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Cytosinium–hydrogen maleate–cytosine (1/1/1)

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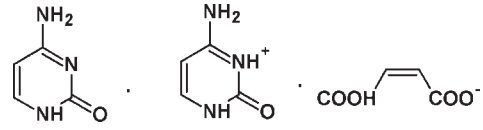
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 17.3.

The title organic salt, $C_4H_6N_3O^+\cdot C_4H_3O_4^-\cdot C_4H_5N_3O$, was synthesized from cytosine base and maleic acid. An intramolecular O—H···O hydrogen bond occurs in the hydrogen maleate anion. The crystal packing is stabilized by intermolecular N—H···O, N—H···N and C—H···O hydrogen bonds, giving rise to a nearly planar two-dimensional network parallel to (101).

Related literature

For background to cytosine, see: Devlin (1986); Johnson & Coghill (1925); Mahan *et al.* (2004). For the structure of cytosine, see: Barker & Marsh (1964) and for that of cytosine monohydrate, see: Jeffrey & Kinoshita (1963); Swamy *et al.* (2001). For the stuctures of inorganic cytosinium salts, see: Mandel (1977); Cherouana *et al.* (2003); Jaskólski (1989); Bagieu-Beucher (1990) and for those of cytosinium salts of organic acids, see: Gdaniec *et al.* (1989); Smith *et al.* (2005); Balasubramanian *et al.* (1996). For the hydrogen maleate anion, see: Madsen & Larsen (1998). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_4H_6N_3O^+\cdot C_4H_3O_4^-\cdot C_4H_5N_3O$
M_r = 338.29
Monoclinic, $C2/c$
a = 27.3226 (5) Å
b = 7.3618 (2) Å
c = 14.6742 (4) Å
β = 93.905 (1)°
V = 2944.77 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 298 K
0.3 × 0.15 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
3490 measured reflections
3485 independent reflections
2603 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.07
3485 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1A—H1A···O4	0.86	1.89	2.7426 (19)	174
N1B—H1B···O2^{i}	0.86	1.91	2.7701 (19)	174
N8A—H8A1···O7B	0.86	2.00	2.8582 (19)	178
N8A—H8A2···O7A^{ii}	0.86	2.04	2.8329 (19)	153
N3B—H3B···N3A	0.86	1.98	2.8370 (19)	176
N8B—H8B1···O7A	0.86	1.99	2.8458 (19)	173
N8B—H8B2···O7B^{iii}	0.86	2.06	2.8491 (18)	153
O3—H3···O1	1.17 (2)	1.25 (2)	2.4167 (16)	173 (2)
C6B—H6B···O1^{i}	0.93	2.50	3.186 (2)	131
C5B—H5B···O2^{iv}	0.93	2.42	3.330 (2)	165
C5A—H5A···O4^{ii}	0.93	2.37	3.296 (2)	175

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

Data collection: *KappaCCD Server Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2509).

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