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Morpholin-4-ium hydrogen tartrate

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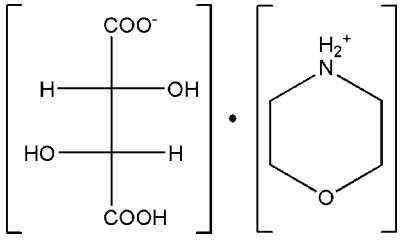
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.097; data-to-parameter ratio = 13.0.

In the title molecular salt, $C_4H_{10}NO^+\cdot C_4H_5O_6^-$, the morpholinium cation adopts a chair conformation. The conformation of the C—C—C—C backbone of the monotartrate anion is close to *anti* [torsion angle = 173.18 (17)°], which is supported by two intramolecular O—H···O hydrogen bonds. In the crystal, the components are linked by N—H—O and O—H—O hydrogen bonds, generating (001) sheets.

Related literature

For a related structure, see: Ruble *et al.* (1976).



Experimental

Crystal data

$C_4H_{10}NO^+\cdot C_4H_5O_6^-$
M_r = 237.21
Orthorhombic, $P2_12_12_1$
a = 7.2601 (15) Å
b = 9.1716 (18) Å
c = 16.283 (3) Å
V = 1084.2 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 293 K
0.36 × 0.32 × 0.28 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.954, T_{max} = 0.966
8960 measured reflections
1903 independent reflections
1747 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.097
S = 1.17
1903 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.90	2.05	2.918 (3)	162
N1—H1B···O2^{ii}	0.90	1.95	2.790 (3)	154
O1—H1···O2	0.82	2.09	2.600 (2)	120
O1—H1···O4^{iii}	0.82	2.40	3.068 (2)	139
O5—H5···O3^{iv}	0.82	1.73	2.529 (2)	165
O6—H6···O4	0.82	2.20	2.674 (2)	117
O6—H6···O1^{v}	0.82	2.24	2.996 (2)	153

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

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*.

The author thanks an anonymous advisor from the Ordered Matter Science Research Centre, Southeast University, for great help in the revision of this paper.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6576).

References

Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Ruble, J. R., Hite, G. & Soares, J. R. (1976). *Acta Cryst.* B**32**, 136–140.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o289 [doi:10.1107/S1600536811055759]

Morpholin-4-ium hydrogen tartrate

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S1. Experimental

0.87 g (0.01 mol) of morpholine was firstly dissolved in 30 ml of ethanol, to which 1.50 g (0.01 mol) of tartaric acid was added at ambient temperature. Colourless blocks were obtained by the slow evaporation of the above solution after 3 days in air.

The dielectric constant of the compound as a function of temperature indicates that the permittivity is basically temperature-independent ($\varepsilon = C/(T–T_0)$), suggesting that this compound is not ferroelectric or there may be no distinct phase transition occurring within the measured temperature (below the melting point).

S2. Refinement

The absolute structure is indeterminate based on the present model. H atoms were placed in calculated positions (N—H = 0.89 Å; C—H = 0.93Å for C*sp*^{2} atoms and C—H = 0.96Å and 0.97Å for C*sp*^{3} atoms), assigned fixed U_{iso} values [U_{iso} = 1.2*U*eq(C*sp*^{2}) and 1.5*U*eq(C*sp*^{3},*N*)] and allowed to ride.

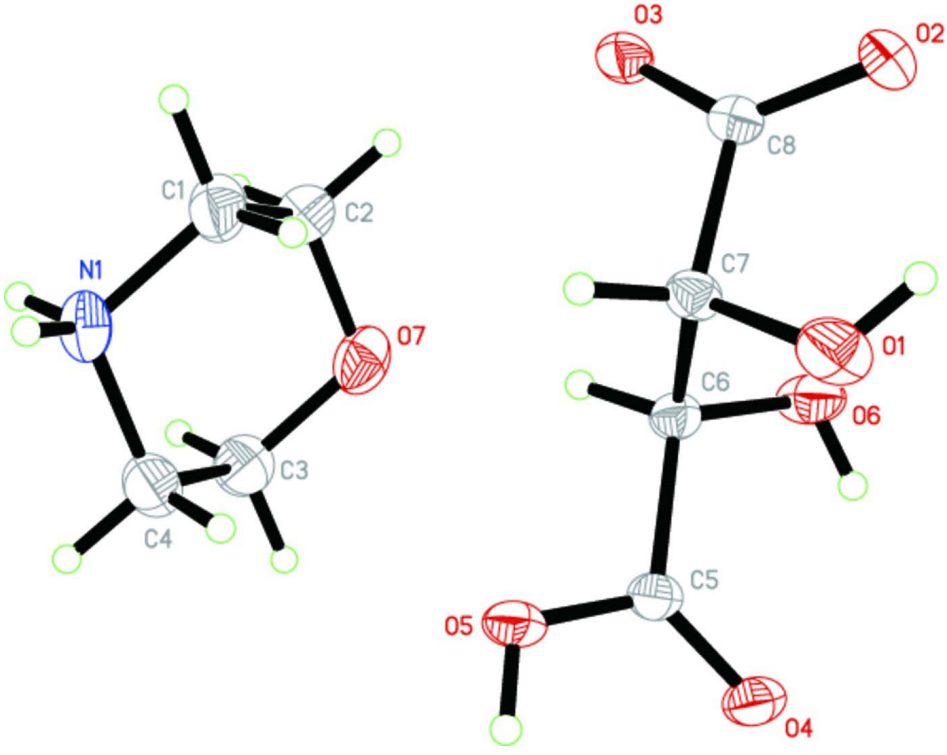

Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

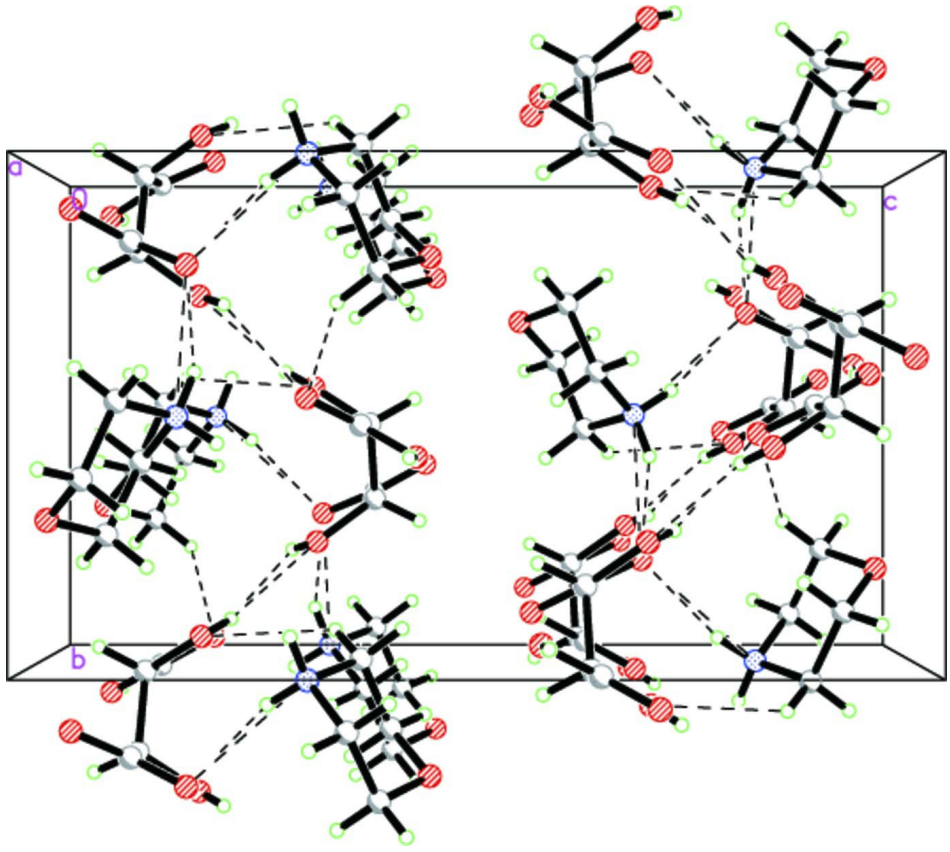

Figure 2

Crystal structure of the title compound with view along the *b* axis. Intermolecular interactions are shown as dashed lines.

Morpholin-4-ium hydrogen tartrate

Crystal data

$C_4H_{10}NO^+·C_4H_5O_6^-$
M_r = 237.21
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 7.2601 (15) Å
b = 9.1716 (18) Å
c = 16.283 (3) Å
V = 1084.2 (4) Å^3
Z = 4

$F(000)$ = 504
D_x = 1.453 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1903 reflections
θ = 3.4–26.4°
μ = 0.13 mm^{-1}
T = 293 K
Block, colourless
0.36 × 0.32 × 0.28 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans

Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.954, T_{max} = 0.966
8960 measured reflections
1903 independent reflections
1747 reflections with I > \2s(I)

R_{int} = 0.060
θ_{max} = 25°, θ_{min} = 3.1°
h = −8→8
k = −10→10
l = −19→19
3 standard reflections every 180 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.097
S = 1.17
1903 reflections
146 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
$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2 + 0.0989P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.095
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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}
O7	0.3787 (3)	0.3058 (2)	0.55071 (10)	0.0542 (5)
N1	0.4758 (3)	0.4978 (2)	0.68097 (11)	0.0426 (5)
H1A	0.4382	0.4480	0.7256	0.051*
H1B	0.5249	0.5827	0.6979	0.051*
C1	0.3161 (4)	0.5269 (3)	0.62661 (15)	0.0510 (7)
H1C	0.3541	0.5882	0.5811	0.061*
H1D	0.2210	0.5780	0.6570	0.061*
C2	0.2413 (4)	0.3847 (3)	0.59447 (15)	0.0508 (7)
H2A	0.1973	0.3262	0.6400	0.061*
H2B	0.1378	0.4039	0.5584	0.061*
C3	0.5307 (4)	0.2735 (3)	0.60333 (15)	0.0519 (7)
H3A	0.6219	0.2178	0.5731	0.062*
H3B	0.4885	0.2143	0.6490	0.062*
C4	0.6178 (4)	0.4113 (3)	0.63583 (16)	0.0504 (7)
H4A	0.7186	0.3871	0.6725	0.060*
H4B	0.6668	0.4684	0.5907	0.060*
O1	0.4383 (2)	0.75847 (19)	0.31549 (10)	0.0494 (5)
H1	0.3531	0.7781	0.2843	0.074*
O2	0.08530 (19)	0.71085 (17)	0.31349 (8)	0.0358 (4)
O3	0.08075 (18)	0.60421 (18)	0.43779 (9)	0.0394 (4)
O4	0.73405 (19)	0.46475 (19)	0.31136 (9)	0.0418 (4)

O5	0.73379 (19)	0.58152 (19)	0.43315 (9)	0.0410 (4)
H5	0.8459	0.5815	0.4269	0.062*
O6	0.3670 (2)	0.44104 (19)	0.31002 (10)	0.0474 (5)
H6	0.4483	0.4105	0.2796	0.071*
C5	0.6557 (3)	0.5186 (2)	0.36993 (13)	0.0312 (5)
C6	0.4477 (3)	0.5161 (3)	0.37717 (12)	0.0304 (5)
H6A	0.4145	0.4652	0.4280	0.036*
C7	0.3714 (3)	0.6722 (2)	0.38132 (13)	0.0304 (5)
H7	0.4082	0.7168	0.4335	0.036*
C8	0.1603 (3)	0.6624 (2)	0.37789 (13)	0.0284 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O7	0.0728 (12)	0.0500 (12)	0.0397 (9)	0.0035 (11)	−0.0084 (9)	−0.0083 (9)
N1	0.0568 (12)	0.0357 (12)	0.0351 (10)	−0.0088 (10)	0.0062 (9)	−0.0021 (9)
C1	0.0662 (17)	0.0440 (17)	0.0427 (13)	0.0129 (14)	0.0084 (12)	0.0050 (12)
C2	0.0513 (15)	0.0540 (18)	0.0472 (14)	0.0009 (14)	−0.0056 (12)	0.0016 (12)
C3	0.0590 (16)	0.0467 (18)	0.0499 (15)	0.0103 (14)	−0.0012 (13)	−0.0094 (13)
C4	0.0462 (15)	0.0577 (18)	0.0472 (14)	−0.0024 (14)	0.0061 (12)	−0.0044 (13)
O1	0.0317 (8)	0.0551 (12)	0.0614 (11)	−0.0088 (8)	0.0021 (8)	0.0244 (9)
O2	0.0332 (8)	0.0366 (9)	0.0377 (8)	0.0004 (7)	−0.0087 (7)	0.0026 (7)
O3	0.0229 (8)	0.0569 (11)	0.0384 (8)	−0.0009 (7)	0.0019 (7)	0.0068 (8)
O4	0.0298 (8)	0.0526 (11)	0.0429 (9)	0.0040 (8)	0.0065 (7)	−0.0073 (8)
O5	0.0211 (7)	0.0579 (11)	0.0441 (9)	0.0001 (7)	0.0015 (7)	−0.0070 (8)
O6	0.0299 (8)	0.0554 (11)	0.0568 (10)	0.0005 (8)	0.0002 (8)	−0.0227 (9)
C5	0.0257 (10)	0.0330 (13)	0.0349 (11)	0.0021 (10)	0.0013 (9)	0.0033 (10)
C6	0.0255 (10)	0.0337 (13)	0.0318 (11)	−0.0008 (10)	0.0023 (8)	−0.0002 (10)
C7	0.0244 (10)	0.0323 (13)	0.0344 (11)	−0.0025 (10)	−0.0003 (8)	0.0031 (10)
C8	0.0255 (10)	0.0245 (12)	0.0351 (11)	0.0000 (10)	−0.0015 (9)	−0.0034 (10)

Geometric parameters (Å, º)

O7—C2	1.423 (3)	C4—H4B	0.9700
O7—C3	1.428 (3)	O1—C7	1.418 (2)
N1—C1	1.483 (3)	O1—H1	0.8203
N1—C4	1.494 (3)	O2—C8	1.263 (2)
N1—H1A	0.9006	O3—C8	1.253 (2)
N1—H1B	0.8996	O4—C5	1.216 (2)
C1—C2	1.507 (4)	O5—C5	1.309 (2)
C1—H1C	0.9700	O5—H5	0.8200
C1—H1D	0.9700	O6—C6	1.419 (2)
C2—H2A	0.9700	O6—H6	0.8198
C2—H2B	0.9700	C5—C6	1.515 (3)
C3—C4	1.510 (4)	C6—C7	1.536 (3)
C3—H3A	0.9700	C6—H6A	0.9800
C3—H3B	0.9700	C7—C8	1.536 (3)
C4—H4A	0.9700	C7—H7	0.9800

C2—O7—C3	110.29 (17)	N1—C4—H4A	109.9
C1—N1—C4	109.97 (18)	C3—C4—H4A	109.9
C1—N1—H1A	109.6	N1—C4—H4B	109.9
C4—N1—H1A	109.7	C3—C4—H4B	109.9
C1—N1—H1B	109.7	H4A—C4—H4B	108.3
C4—N1—H1B	109.7	C7—O1—H1	109.4
H1A—N1—H1B	108.2	C5—O5—H5	109.4
N1—C1—C2	109.5 (2)	C6—O6—H6	109.5
N1—C1—H1C	109.8	O4—C5—O5	126.37 (18)
C2—C1—H1C	109.8	O4—C5—C6	121.5 (2)
N1—C1—H1D	109.8	O5—C5—C6	112.16 (18)
C2—C1—H1D	109.8	O6—C6—C5	111.03 (17)
H1C—C1—H1D	108.2	O6—C6—C7	109.70 (17)
O7—C2—C1	111.2 (2)	C5—C6—C7	110.44 (18)
O7—C2—H2A	109.4	O6—C6—H6A	108.5
C1—C2—H2A	109.4	C5—C6—H6A	108.5
O7—C2—H2B	109.4	C7—C6—H6A	108.5
C1—C2—H2B	109.4	O1—C7—C6	111.28 (16)
H2A—C2—H2B	108.0	O1—C7—C8	110.32 (17)
O7—C3—C4	111.1 (2)	C6—C7—C8	107.67 (18)
O7—C3—H3A	109.4	O1—C7—H7	109.2
C4—C3—H3A	109.4	C6—C7—H7	109.2
O7—C3—H3B	109.4	C8—C7—H7	109.2
C4—C3—H3B	109.4	O3—C8—O2	126.69 (18)
H3A—C3—H3B	108.0	O3—C8—C7	117.18 (18)
N1—C4—C3	109.1 (2)	O2—C8—C7	116.10 (19)

C4—N1—C1—C2	56.0 (3)	O5—C5—C6—C7	61.0 (2)
C3—O7—C2—C1	60.4 (3)	O6—C6—C7—O1	−70.5 (2)
N1—C1—C2—O7	−58.4 (3)	C5—C6—C7—O1	52.2 (2)
C2—O7—C3—C4	−60.4 (3)	O6—C6—C7—C8	50.5 (2)
C1—N1—C4—C3	−55.9 (3)	C5—C6—C7—C8	173.18 (17)
O7—C3—C4—N1	58.0 (3)	O1—C7—C8—O3	−171.64 (18)
O4—C5—C6—O6	1.9 (3)	C6—C7—C8—O3	66.7 (2)
O5—C5—C6—O6	−177.08 (17)	O1—C7—C8—O2	10.1 (3)
O4—C5—C6—C7	−120.0 (2)	C6—C7—C8—O2	−111.5 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*+1/2; (ii) *x*+1/2, −*y*+3/2, −*z*+1; (iii) −*x*+1, *y*+1/2, −*z*+1/2; (iv) *x*+1, *y*, *z*; (v) −*x*+1, *y*−1/2, −*z*+1/2.