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Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.065
wR factor = 0.120
Data-to-parameter ratio = 17.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Imidazolium hydrogen tartronate

Tartronic acid forms the title salt, $\text{C}_3\text{H}_5\text{N}_2^+\cdot\text{C}_3\text{H}_3\text{O}_5^-$, with imidazole. Hydrogen bonds in the crystal link the anions, forming a hydrogen-bonded layer. The cations cross-link the layers, leading to a three-dimensional hydrogen-bonded network.

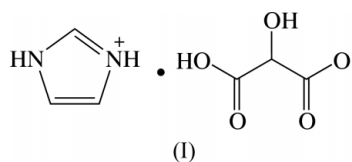
Received 15 October 2003

Accepted 27 October 2003

Online 8 November 2003

Comment

The title compound, (I), was investigated as part of a structural study on $D-\text{H}\cdots A$ hydrogen bonding ($D = \text{N}, \text{O}$ or C ; $A = \text{N}$ or O) in carboxylic acid and pyridine systems (Kashino *et al.*, 2001; Ishida *et al.*, 2001, 2002; Fukunaga *et al.*, 2003). Tartronic acid is of potential interest in crystal engineering for the formation of specific two- or three-dimensional aggregates with organic bases, because the hydroxyl and two carboxyl groups of the acid may act as hydrogen-bond donors as well as acceptors (Taka *et al.*, 1998; Moritani *et al.*, 2001). Furthermore, the acid is an interesting candidate for the selective synthesis and crystallization of optically active substances, because its anion, the hydrogen tartronate ion, is optically active. We report here the packing and hydrogen-bonding patterns of the chiral molecules of hydrogen tartronate, induced by an acid–base interaction involving proton transfer in the crystal structure of (I).



In (I), the asymmetric unit is composed of $\text{C}_3\text{H}_5\text{N}_2^+\cdot\text{C}_3\text{H}_3\text{O}_5^-$ and the crystal is racemic. The imidazolium cation and the hydrogen tartronate anion are held together by $\text{N1}-\text{H1}\cdots\text{O5}$ and $\text{C3}-\text{H5}\cdots\text{O2}$ hydrogen bonds (Fig. 1). In the anion, an intramolecular hydrogen bond, $\text{O1}-\text{H7}\cdots\text{O2}$, is

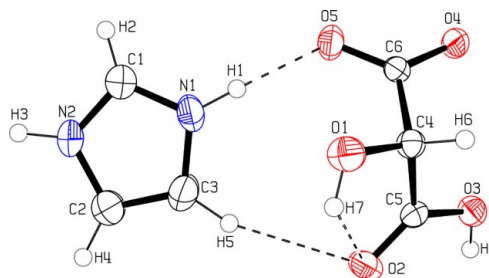


Figure 1

ORTEP-3 (Farrugia, 1997) drawing of the asymmetric unit of (I), with the atomic numbering. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level. $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds are indicated by dashed lines.

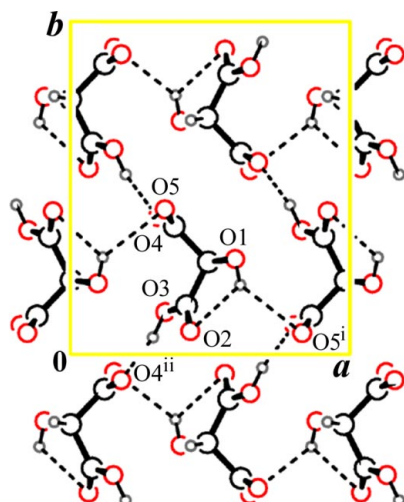


Figure 2
The hydrogen-bonded layer of anions, formed parallel to the *ab* plane (symmetry codes as in Table 2).

observed. The packing of the anions of (I), viewed down the *c* axis, is shown in Fig. 2. The assembly of hydrogen tartronate ions, leading to layers parallel to the *ab* plane, is characterized by a short O3—H8···O4ⁱⁱ hydrogen bond between the carboxyl and carboxylate groups and a long O1—H7···O5ⁱ hydrogen bond between the hydroxyl and carboxylate groups (Table 2). In the layer, adjacent tartronate anions, which are related by a 2₁ screw axis and linked by an O3—H8···O4ⁱⁱ hydrogen bond, form a homochiral helical chain running along the *b* direction. The adjacent anion chains related by the *a* glide plane are linked in the *a* direction by a weak O1—H7···O5ⁱ bond, resulting in the heterochiral layer. These layers are cross-linked in the *c* direction by the imidazolium cations, by way of N1—H1···O5, N2—H3···O4ⁱⁱⁱ, C2—H4···O2^v, C2—H4···O3ⁱⁱⁱ and C3—H5···O2 bonds, leading to a three-dimensional hydrogen-bonded network (Table 2 and Fig. 3).

Experimental

The title crystal was grown by slow evaporation of an ethanol solution of imidazole and tartronic acid in a 1:1 molar ratio.

Crystal data

C ₃ H ₅ N ₂ ⁺ ·C ₃ H ₃ O ₅ ⁻	<i>D</i> _x = 1.525 Mg m ⁻³
<i>M</i> _r = 188.14	Mo Kα radiation
Monoclinic, <i>P</i> 2 ₁ / <i>a</i>	Cell parameters from 25 reflections
<i>a</i> = 8.5516 (15) Å	<i>θ</i> = 11.1–11.5°
<i>b</i> = 10.2077 (17) Å	<i>μ</i> = 0.13 mm ⁻¹
<i>c</i> = 9.392 (3) Å	<i>T</i> = 298 K
<i>β</i> = 91.64 (2)°	Prism, colourless
<i>V</i> = 819.6 (3) Å ³	0.50 × 0.40 × 0.35 mm
<i>Z</i> = 4	

Data collection

Rigaku AFC-5R diffractometer	<i>R</i> _{int} = 0.021
<i>ω</i> -2 <i>θ</i> scans	<i>θ</i> _{max} = 31.0°
Absorption correction: <i>ψ</i> scan (North <i>et al.</i> , 1968)	<i>h</i> = -2 → 12
<i>T</i> _{min} = 0.88, <i>T</i> _{max} = 0.95	<i>k</i> = -14 → 14
6785 measured reflections	<i>l</i> = -13 → 13
2617 independent reflections	3 standard reflections
2032 reflections with <i>I</i> > 2 <i>σ</i> (<i>I</i>)	every 97 reflections
	intensity decay: 4.2%

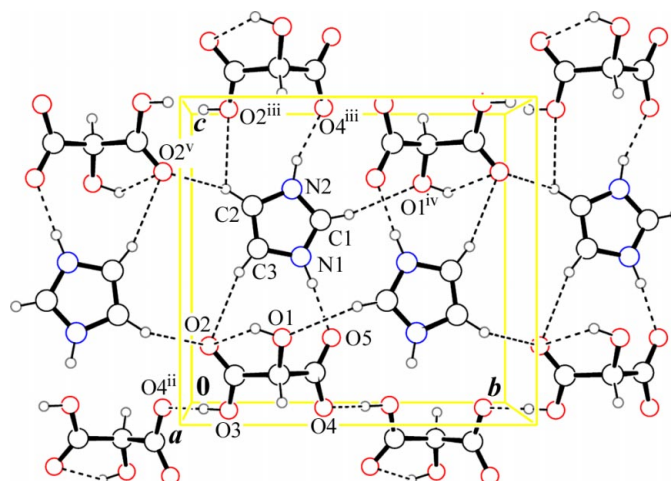


Figure 3
Packing diagram of (I), viewed along the *a* direction, showing N—H···O, O—H···O and C—H···O hydrogen bonds (symmetry codes as in Table 2).

Refinement

Refinement on <i>F</i> ²	(<i>Δ</i> / <i>σ</i>) _{max} = 0.001
<i>R</i> [<i>F</i> ² > 2 <i>σ</i> (<i>F</i> ²)] = 0.065	<i>Δρ</i> _{max} = 0.36 e Å ⁻³
<i>wR</i> (<i>F</i> ²) = 0.120	<i>Δρ</i> _{min} = -0.27 e Å ⁻³
<i>S</i> = 1.01	Extinction correction: Zachariasen (1967)
2617 reflections	Extinction coefficient: 1.43 (12) × 10 ⁻⁵
151 parameters	
All H-atom parameters refined	
<i>w</i> = 1/[<i>σ</i> ² (<i>F</i> _o) + 0.00181 <i>F</i> _o ²]	

Table 1

Selected geometric parameters (Å, °).

O1—C4	1.4089 (12)	N1—C3	1.3659 (18)
O2—C5	1.2138 (12)	N2—C1	1.3169 (15)
O3—C5	1.3031 (12)	N2—C2	1.3651 (18)
O4—C6	1.2622 (12)	C2—C3	1.3420 (18)
O5—C6	1.2383 (12)	C4—C5	1.5279 (13)
N1—C1	1.3200 (15)	C4—C6	1.5384 (13)
C1—N1—C3	108.38 (10)	O1—C4—C5	110.15 (8)
C1—N2—C2	108.80 (10)	O2—C5—O3	126.13 (9)
N1—C1—N2	108.71 (11)	O3—C5—C4	112.94 (8)
N2—C2—C3	106.82 (12)	O4—C6—O5	124.77 (9)
N1—C3—C2	107.28 (12)		

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H7···O2	0.87 (2)	2.18 (2)	2.6552 (12)	113.8 (16)
O1—H7···O5 ⁱ	0.87 (2)	2.48 (2)	3.1150 (16)	130.2 (17)
O3—H8···O4 ⁱⁱ	0.882 (17)	1.665 (17)	2.5361 (14)	169.0 (17)
N1—H1···O5	0.901 (15)	1.825 (16)	2.7116 (15)	167.3 (17)
N2—H3···O4 ⁱⁱⁱ	0.920 (18)	1.875 (19)	2.7662 (14)	162.5 (19)
C1—H2···O1 ^{iv}	0.928 (18)	2.516 (18)	3.3667 (18)	152.5 (13)
C2—H4···O2 ^v	0.98 (2)	2.49 (2)	3.280 (2)	137.6 (19)
C2—H4···O3 ⁱⁱⁱ	0.98 (2)	2.524 (18)	3.1347 (18)	120.2 (14)
C3—H5···O2	0.953 (17)	2.462 (16)	3.3841 (19)	162.7 (15)

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

All H atoms were located in difference Fourier maps and refined isotropically. Refined distances: C–H = 0.927 (18)–0.98 (2), N–H = 0.901 (15)–0.920 (18) and O–H = 0.87 (2)–0.883 (18) Å.

Data collection: *MSC/AFM Diffractometer Control Software* (Molecular Structure Corporation, 1990); cell refinement: *MSC/AFM Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1997–1999); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *TEXSAN for Windows*; molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN for Windows*.

X-ray measurements were made at the X-ray Laboratory of Okayama University.

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