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Piperazine-1,4-diium pyridine-2,3-dicarboxylate methanol monosolvate[1]

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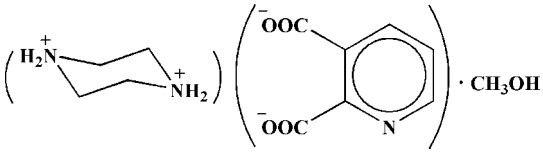
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.034; wR factor = 0.085; data-to-parameter ratio = 19.7.

The title solvated molecular salt, $C_4H_{12}N_2^{2+}\cdot C_7H_3NO_4^{2-}\cdot CH_3OH$ or $(pipzH_2)(py\text{-}2,3\text{-}dc)\cdot MeOH$, was prepared by the reaction of pyridine-2,3-dicarboxylic acid (py-2,3-dcH_2) and piperazine (pipz) in methanol (MeOH) as solvent. One of the two carboxylate groups of the acid fragment is nearly perpendicular to the pyridine ring and the other is almost in its plane [C—C—C—O torsion angles = −85.50 (11) and 88.07 (11)° and N—C—C—O torsion angles = −176.31 (8) and 5.41 (13)°]. In the crystal, the components are linked by O—H···O, N—H···O and C—H···O hydrogen bonds, generating a three-dimensional network.

Related literature

For similar ion pairs, see: Aghabozorg, Manteghi & Ghadermazi (2008); Aghabozorg, Manteghi & Sheshmani (2008). For related metal complexes, see: Barszcz *et al.* (2010); Li & Li (2004).



Experimental

Crystal data

$C_4H_{12}N_2^{2+}\cdot C_7H_3NO_4^{2-}\cdot CH_4O$
M_r = 285.30
Monoclinic, $P2_1/n$
a = 8.2541 (6) Å
b = 11.8988 (8) Å
c = 13.8197 (9) Å
β = 90.288 (2)°
V = 1357.27 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEXII diffractometer
16044 measured reflections
3579 independent reflections
3189 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.085
S = 1.03
3579 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 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
N2—H2A···O4^{i}	0.90	1.74	2.6257 (11)	168
N2—H2B···O2	0.90	1.89	2.7274 (11)	155
N3—H3A···O1^{ii}	0.90	1.85	2.7379 (11)	169
N3—H3B···O3^{iii}	0.90	1.86	2.7393 (11)	166
O5—H5A···O1	0.85	1.84	2.6867 (10)	171
C3—H3···O5^{iv}	0.95	2.41	3.3163 (13)	159

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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) and *Mercury* (Macrae *et al.*, 2008); 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: OM2416).

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[1] In memory of our great professor, Dr Hossein Aghabozorg, who passed away recently.