.5405	0.8182	0.043*
H1B	0.6812	0.4603	0.7926	0.043*
H1C	0.8057	0.5313	0.8016	0.043*
N2	0.1923 (3)	0.84765 (12)	0.8146 (3)	0.0366 (5)
C3	−0.0997 (4)	0.72136 (13)	0.7603 (4)	0.0284 (5)
H3A	−0.1982	0.6795	0.7416	0.034*
C5	−0.0222 (4)	0.85903 (14)	0.7611 (4)	0.0346 (6)
H5A	−0.0727	0.9110	0.7423	0.042*
C1	0.2585 (4)	0.77203 (14)	0.8423 (4)	0.0308 (6)
H1D	0.4069	0.7628	0.8816	0.037*
C6	0.2143 (3)	0.62372 (13)	0.8475 (3)	0.0248 (5)
C7	0.6080 (4)	0.52001 (14)	0.5385 (3)	0.0278 (5)
H7B	0.7182	0.4959	0.4773	0.033*
H7A	0.5977	0.5758	0.5025	0.033*
C4	−0.1726 (4)	0.79878 (14)	0.7320 (4)	0.0326 (6)
H4A	−0.3202	0.8098	0.6942	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0329 (10)	0.0209 (9)	0.0674 (13)	−0.0021 (7)	0.0086 (9)	−0.0007 (8)
O2	0.0237 (9)	0.0340 (10)	0.0633 (13)	0.0046 (7)	0.0006 (8)	−0.0115 (9)
C2	0.0247 (11)	0.0225 (11)	0.0210 (11)	−0.0010 (9)	0.0058 (9)	−0.0012 (9)
N1	0.0268 (10)	0.0222 (10)	0.0342 (11)	0.0025 (8)	0.0016 (8)	−0.0010 (8)
N2	0.0402 (12)	0.0247 (11)	0.0466 (13)	−0.0054 (9)	0.0128 (10)	−0.0029 (9)
C3	0.0278 (12)	0.0223 (12)	0.0346 (13)	−0.0024 (9)	0.0050 (10)	−0.0004 (10)
C5	0.0485 (15)	0.0214 (13)	0.0370 (14)	0.0037 (11)	0.0158 (12)	0.0031 (10)
C1	0.0262 (12)	0.0286 (13)	0.0383 (14)	−0.0031 (10)	0.0081 (10)	−0.0022 (10)
C6	0.0257 (12)	0.0234 (12)	0.0253 (12)	0.0000 (9)	0.0057 (9)	−0.0028 (9)
C7	0.0266 (12)	0.0236 (12)	0.0326 (13)	−0.0029 (9)	0.0048 (10)	0.0022 (10)
C4	0.0299 (13)	0.0308 (13)	0.0370 (14)	0.0047 (10)	0.0069 (11)	0.0044 (11)

Geometric parameters (Å, º)

O1—C6	1.247 (3)	N2—C1	1.341 (3)
O2—C6	1.257 (3)	C3—C4	1.382 (3)
C2—C3	1.387 (3)	C3—H3A	0.9300
C2—C1	1.389 (3)	C5—C4	1.373 (3)
C2—C6	1.509 (3)	C5—H5A	0.9300
N1—C7	1.476 (3)	C1—H1D	0.9300
N1—H1A	0.9005	C7—C7^{i}	1.510 (4)
N1—H1B	0.9004	C7—H7B	0.9700
N1—H1C	0.9004	C7—H7A	0.9700
N2—C5	1.337 (3)	C4—H4A	0.9300
C3—C2—C1	116.9 (2)	N2—C1—C2	124.7 (2)
C3—C2—C6	122.82 (19)	N2—C1—H1D	117.6
C1—C2—C6	120.2 (2)	C2—C1—H1D	117.6
C7—N1—H1A	110.7	O1—C6—O2	124.1 (2)
C7—N1—H1B	110.0	O1—C6—C2	119.0 (2)
H1A—N1—H1B	114.6	O2—C6—C2	116.87 (19)
C7—N1—H1C	109.6	N1—C7—C7^{i}	110.1 (2)
H1A—N1—H1C	107.1	N1—C7—H7B	109.6
H1B—N1—H1C	104.5	C7^{i}—C7—H7B	109.6
C5—N2—C1	116.2 (2)	N1—C7—H7A	109.6
C4—C3—C2	119.6 (2)	C7^{i}—C7—H7A	109.6
C4—C3—H3A	120.2	H7B—C7—H7A	108.2
C2—C3—H3A	120.2	C5—C4—C3	118.5 (2)
N2—C5—C4	124.1 (2)	C5—C4—H4A	120.7
N2—C5—H5A	118.0	C3—C4—H4A	120.7
C4—C5—H5A	118.0		
C1—C2—C3—C4	0.2 (3)	C3—C2—C6—O1	1.0 (3)
C6—C2—C3—C4	−179.1 (2)	C1—C2—C6—O1	−178.3 (2)
C1—N2—C5—C4	−0.7 (4)	C3—C2—C6—O2	−178.8 (2)

C5—N2—C1—C2	1.0 (4)	C1—C2—C6—O2	1.9 (3)
C3—C2—C1—N2	−0.7 (4)	N2—C5—C4—C3	0.3 (4)
C6—C2—C1—N2	178.6 (2)	C2—C3—C4—C5	0.0 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···N2^{ii}	0.90	2.24	2.971 (3)	138
N1—H1*C*···O1^{iii}	0.90	1.85	2.729 (3)	164
N1—H1*A*···O2	0.90	1.83	2.711 (3)	166

Symmetry codes: (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*+1, *y*, *z*.