$S = 1.56$
1059 reflections
127 parameters
H atoms treated using a riding model
$w = 1/[\sigma^2(F) + 0.0008F^2]$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
N1	0.72058 (9)	0.83028 (9)	0.9271 (4)	0.0379 (14)
C1	0.75047 (13)	0.88604 (12)	0.9092 (6)	0.0559 (20)
C2	0.66158 (12)	0.83080 (12)	0.8929 (5)	0.0411 (17)
O2	0.63641 (8)	0.87533 (9)	0.8498 (4)	0.0589 (14)
N3	0.63326 (9)	0.77892 (10)	0.9079 (4)	0.0443 (15)
C3	0.57093 (13)	0.77953 (15)	0.8660 (7)	0.074 (3)
C4	0.65969 (12)	0.72629 (12)	0.9550 (4)	0.0424 (16)
O4	0.62912 (9)	0.68245 (9)	0.9629 (4)	0.0637 (16)
C5	0.72019 (11)	0.72830 (11)	0.9949 (4)	0.0350 (14)
C51	0.74753 (12)	0.67496 (11)	1.0559 (4)	0.0397 (16)
N5	0.80196 (10)	0.67109 (9)	1.0894 (4)	0.0438 (14)
O5	0.81672 (9)	0.61491 (9)	1.1516 (4)	0.0618 (15)
C6	0.74957 (11)	0.78094 (11)	0.9800 (4)	0.0341 (14)
N6	0.80628 (9)	0.78507 (9)	1.0154 (4)	0.0415 (15)

Table 2. *Selected geometric parameters* (Å, °)

N1—C1	1.465 (4)	C4—O4	1.234 (3)
N1—C2	1.382 (3)	C4—C5	1.424 (4)
N1—C6	1.371 (3)	C5—C51	1.447 (4)
C2—O2	1.218 (3)	C5—C6	1.395 (4)
C2—N3	1.368 (4)	C51—N5	1.280 (4)
N3—C3	1.468 (4)	N5—O5	1.408 (3)
N3—C4	1.398 (4)	C6—N6	1.335 (3)
C1—N1—C2	116.20 (22)	N3—C4—C5	116.44 (23)
C1—N1—C6	121.50 (22)	O4—C4—C5	125.3 (3)
C2—N1—C6	122.27 (22)	C4—C5—C51	117.20 (23)
N1—C2—O2	121.3 (3)	C4—C5—C6	119.35 (23)
N1—C2—N3	116.75 (23)	C51—C5—C6	123.41 (24)
O2—C2—N3	121.96 (25)	C5—C51—N5	122.72 (24)
C2—N3—C3	116.40 (23)	C51—N5—O5	110.93 (22)
C2—N3—C4	124.72 (22)	N1—C6—C5	120.40 (23)
C3—N3—C4	118.86 (24)	N1—C6—N6	117.94 (22)
N3—C4—O4	118.2 (3)	C5—C6—N6	121.66 (23)

Data reduction: *NRCVAX DATRD2* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX SOLVER*. Program(s) used to refine structure: *NRCVAX LSTSQ*. Molecular graphics: *NRCVAX* and *PLUTON92* (Spek, 1992). Software used to prepare material for publication: *NRCVAX TABLES*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, torsion angles and complete geometry have been deposited with the IUCr (Reference: HA1109). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4-Amino-2-methylthio-6-oxo-1,6-dihydropyrimidine and its 1-Methyl Derivative and 4-Amino-2-methoxy-1-methyl-6-oxo-1,6-dihydropyrimidine and its 5-Nitroso Derivative

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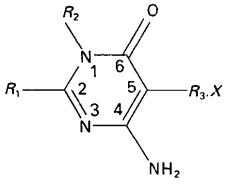
Abstract

The molecular structures of 4-amino-2-methylthio-6-oxo-1,6-dihydropyrimidine trihydrate (AMT, $C_5H_7N_3OS.3H_2O$), 4-amino-1-methyl-2-methylthio-6-oxo-1,6-dihydropyrimidine (AMEMT, $C_6H_9N_3OS$), 4-amino-2-methoxy-1-methyl-6-oxo-1,6-dihydropyrimidine (AMH, $C_6H_9N_3O_2$) and 4-amino-2-methoxy-1-methyl-5-nitroso-6-oxo-1,6-dihydropyrimidine monohydrate (AMEMONO, $C_6H_8N_4O_3.H_2O$) show that, as has been reported for analogous compounds, there is extensive electron delocalization in the pyrimidine rings of all four compounds.

Comment

Knowledge of the molecular structure of free pyrimidine ligands is of interest because it permits an understanding

of the changes in the bond lengths in the proximity of the donor atoms when complex formation takes place. This leads to a better understanding of the spectral and magnetic properties of such metal complexes. Structural studies of free uracil derivatives have been reported by Low, Howie, Hueso-Ureña & Moreno-Carretero (1992, and references cited therein), Hueso-Ureña *et al.* (1992), Kivekäs, Sundberg, Ruiz & Colacio (1991), Romero-Molina *et al.* (1990) and Dattagupta, Kroger & Saenger (1977). We now report the crystal structures of four 6-oxopyrimidine derivatives, each with 4-amino and 2-methylthio or 2-methoxy substituents.



$R_1 = CH_3S$; AMT, AMEMT
$R_1 = CH_3O$; AMH, AMEMONO
$R_2 = H$; AMT
$R_2 = CH_3$; AMEMT, AMH, AMEMONO
$R_3 = H$; AMT, AMEMT, AMH
$R_3 = NO$; AMEMONO
$X = 3H_2O$; AMT
$X = H_2O$; AMEMONO

In most cases the bond lengths indicate that substantial delocalization exists. The only exceptions are the C2═N3 and C6—N1 bonds which exhibit practically pure double- and single-bond character, respectively. This delocalization extends to the exocyclic substituents, especially in the case of the C6—O6 and C4—N4 bonds, which are longer and shorter, respectively, than those corresponding to double C═O and single C—N bonds, except in the case of the nitroso compound in which both these bonds show true double-bond character (Ladd, 1979). This may explain why the —NH_2 group does not show the expected chemical properties of a true primary amino group (Brown, 1970).

In the nitroso compound, the presence of the 5-nitroso group, as well as shortening the C6—O6 and C4—N4 bonds, increases the C4—C5 and C5—C6 bond lengths and slightly decreases the N3—C4, C6—N1 and C2—O2 bond lengths.

In both methylthio compounds, the lengths of the C2—S2 bonds appear to be intermediate between those of single and double bonds as a consequence of the polarizability of the S atom. In contrast, as may be expected, the C21—S2 bond lengths show pure single-bond character. In both methoxy compounds, the C2—O2 bonds also appear to have lengths between those of single and double bonds, but the C21—O2 bond lengths are slightly longer than expected for a pure single bond.

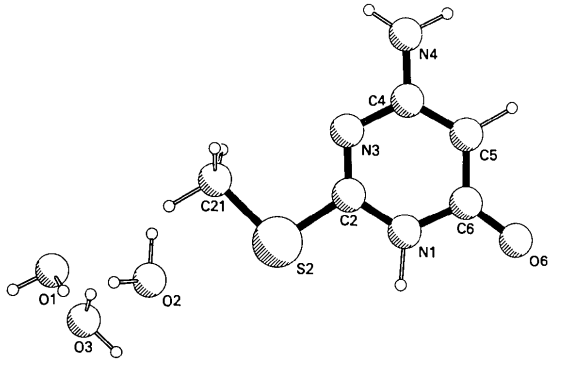


Fig. 1. Molecular drawing of AMT showing the atom-numbering scheme.

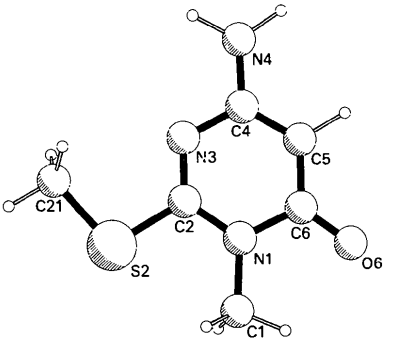


Fig. 2. Molecular drawing of AMEMT showing the atom-numbering scheme.

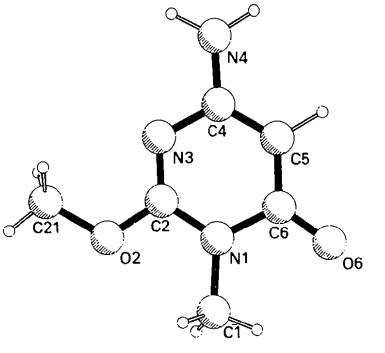


Fig. 3. Molecular drawing of AMH showing the atom-numbering scheme.

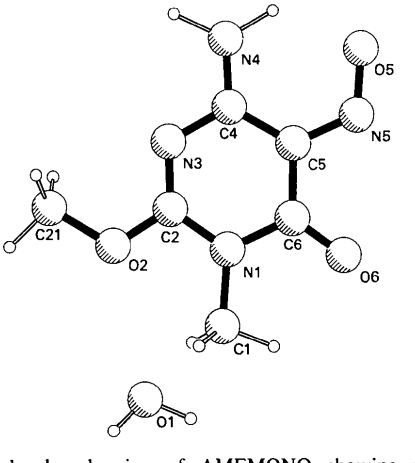


Fig. 4. Molecular drawing of AMEMONO showing the atom-numbering scheme.

All these conclusions are in accordance with previously reported data for analogous compounds (Low *et al.*, 1992; Moreno-Carretero, Salas-Peregrin, Colacio-Rodriguez, Sanchez-Sanchez & Nieto-Garcia, 1986; Romero-Molina, Moreno-Carretero, Ruiz-Sanchez, Sanchez-Sanchez & Nieto-Garcia, 1986; Romero-Molina *et al.*, 1990).

Experimental

The crystals were obtained from aqueous solutions following previously reported methods (Baker, Joseph & Schaud, 1954; Hendrix, 1915).

AMT

Crystal data

$C_5H_7N_3OS.3H_2O$
M_r = 211.23
Triclinic
$P\bar{1}$
a = 6.848 (4) Å
b = 6.865 (2) Å
c = 11.763 (4) Å
α = 76.880 (2)°
β = 98.86 (3)°
γ = 111.50 (3)°
V = 499.6 (4) Å^3
Z = 2
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 14 reflections
θ = 8.00–10.50°
μ = 0.26 mm^{-1}
T = 293 K
Prism
0.60 × 0.30 × 0.10 mm
Colourless

Data collection

Nicolet $P3$ four-circle diffractometer
ω scans
Absorption correction: none
1741 measured reflections
1738 independent reflections
1438 observed reflections [$I > 2.5\sigma(I)$]
R_{int} = 0.019
θ_{max} = 25.00°
$h = -8 \rightarrow 7$
$k = 0 \rightarrow 8$
$l = -13 \rightarrow 13$
2 standard reflections monitored every 50 reflections
intensity variation: 2.2%

Refinement

Refinement on F
R = 0.036
wR = 0.041
S = 2.80
1438 reflections
118 parameters
All H-atom parameters refined
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* AMT

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N1	0.3550 (3)	0.7087 (3)	0.02900 (16)	0.0339 (12)
C2	0.2674 (4)	0.5046 (4)	0.08754 (20)	0.0312 (15)
S2	0.28555 (11)	0.48164 (11)	0.23947 (5)	0.0411 (4)
C21	0.1773 (5)	0.1970 (4)	0.28788 (24)	0.0560 (20)
N3	0.1784 (3)	0.3392 (3)	0.03780 (16)	0.0347 (13)
C4	0.1781 (4)	0.3828 (4)	−0.08254 (20)	0.0324 (14)
N4	0.0877 (4)	0.2130 (3)	−0.13393 (18)	0.0485 (16)
C5	0.2626 (4)	0.5866 (4)	−0.14828 (20)	0.0349 (15)
C6	0.3561 (4)	0.7583 (4)	−0.09166 (20)	0.0333 (15)
O6	0.4422 (3)	0.9518 (3)	−0.14049 (14)	0.0476 (12)
O1*W*	0.3796 (3)	0.0738 (3)	0.62784 (14)	0.0455 (12)
O2*W*	0.2708 (3)	0.7495 (3)	0.50653 (16)	0.0494 (12)
O3*W*	0.1255 (3)	0.3147 (3)	0.60304 (16)	0.0505 (12)

Table 2. *Selected geometric parameters* (Å, °) *for* AMT

N1—C2	1.368 (3)	N3—C4	1.379 (3)
N1—C6	1.383 (3)	C4—N4	1.335 (3)
C2—S2	1.7471 (24)	C4—C5	1.394 (3)
C2—N3	1.299 (3)	C5—C6	1.384 (3)
S2—C21	1.804 (3)	C6—O6	1.275 (3)
N1···O6^{i}	2.745 (3)	*OW*3···*OW*2^{iv}	2.743 (3)
*OW*2···*OW*1^{ii}	2.729 (3)	*OW*1···*OW*3	2.753 (3)
*OW*2···*OW*1^{iii}	2.805 (3)	*OW*1···O6^{v}	2.679 (3)
*OW*3···*OW*2	2.797 (3)	N4···*OW*3^{vi}	3.043 (3)
C2—N1—C6	122.20 (19)	N3—C4—C5	123.98 (20)
N1—C2—S2	113.82 (17)	N4—C4—C5	121.19 (21)
N1—C2—N3	124.66 (20)	C4—C5—C6	119.43 (21)
S2—C2—N3	121.52 (18)	N1—C6—C5	115.07 (20)
C2—S2—C21	102.08 (12)	N1—C6—O6	118.90 (20)
C2—N3—C4	114.65 (19)	C5—C6—O6	126.02 (21)
N3—C4—N4	114.82 (20)		

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

AMEMT

Crystal data

$C_6H_9N_3OS$
M_r = 171.22
Monoclinic
$P2_1/c$
a = 7.594 (5) Å
b = 9.821 (6) Å
c = 11.271 (6) Å
β = 109.83 (4)°
V = 790.8 (8) Å^3
Z = 4
D_x = 1.438 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 14 reflections
θ = 8.00–11.50°
μ = 0.34 mm^{-1}
T = 293 K
Prism
0.60 × 0.40 × 0.40 mm
Colourless

Data collection

Nicolet $P3$ four-circle diffractometer
ω scans
Absorption correction: none
1501 measured reflections
1395 independent reflections
1222 observed reflections [$I > 2.5\sigma(I)$]
R_{int} = 0.036
θ_{max} = 25.00°
$h = -9 \rightarrow 8$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 13$
2 standard reflections monitored every 50 reflections
intensity variation: 2.0%

Refinement

Refinement on F
R = 0.041
wR = 0.050
S = 4.27
1222 reflections
100 parameters
All H-atom parameters refined
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters* ($Å^2$) *for* AMEMT

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
N1	0.2433 (3)	0.03953 (20)	0.44487 (17)	0.0378 (12)
C1	0.2979 (4)	0.1803 (3)	0.4295 (3)	0.0517 (18)
C2	0.2776 (3)	−0.0164 (3)	0.56174 (20)	0.0352 (14)
S2	0.39421 (10)	0.08976 (7)	0.68882 (6)	0.0472 (4)
C21	0.4181 (5)	−0.0210 (3)	0.81904 (24)	0.0681 (21)
N3	0.2332 (3)	−0.14038 (20)	0.58209 (17)	0.0390 (12)
C4	0.1493 (3)	−0.21959 (25)	0.47767 (21)	0.0396 (14)
N4	0.1077 (4)	−0.34830 (23)	0.50220 (20)	0.0570 (15)
C5	0.1123 (4)	−0.1732 (3)	0.35694 (22)	0.0437 (15)
C6	0.1548 (3)	−0.0389 (3)	0.33505 (21)	0.0418 (14)
O6	0.1254 (3)	0.01526 (19)	0.23004 (14)	0.0573 (13)

Table 4. *Selected geometric parameters* (Å, °) *for* AMEMT

N1—C1	1.470 (3)	N3—C4	1.374 (3)
N1—C2	1.368 (3)	C4—N4	1.354 (3)
N1—C6	1.419 (3)	C4—C5	1.371 (3)
C2—S2	1.750 (3)	C5—C6	1.399 (4)
C2—N3	1.305 (3)	C6—O6	1.247 (3)
S2—C21	1.786 (3)		
N4···O6^{i}	3.011 (3)	N4···O6^{ii}	2.939 (3)
C1—N1—C2	121.45 (20)	N3—C4—N4	115.23 (20)
C1—N1—C6	118.46 (20)	N3—C4—C5	122.78 (23)
C2—N1—C6	120.08 (20)	N4—C4—C5	121.98 (22)
N1—C2—S2	115.30 (18)	C4—C5—C6	120.43 (22)
N1—C2—N3	124.60 (21)	N1—C6—C5	115.29 (20)
S2—C2—N3	120.09 (17)	N1—C6—O6	118.42 (23)
C2—S2—C21	101.07 (13)	C5—C6—O6	126.27 (23)
C2—N3—C4	116.77 (20)		

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

AMH

Crystal data

$C_6H_9N_3O_2$
$M_r = 155.15$
Monoclinic
$P2_1/n$
$a = 7.399$ (4) Å
$b = 9.964$ (6) Å
$c = 10.773$ (6) Å
$\beta = 109.96$ (4)°
$V = 746.5$ (7) $Å^3$
$Z = 4$
$D_x = 1.381$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 14 reflections
$\theta = 10.00$–$12.50°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Needle
0.70 × 0.20 × 0.20 mm
Colourless

Data collection

Nicolet $P3$ four-circle diffractometer
ω scans
Absorption correction: none
1416 measured reflections
1317 independent reflections
883 observed reflections [$I > 2.5\sigma(I)$]
$R_{int} = 0.026$
$\theta_{max} = 24.95°$
$h = -8 \rightarrow 8$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow 12$
2 standard reflections monitored every 50 reflections
intensity variation: 2.5%

Refinement

Refinement on F
$R = 0.042$
$wR = 0.039$
$S = 2.72$
883 reflections
100 parameters
All H-atom parameters refined
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e $Å^{-3}$
$\Delta\rho_{min} = -0.20$ e $Å^{-3}$
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B)

Table 5. *Fractional atomic coordinates and equivalent isotropic displacement parameters* ($Å^2$) *for* AMH

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
N1	0.2108 (3)	0.53560 (21)	0.96443 (21)	0.0448 (14)
C1	0.1447 (5)	0.6758 (3)	0.9589 (3)	0.0611 (21)
C2	0.2990 (4)	0.4730 (3)	1.08211 (24)	0.0453 (18)
O2	0.3136 (3)	0.55247 (19)	1.18476 (18)	0.0584 (12)
C21	0.4012 (5)	0.4937 (3)	1.3140 (3)	0.0768 (23)
N3	0.3628 (3)	0.35126 (23)	1.09781 (19)	0.0457 (14)
C4	0.3358 (4)	0.2793 (3)	0.98429 (25)	0.0430 (17)
N4	0.3991 (3)	0.15158 (23)	1.00274 (21)	0.0576 (16)
C5	0.2490 (4)	0.3329 (3)	0.86099 (24)	0.0486 (19)
C6	0.1818 (4)	0.4648 (3)	0.8457 (3)	0.0476 (18)
O6	0.0978 (3)	0.52326 (20)	0.73910 (16)	0.0652 (15)

Table 6. *Selected geometric parameters* (Å, °) *for* AMH

N1—C1	1.474 (4)	N3—C4	1.372 (3)
N1—C2	1.363 (3)	C4—N4	1.347 (4)
N1—C6	1.412 (3)	C4—C5	1.371 (4)
C2—O2	1.334 (3)	C5—C6	1.395 (4)
C2—N3	1.292 (4)	C6—O6	1.248 (3)
O2—C21	1.444 (4)		
N4···O6^{i}	3.021 (3)	N4···O6^{ii}	2.909 (3)
C1—N1—C2	121.20 (22)	N3—C4—N4	115.14 (22)
C1—N1—C6	119.41 (22)	N3—C4—C5	122.49 (24)
C2—N1—C6	119.39 (23)	N4—C4—C5	122.36 (23)
N1—C2—O2	112.18 (25)	C4—C5—C6	120.78 (23)
N1—C2—N3	126.08 (23)	N1—C6—C5	115.23 (23)
O2—C2—N3	121.74 (23)	N1—C6—O6	118.3 (3)
C2—O2—C21	116.19 (22)	C5—C6—O6	126.46 (24)
C2—N3—C4	116.03 (22)		

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

AMEMONO

Crystal data

$C_6H_8N_4O_3.H_2O$
$M_r = 202.17$
Triclinic
$P\bar{1}$
$a = 7.415$ (2) Å
$b = 7.419$ (3) Å
$c = 8.759$ (3) Å
$\alpha = 92.24$ (3)°
$\beta = 92.55$ (3)°
$\gamma = 69.21$ (3)°
$V = 449.9$ (3) $Å^3$
$Z = 2$
$D_x = 1.492$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 14 reflections
$\theta = 10.00$–$12.00°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prism
0.50 × 0.50 × 0.50 mm
Violet

Data collection

Nicolet $P3$ four-circle diffractometer
ω scans
Absorption correction: none
$R_{int} = 0.004$
$\theta_{max} = 24.95°$
$h = -8 \rightarrow 8$
$k = 0 \rightarrow 8$
$l = -10 \rightarrow 10$

1580 measured reflections
1579 independent reflections
1310 observed reflections
$[I > 2.5\sigma(I)]$
2 standard reflections
monitored every 50
reflections
intensity variation: 3.0%

Refinement

Refinement on F
$R = 0.041$
$wR = 0.047$
$S = 3.92$
1310 reflections
127 parameters
All H-atom parameters
refined
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} = < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: none
Atomic scattering factors
from *International Tables*
for X-ray Crystallography
(1974, Vol. IV, Table
2.2B)

Table 7. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* AMEMONO

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
N1	0.30316 (23)	0.28987 (22)	0.36718 (18)	0.0374 (9)
C1	0.3439 (3)	0.4186 (3)	0.25940 (25)	0.0517 (14)
C2	0.3167 (3)	0.1075 (3)	0.32383 (21)	0.0332 (10)
O2	0.37205 (21)	0.06273 (19)	0.18203 (14)	0.0441 (9)
C21	0.3656 (4)	−0.1192 (3)	0.11716 (23)	0.0536 (14)
N3	0.28479 (22)	−0.01775 (21)	0.40813 (17)	0.0340 (9)
C4	0.2262 (3)	0.0379 (3)	0.55264 (20)	0.0308 (10)
N4	0.19334 (24)	−0.09096 (22)	0.63486 (18)	0.0392 (10)
C5	0.2032 (3)	0.2275 (3)	0.61155 (20)	0.0355 (10)
N5	0.1429 (3)	0.30054 (24)	0.75182 (19)	0.0458 (10)
O5	0.10369 (23)	0.19212 (21)	0.84278 (16)	0.0549 (10)
C6	0.2457 (3)	0.3593 (3)	0.51437 (21)	0.0391 (12)
O6	0.2321 (3)	0.52428 (21)	0.55220 (18)	0.0624 (11)
O1*W*	0.0973 (3)	0.70649 (24)	0.87500 (18)	0.0751 (13)

Table 8. *Selected geometric parameters* (Å, °) *for* AMEMONO

N1—C1	1.482 (3)	C4—N4	1.3140 (24)
N1—C2	1.3605 (24)	C4—C5	1.434 (3)
N1—C6	1.3965 (25)	C5—N5	1.3518 (24)
C2—O2	1.3182 (22)	C5—C6	1.444 (3)
C2—N3	1.3002 (24)	N5—O5	1.2663 (24)
O2—C21	1.4594 (25)	C6—O6	1.2257 (23)
N3—C4	1.3573 (23)		
N4···O6^{i}	2.8337 (23)	O*W*1···N5	3.067 (3)
N4···O5	2.6433 (23)	O*W*1···O5^{ii}	2.8784 (23)
C1—N1—C2	121.08 (16)	N3—C4—C5	121.18 (16)
C1—N1—C6	119.14 (15)	N4—C4—C5	122.24 (16)
C2—N1—C6	119.76 (15)	C4—C5—N5	126.66 (17)
N1—C2—O2	112.82 (16)	C4—C5—C6	118.68 (16)
N1—C2—N3	126.47 (17)	N5—C5—C6	114.66 (16)
O2—C2—N3	120.70 (16)	C5—N5—O5	117.80 (16)
C2—O2—C21	117.18 (15)	N1—C6—C5	116.03 (15)
C2—N3—C4	117.84 (15)	N1—C6—O6	119.41 (18)
N3—C4—N4	116.57 (15)	C5—C6—O6	124.55 (18)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, 1-y, 2-z$.

Data collection and cell refinement: Nicolet *P*3 software. Data reduction: *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989). Structure refinement: *NRCVAX*. Program used to solve structures: *SHELX*86 (Sheldrick, 1985). Programs used to produce molecular graphics: *PLUTON*92 (Spek, 1992).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HA1089). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acetamide Hydrochloride

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Abstract

The title compound, acetamide hydrochloride (I), $C_2H_6NO^+.Cl^-$, has a planar network of infinite hydrogen bonds connecting the $C_2H_6NO^+$ cation to three different Cl^- anions and *vice versa*, *via* one O—H···Cl and two N—H···Cl hydrogen bonds.