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Cytosinium oxalate monohydrate

Karim Bouchouit,[a] Nourredine Benali-Cherif,[b]* Slimane Dahaoui,[c] El-Eulmi Bendeif[c] and Claude Lecomte[c]

[a]Faculté des Sciences, Département de Chimie, Université de Jijel, 18000 Jijel, Algeria, [b]Institut des Sciences Exactes, Technologie et Informatique, Centre Universitaire de Khenchela, 40000 Khenchela, Algeria, and [c]Laboratoire de Cristallographie et Modélisation, des Matériaux Minéraux et Biologiques (LCM3B), Université Henri Poincaré Nancy I, UPRESA CNRS 7036, BP 239, 54506 Vandoeuvre les Nancy, France

Correspondence e-mail: benalicherif@hotmail.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.050
wR factor = 0.120
Data-to-parameter ratio = 22.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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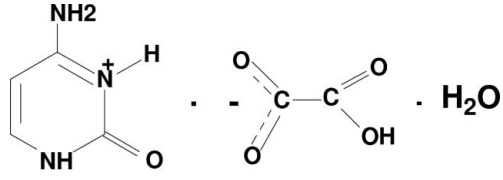
In the title compound, $C_4H_6N_3O^+\cdot C_2HO_4^-\cdot H_2O$, the cytosine molecule is protonated and oxalic acid is in the monoionized state. The structure is stabilized by O—H···O and N—H···O hydrogen bonds, and van der Waals interactions. The water molecules are also found to mediate interactions between oxalate anions and cytosinium cations.

Comment

X-ray studies on crystalline complexes of amino acids with carboxylic acids have provided a wealth of information regarding intermolecular interactions and biomolecular aggregation patterns (Vijayan, 1988; Prasad & Vijayan, 1993). The crystal structures of glycinium oxalate (Subha Nandhini *et al.*, 2001*a*), sarcosinium oxalate monohydrate (Krishnakumar *et al.*, 1998) and L-alaninium oxalate (Subha Nandhini *et al.*, 2001*b*) have been elucidated.

This work is part of our research on structural studies of hybrid compounds based on 'organic matrix-inorganic acids' and 'organic matrix-organic acids': guaninium dinitrate hydrate (Bouchouit *et al.*, 2002), D-phenylglycinium nitrate (Bouchouit *et al.*, 2004), guaninium dihydrogenphosphite dihydrate (Bendheif *et al.*, 2003) and *m*-carboxyphenylammonium nitrate (Benali-Cherif *et al.*, 2002).

The present study reports the crystal structure of an 'organic matrix-organic acid' hybrid compound, (I), formed by reaction of cytosine with oxalic acid.



(I)

The asymmetric unit contains one cytosinium cation, one semi-oxalate anion and a water molecule. Cytosine is monoprotonated at atom N1 and oxalic acid is mono-deprotonated.

Geometrical parameters of the cytosinium cations are found to be in agreement with those of other similar structures of cytosinium nitrate (Cherouana *et al.*, 2003), cytosine (Barker & Marsh, 1964) and cytosine monohydrate (Jeffrey & Kinoshita, 1963).

The cytosinium cations is connected to $HC_2O_4^-$ anions by six N—H···O hydrogen bonds (Table 1).

The semi-oxalate ions have a planar geometry. Bond distances around atom C3 indicate a carboxylate group with delocalization of the negative charge between atoms O3 and

O4. Bond distances around atom C1 are consistent with a carboxylic acid group.

Water molecules play an important role in the cohesion and the stability of the crystal structure; they are involved in three hydrogen bonds connecting one oxalate anion and a cytosinium cation as donor (O1*w*—H2*w*···O2 and O1*w*—H1*w*···O7) and another oxalate anion as acceptor (O1*w*···H—O1) (Table 1). No hydrogen bonds were observed between water molecules.

Experimental

The title compound, (I), was crystallized by slow evaporation of an aqueous solution of cytosine and oxalic acid in a 1:1 stoichiometric ratio.

Crystal data

$C_4H_6N_3O^+\cdot C_2HO_4^-\cdot H_2O$	D_x = 1.657 Mg m^{-3}
M_r = 219.16	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3139 reflections
a = 3.6230 (3) Å	θ = 1.0–32.7°
b = 11.9750 (2) Å	μ = 0.15 mm^{-1}
c = 20.2509 (2) Å	T = 293 (2) K
β = 91.484 (3)°	Prism, colorless
V = 878.30 (7) Å^3	0.20 × 0.20 × 0.15 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	R_{int} = 0.021
φ scans	θ_{max} = 32.7°
12842 measured reflections	$h = -5 \rightarrow 5$
3139 independent reflections	$k = -18 \rightarrow 18$
2226 reflections with $I > 2\sigma(I)$	$l = -30 \rightarrow 30$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.627P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.050	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.120	$\Delta\rho_{max}$ = 0.37 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
3139 reflections	
143 parameters	
H atoms treated by a mixture of independent and constrained refinement	

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O4	0.86	1.94	2.7874 (15)	170
N8—H8*a*···O3	0.86	1.87	2.7267 (17)	173
N8—H8*b*···O3^{i}	0.86	2.10	2.7397 (15)	131
N8—H8*b*···O1^{i}	0.86	2.58	3.4071 (17)	161
N1—H1···O2^{ii}	0.86	2.09	2.9127 (16)	160
N1—H1···O4^{ii}	0.86	2.37	2.9445 (16)	124
O1—H1*a*···O1*w*	0.82	1.76	2.5592 (16)	165
O1*w*—H2*w*···O2^{iii}	0.85 (1)	2.02 (1)	2.8322 (16)	159 (2)
O1*w*—H1*w*···O7^{iv}	0.85 (1)	1.98 (1)	2.8247 (16)	170 (2)

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

All H atoms were located in Fourier maps; those attached to C and N were treated as riding on their parent atoms, with C—H =0.93 and N—H = 0.86 Å and U_{iso} = 1.2U_{eq}(C,N). For the water molecule, the

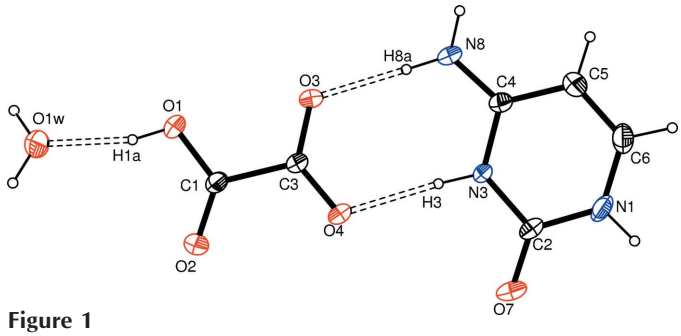


Figure 1
ORTEP-3 (Farrugia, 1997) view of the title compound, with the atomic labelling scheme. Displacement are drawn at the 50% probability level. Hydrogen bonds are drawn as dashed lines.

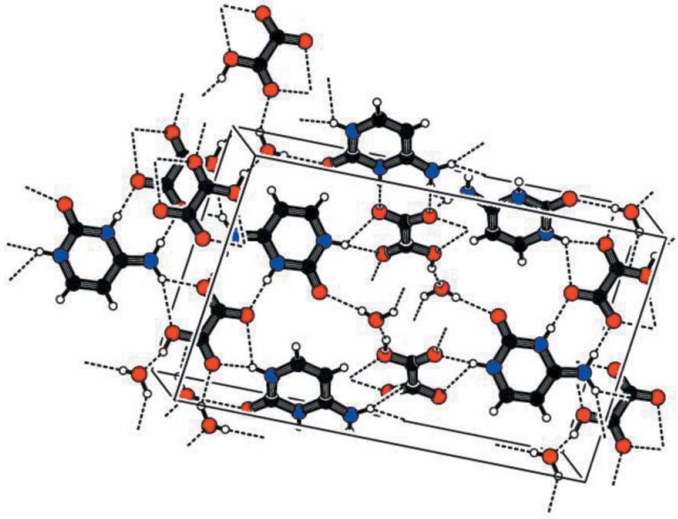


Figure 2
PLATON (Spek, 2003) diagram of the layered packing in the title compound. Hydrogen bonds are drawn as dashed lines.

O*w*—H and H···H distances were restrained to 0.85 (1) and 1.39 (2) Å, respectively, and the H atoms were refined with U_{iso} = 1.2U_{eq}(O*w*).

Data collection: *KappaCCD Reference Manual* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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