Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cytosinium hydrogen selenite

Radhwane Takouachet, Rim Benali-Cherif and Nourredine Benali-Cherif*

Laboratoire des Structures, Propriétés et Interactions InterAtomiques, Université Abbes Laghrour-Khenchela, 40000 Khenchela, Algeria
Correspondence e-mail: benalicherif@hotmail.com

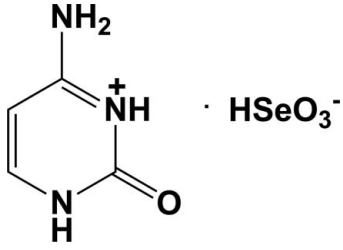
Received 14 January 2014; accepted 17 January 2014

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.042; wR factor = 0.098; data-to-parameter ratio = 12.0.

In the crystal structure of the title salt, $C_4H_6N_3O^+\cdot HSeO_3^-$, systematic name 6-amino-2-methylidene-2,3-dihydropyrimidin-1-ium hydrogen selenite, the hydrogenselenite anions and the cytosinium cations are linked *via* N—H···O, N—H···Se, O—H···O, O—H··Se and C—H···O hydrogen bonds, forming a three-dimensional framework.

Related literature

For the crystal structure of cytosine, see: Barker & Marsh (1964), and of cytosine monohydrate, see: Jeffrey & Kinoshita (1963). For examples of some inorganic cytosinium salts, see: Mandel (1977); Bagieu-Beucher (1990). For examples of the structures of cytosinium salts of organic acids, see: Gdaniec *et al.* (1989); Smith *et al.* (2005). For examples of the structure of the hydrogenselenite anion, see: Richie & Harrison (2003); Wang *et al.* (2006); Chomnilpan *et al.* (1981).



Experimental

Crystal data

$C_4H_6N_3O^+\cdot HSeO_3^-$
M_r = 240.09
Orthorhombic, $Pca2_1$
a = 7.0051 (3) Å
b = 8.6342 (2) Å
c = 12.7131 (3) Å
V = 768.93 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.86 mm^{-1}
T = 293 K
0.20 × 0.15 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.295, T_{max} = 0.369
4568 measured reflections
1494 independent reflections
1283 reflections with $I > 2\sigma(I)$
R_{int} = 0.067

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
S = 1.04
1494 reflections
125 parameters
7 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Absolute structure: Flack parameter determined using 518 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.02 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Se1^{i}	0.85 (3)	3.04 (6)	3.789 (9)	148 (9)
N1—H1A···O3^{i}	0.85 (3)	1.93 (3)	2.785 (10)	176 (10)
N2—H2A···O4^{ii}	0.86 (3)	1.97 (5)	2.798 (12)	160 (10)
N3—H3A···Se1^{iii}	0.84 (3)	3.06 (3)	3.896 (12)	174 (7)
N3—H3A···O2^{iii}	0.84 (3)	2.42 (7)	3.126 (12)	141 (8)
N3—H3A···O4^{iii}	0.84 (3)	2.42 (4)	3.196 (17)	152 (8)
N3—H3B···O3^{ii}	0.84 (3)	1.95 (4)	2.772 (12)	166 (12)
O2—H2···Se1^{iv}	0.81 (3)	2.97 (6)	3.691 (7)	149 (10)
O2—H2···O4^{iv}	0.81 (3)	1.87 (3)	2.682 (10)	180 (14)
C3—H3···O1^{v}	0.93	2.46	3.168 (12)	133
C4—H4···O2^{vi}	0.93	2.31	3.196 (11)	159

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

Data collection: *COLLECT* (Hooft, 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: *SHELXL2013* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2013* and *PLATON*.

We are grateful to Dr M. Giorgi, Faculté des Sciences et Techniques de Saint Jeŕome, Marseille, France, for providing access to the X-ray diffraction facilities. We also thank Abbes Laghrour Khenchela University, le Ministére de l'Enseignement Supérieur et de la Recherche Scientifique–Algeria and the Direction Générale de la Recherche Scientifique et du Développement Technologique–Algeria for financial support.

Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2689).

References

Bagieu-Beucher, M. (1990). *Acta Cryst.* C**46**, 238–240.
Barker, D. L. & Marsh, R. E. (1964). *Acta Cryst.* **17**, 1581–1587.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.
Chomnilpan, S., Liminga, R., Sonneveld, E. J. & Visser, J. W. (1981). *Acta Cryst.* B**37**, 2217–2220.
Gdaniec, M., Brycki, B. & Szafran, M. (1989). *J. Mol. Struct.* pp. 57–64.

Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Jeffrey, G. A. & Kinoshita, Y. (1963). *Acta Cryst.* **16**, 20–28.
Mandel, N. S. (1977). *Acta Cryst.* B**33**, 1079–1082.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C.W. Carter Jr & R.M. Sweet, pp. 307–326. New York: Academic Press.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Ritchie, L. K. & Harrison, W. T. A. (2003). *Acta Cryst.* E**59**, o1296–o1298.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Smith, G., Wermuth, U. D. & Healy, P. C. (2005). *Acta Cryst.* E**61**, o746–o748.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wang, J.-J., Tessier, C. & Holm, R. H. (2006). *Inorg. Chem.* **45**, 2979–2988.

supporting information

Acta Cryst. (2014). E**70**, o186–o187 [doi:10.1107/S1600536814001275]

Cytosinium hydrogen selenite

Radhwane Takouachet, Rim Benali-Cherif and Nourredine Benali-Cherif

S1. Comment

The crystal structure of cytosine (Barker & Marsh, 1964) and cytosine monohydrate (Jeffrey & Kinoshita, 1963) were determined many years ago. Many inorganic cytosinium salts have been synthesized, including the hydrochloride (Mandel, 1977) and the dihydrogenmonophosphate (Bagieu-Beucher, 1990) salts. Cytosinium salts of organic acids are also common, these include for example, cytosinium trichloroacetate (Gdaniec *et al.*, 1989) and cytosinium 3,5-dinitro-salicylate (Smith *et al.*, 2005). We report herein on the molecular structure of a new cytosinium salt formed by the reaction of cytosine with selenious acid.

The structure of the title salt is illustrated in Fig. 1. The $HSeO_3^-$ ion is pyramidal with two short Se—O bonds, Se1—O3 = 1.634 (8) A° and Se1—O4 = 1.686 (6) A°, and a longer Se—OH bond, Se1—O2 = 1.738 (7) A°. These values are very similar to those described in the literature (Richie & Harrison, 2003; Wang *et al.*, 2006; Chomnilpan *et al.*, 1981). The geometry of this inorganic moiety clearly implies that one proton was transferred from selenious acid to cytosine.

In the crystal, the anions and cations are linked *via* N—H···O/Se, O-H···O/Se and C-H···O hydrogen bonds forming a three-dimensional framework (Table 1 and Fig. 2).

S2. Experimental

Selenious acid (H_2SeO_3) was added to an aqueous solution of cytosine in the stoichiometric ratio 1:1, at room temperature. After four weeks colourless prismatic crystals of the title salt were obtained.

S3. Refinement

All the H atoms could be located in difference Fourier maps and this was confirmed by plotting difference Fourier maps using the ContourDif routine in PLATON (Spek, 2009). In the final cycles of refinement the NH_2 distances were restrained to N-H = 0.86 (2) and H···H = 1.33 (2) Å with $U_{iso}(H) = 1.2U_{eq}(N)$. The OH distance was restrained to O-H = 0.82 (2) Å with $U_{iso}(H) = 1.5U_{eq}(O)$. The C bound H atoms were included in calculated positions and treated as riding atoms: C-H = 0.93 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

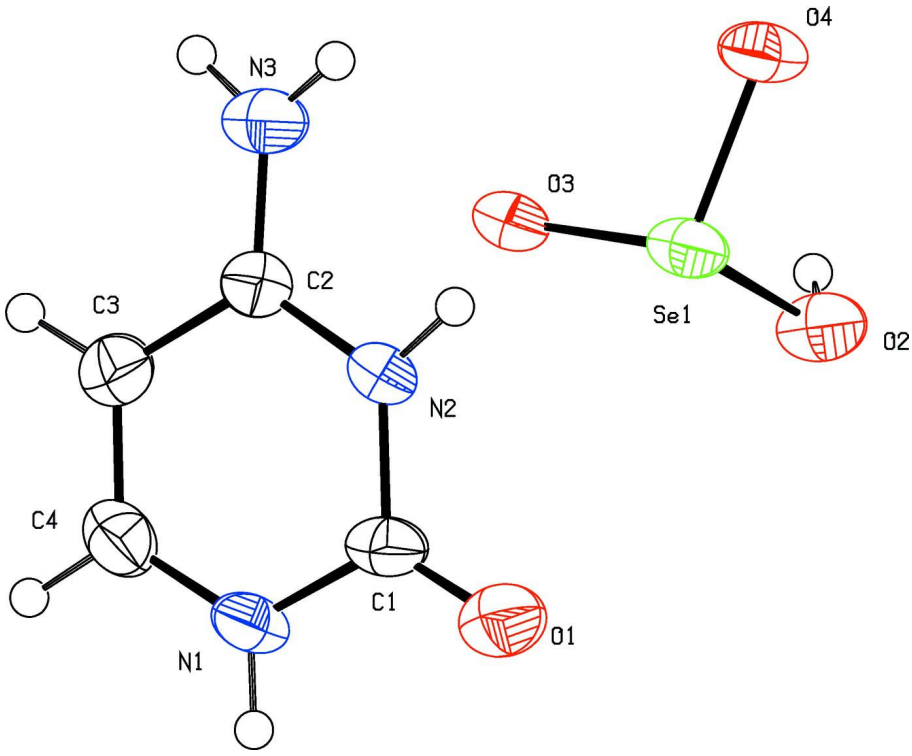


Figure 1

A view of the molecular structure of the title salt, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

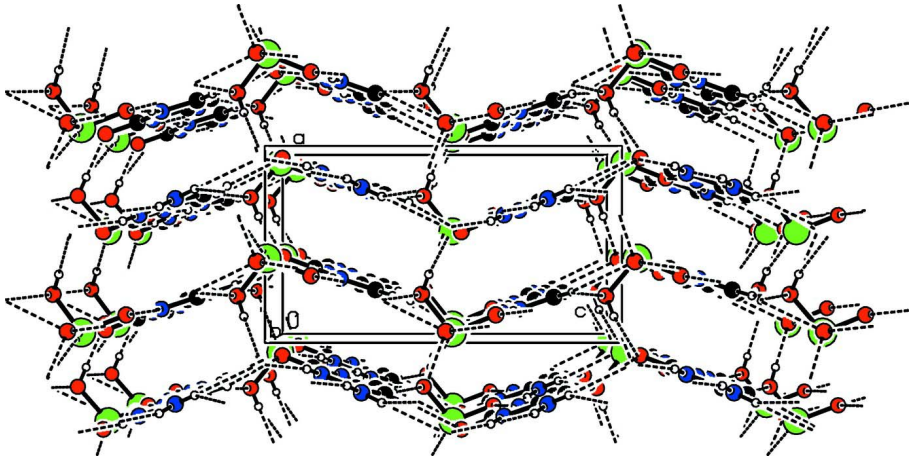


Figure 2

A view along the b axis of the crystal packing of the title compound. The hydrogen-bonds are shown as dashed lines (See Table 1 for details).

6-Amino-2-methylidene-2,3-dihydropyrimidin-1-ium hydrogen selenite

Crystal data

$C_4H_6N_3O^+·HSeO_3^-$
M_r = 240.09

Orthorhombic, $Pca2_1$
a = 7.0051 (3) Å

b = 8.6342 (2) Å
c = 12.7131 (3) Å
V = 768.93 (4) Å^3
Z = 4
$F(000)$ = 472
D_x = 2.074 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 5415 reflections
θ = 3.8–29.5°
μ = 4.86 mm^{-1}
T = 293 K
Prism, colourless
0.20 × 0.15 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega - \theta$ scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.295, T_{max} = 0.369

4568 measured reflections
1494 independent reflections
1283 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 26.0°, θ_{min} = 3.8°
h = −8→8
k = −10→10
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.098
S = 1.04
1494 reflections
125 parameters
7 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.8215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.018 (4)
Absolute structure: Flack parameter determined using 518 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.02 (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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.9370 (10)	0.0316 (8)	0.0502 (5)	0.050 (2)
N1	0.8269 (12)	−0.0384 (8)	0.2127 (7)	0.0392 (19)
H1A	0.832 (17)	−0.134 (5)	0.194 (8)	0.047*
N2	0.8534 (12)	0.2200 (8)	0.1669 (6)	0.0363 (17)
H2A	0.885 (14)	0.300 (8)	0.130 (7)	0.044*
N3	0.7775 (19)	0.4148 (8)	0.2818 (10)	0.047 (3)
H3A	0.732 (17)	0.455 (9)	0.337 (5)	0.056*
H3B	0.817 (16)	0.489 (8)	0.245 (6)	0.056*
C1	0.8779 (14)	0.0666 (10)	0.1365 (8)	0.037 (2)
C2	0.7901 (14)	0.2661 (10)	0.2619 (8)	0.036 (2)

C3	0.7485 (14)	0.1527 (10)	0.3383 (8)	0.041 (2)
H3	0.7088	0.1799	0.4056	0.049*
C4	0.7686 (17)	0.0029 (10)	0.3095 (8)	0.041 (2)
H4	0.7413	−0.0742	0.3583	0.049*
Se1	0.43127 (11)	0.36795 (7)	0.02452 (11)	0.0378 (4)
O2	0.2460 (11)	0.3114 (7)	−0.0579 (6)	0.0444 (16)
H2	0.147 (10)	0.350 (12)	−0.038 (10)	0.067*
O3	0.3461 (15)	0.3439 (7)	0.1431 (6)	0.054 (2)
O4	0.4180 (9)	0.5615 (6)	0.0084 (8)	0.0432 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.063 (4)	0.039 (3)	0.048 (6)	0.004 (3)	0.007 (3)	−0.006 (3)
N1	0.051 (5)	0.022 (3)	0.045 (5)	0.001 (3)	−0.005 (4)	0.003 (3)
N2	0.051 (4)	0.023 (4)	0.035 (4)	0.000 (3)	−0.001 (3)	0.004 (3)
N3	0.062 (8)	0.029 (3)	0.049 (5)	0.002 (5)	0.004 (5)	−0.004 (4)
C1	0.038 (5)	0.024 (4)	0.047 (6)	−0.001 (4)	−0.004 (4)	−0.004 (4)
C2	0.043 (7)	0.030 (4)	0.035 (6)	0.004 (4)	−0.002 (5)	−0.001 (4)
C3	0.050 (6)	0.036 (5)	0.036 (5)	−0.004 (4)	0.000 (4)	−0.002 (4)
C4	0.045 (6)	0.035 (5)	0.042 (6)	−0.003 (4)	−0.003 (5)	0.009 (4)
Se1	0.0425 (5)	0.0233 (4)	0.0475 (5)	0.0031 (3)	−0.0018 (7)	−0.0008 (7)
O2	0.046 (4)	0.035 (3)	0.053 (4)	0.002 (3)	−0.002 (3)	−0.009 (3)
O3	0.098 (6)	0.022 (3)	0.041 (4)	0.005 (3)	−0.001 (4)	0.002 (3)
O4	0.052 (3)	0.023 (3)	0.055 (5)	−0.001 (2)	0.003 (4)	−0.001 (3)

Geometric parameters (Å, º)

O1—C1	1.211 (11)	N3—H3B	0.84 (3)
N1—C4	1.345 (14)	C2—C3	1.409 (13)
N1—C1	1.374 (13)	C3—C4	1.352 (12)
N1—H1A	0.85 (3)	C3—H3	0.9300
N2—C2	1.346 (11)	C4—H4	0.9300
N2—C1	1.391 (11)	Se1—O3	1.634 (8)
N2—H2A	0.86 (3)	Se1—O4	1.686 (6)
N3—C2	1.312 (12)	Se1—O2	1.738 (7)
N3—H3A	0.84 (3)	O2—H2	0.81 (3)
C4—N1—C1	123.3 (7)	N3—C2—C3	122.2 (10)
C4—N1—H1A	121 (7)	N2—C2—C3	118.7 (8)
C1—N1—H1A	115 (7)	C4—C3—C2	117.2 (9)
C2—N2—C1	124.9 (8)	C4—C3—H3	121.4
C2—N2—H2A	110 (7)	C2—C3—H3	121.4
C1—N2—H2A	125 (7)	N1—C4—C3	122.2 (8)
C2—N3—H3A	126 (6)	N1—C4—H4	118.9
C2—N3—H3B	128 (6)	C3—C4—H4	118.9
H3A—N3—H3B	106 (5)	O3—Se1—O4	102.6 (4)
O1—C1—N1	124.3 (9)	O3—Se1—O2	104.3 (5)

O1—C1—N2	122.1 (9)	O4—Se1—O2	99.4 (4)
N1—C1—N2	113.6 (8)	Se1—O2—H2	110 (9)
N3—C2—N2	119.0 (9)		
C4—N1—C1—O1	177.3 (10)	C1—N2—C2—C3	1.5 (15)
C4—N1—C1—N2	−3.4 (14)	N3—C2—C3—C4	−179.2 (12)
C2—N2—C1—O1	−179.4 (10)	N2—C2—C3—C4	−2.4 (15)
C2—N2—C1—N1	1.3 (13)	C1—N1—C4—C3	2.7 (17)
C1—N2—C2—N3	178.4 (10)	C2—C3—C4—N1	0.4 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Se1^{i}	0.85 (3)	3.04 (6)	3.789 (9)	148 (9)
N1—H1*A*···O3^{i}	0.85 (3)	1.93 (3)	2.785 (10)	176 (10)
N2—H2*A*···O4^{ii}	0.86 (3)	1.97 (5)	2.798 (12)	160 (10)
N3—H3*A*···Se1^{iii}	0.84 (3)	3.06 (3)	3.896 (12)	174 (7)
N3—H3*A*···O2^{iii}	0.84 (3)	2.42 (7)	3.126 (12)	141 (8)
N3—H3*A*···O4^{iii}	0.84 (3)	2.42 (4)	3.196 (17)	152 (8)
N3—H3*B*···O3^{ii}	0.84 (3)	1.95 (4)	2.772 (12)	166 (12)
O2—H2···Se1^{iv}	0.81 (3)	2.97 (6)	3.691 (7)	149 (10)
O2—H2···O4^{iv}	0.81 (3)	1.87 (3)	2.682 (10)	180 (14)
C3—H3···O1^{v}	0.93	2.46	3.168 (12)	133
C4—H4···O2^{vi}	0.93	2.31	3.196 (11)	159

Symmetry codes: (i) *x*+1/2, −*y*, *z*; (ii) *x*+1/2, −*y*+1, *z*; (iii) −*x*+1, −*y*+1, *z*+1/2; (iv) *x*−1/2, −*y*+1, *z*; (v) −*x*+3/2, *y*, *z*+1/2; (vi) −*x*+1, −*y*, *z*+1/2.