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2-Amino-4,6-dimethylpyrimidin-1-ium chloride

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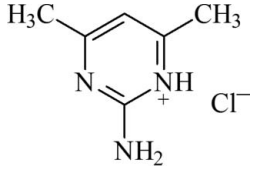
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.105; data-to-parameter ratio = 17.4.

In the title compound, $C_6H_{10}N_3^+\cdot Cl^-$, the cation is essentially planar with an r.m.s. deviations of the fitted atoms of 0.008 Å. In the crystal, adjacent ions are linked by weak N—H···Cl hydrogen bonds involving the pyrimidine and amine N atoms, forming a three-dimensional network. C—H···π interactions between the methyl and pyrimidine groups and π–π stacking [centroid–centroid distance = 3.474 (1) Å] between parallel pyrimidine ring systems are also observed.

Related literature

For the crystal structures of 2-aminopyrimidinium salts with other anions, see: Cheng *et al.* (2010); Eshtiagh-Hosseini *et al.* (2010); Hu & Yeh (2012).



Experimental

Crystal data

$C_6H_{10}N_3^+\cdot Cl^-$
M_r = 159.62
Monoclinic, $C2/c$
a = 16.372 (4) Å
b = 8.795 (2) Å
c = 12.007 (3) Å
β = 108.133 (5)°
V = 1642.9 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 273 K
0.4 × 0.4 × 0.3 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.869, T_{max} = 0.982
5044 measured reflections
1620 independent reflections
1008 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 0.90
1620 reflections
93 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

Cg1 is the centroid of the C1–C4/N2/N3 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl^{i}	0.86	2.42	3.260 (2)	167
N1—H1B···Cl^{ii}	0.86	2.57	3.262 (2)	138
N2—H2N···Cl	0.86	2.22	3.042 (2)	161
C5—H5A···$Cg1^{iii}$	0.96	3.00	3.446 (3)	110

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

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97*.

We are grateful to the National Science Council of the Republic of China and the Taoyuan Innovation Institute of Technology for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2128).

References

Brandenburg, K. (2010). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2010). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cheng, X.-L., Gao, S. & Ng, S. W. (2010). *Acta Cryst.* E**66**, o127.
Eshtiagh-Hosseini, H., Mahjoobizadeh, M. & Mirzaei, M. (2010). *Acta Cryst.* E**66**, o2210.
Hu, H.-L. & Yeh, C.-W. (2012). *Acta Cryst.* E**68**, o2925.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2012). E**68**, o3372 [doi:10.1107/S1600536812046569]

2-Amino-4,6-dimethylpyrimidin-1-ium chloride

Hui-Ling Hu and Chun-Wei Yeh

S1. Comment

There are several supramolecular structures containing 2-aminopyrimidinium cations with other anions constructed by hydrogen bonds (Cheng, *et al.* 2010; Eshtiagh-Hosseini, *et al.* 2010; Hu, *et al.* 2012). The asymmetric unit of the title molecule, $C_6H_{10}N_3^+$, Cl^-, consists a mono-protonated 2-amino-4,6-dimethylpyrimidine and one chloride anion (Fig. 1). The protonated pyrimidine groups are flat and these carbon/nitrogen atoms of mean devition from plane are 0.008 Å. The cations and anions are interlinked through N—H···Cl hydrogen bonds which are found between the H atoms bound to the pyrimidine and amine N atoms and the chloride anions showing the three-dimensional net (Fig. 2, Tab. 1). In the crystal, the weak C—H···pi interactions between the methyl and pyrimidinyl groups and the pi···pi stacking between parallel pyrimidine ring systems are observed, respectively [3.474 (1) Å], while *Cg1* is the centers of C1—C4/N2—N3.

S2. Experimental

An aqueous solution (5.0 ml) of zinc chloride (1.0 mmol) was layered carefully over a methanolic solution (5.0 ml) of 2-amino-4,6-dimethylpyrimidine (2.0 mmol) in a tube. Yellow crystals were obtained after several weeks. These were washed with methanol and collected in 83.5% yield.

S3. Refinement

H atoms bound to C atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 - 0.96 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C/N).

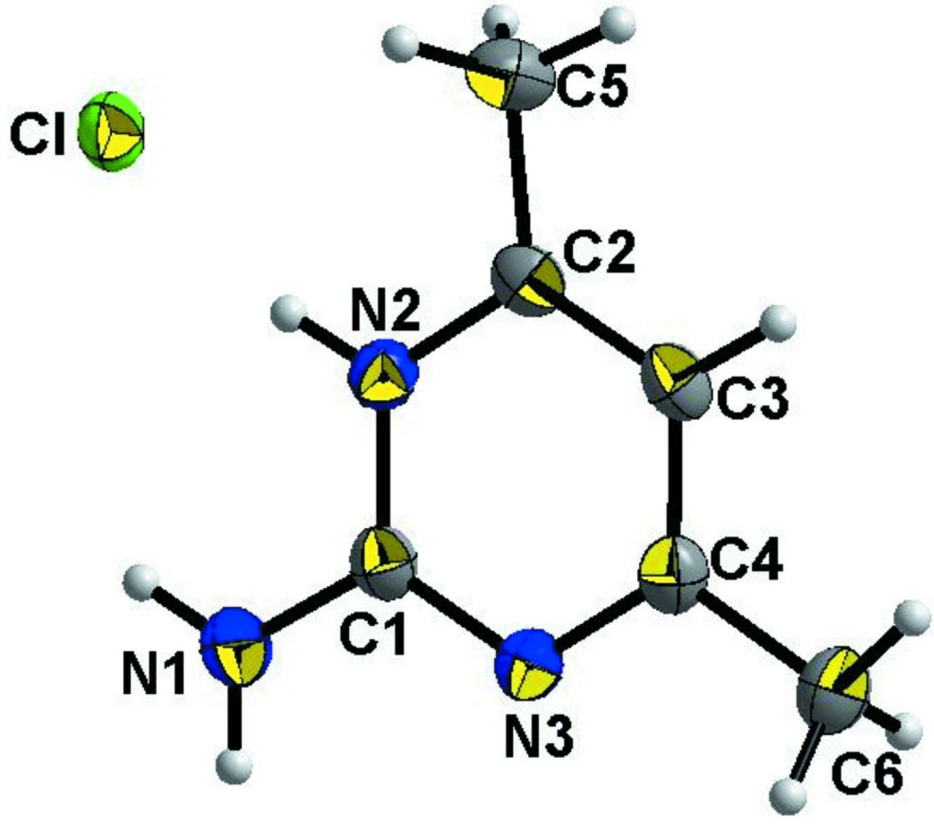


Figure 1

An *ORTEP* view of the title compound with the atom-labelling scheme.Thermal ellipsoids are drawn at 30% probability level, and H atoms are represented by small spheres of arbitrary radii.

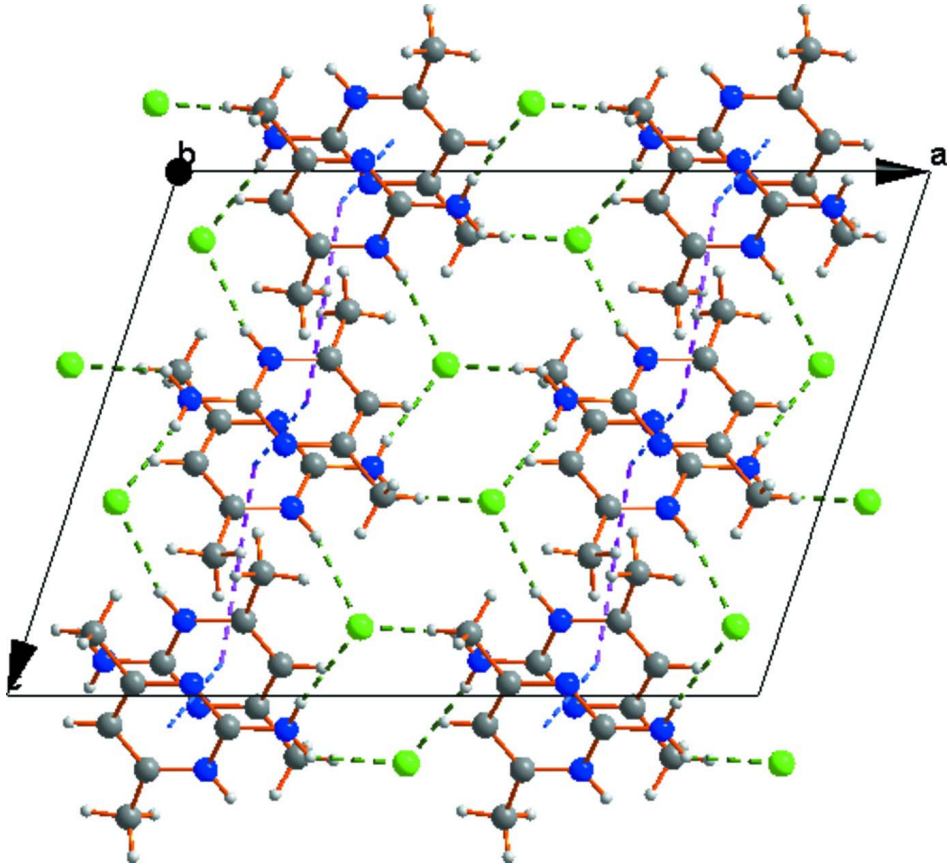


Figure 2

The packing diagram shows the N—H···Cl and C—H···pi hydrogen bonds and pi—pi stacking interactions forming the three-dimensional net.

2-Amino-4,6-dimethylpyrimidin-1-ium chloride

Crystal data

$C_6H_{10}N_3^+\cdot Cl^-$
M_r = 159.62
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 16.372 (4) Å
b = 8.795 (2) Å
c = 12.007 (3) Å
β = 108.133 (5)°
V = 1642.9 (8) Å^3
Z = 8
F(000) = 672
D_x = 1.291 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1118 reflections
θ = 2.7–22.9°
μ = 0.40 mm^{-1}
T = 273 K
Block, yellow
0.4 × 0.4 × 0.3 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.869, T_{max} = 0.982
5044 measured reflections
1620 independent reflections
1008 reflections with $I > 2\sigma(I)$

R_{int} = 0.046
θ_{max} = 26.0°, θ_{min} = 2.6°
h = −19→20
k = −10→10
l = −14→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 0.90
1620 reflections
93 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Cl	0.06044 (4)	0.20186 (8)	0.63062 (5)	0.0635 (3)
C1	0.19281 (13)	0.0360 (3)	0.9384 (2)	0.0456 (6)
C2	0.28190 (14)	0.1835 (2)	0.8578 (2)	0.0476 (6)
C3	0.35098 (14)	0.1274 (3)	0.9429 (2)	0.0524 (6)
H3A	0.4063	0.1584	0.9477	0.063*
C4	0.33775 (13)	0.0227 (3)	1.0228 (2)	0.0490 (6)
C5	0.28542 (16)	0.2952 (3)	0.7666 (2)	0.0639 (7)
H5A	0.2522	0.3834	0.7718	0.096*
H5B	0.2623	0.2499	0.6905	0.096*
H5C	0.3440	0.3244	0.7785	0.096*
C6	0.41211 (15)	−0.0414 (3)	1.1175 (2)	0.0682 (8)
H6A	0.3997	−0.0390	1.1906	0.102*
H6B	0.4625	0.0183	1.1242	0.102*
H6C	0.4219	−0.1445	1.0987	0.102*
N1	0.11391 (11)	−0.0037 (2)	0.93458 (18)	0.0598 (6)
H1A	0.1063	−0.0665	0.9853	0.072*
H1B	0.0703	0.0334	0.8814	0.072*
N2	0.20317 (11)	0.1349 (2)	0.85719 (15)	0.0470 (5)
H2N	0.1585	0.1678	0.8037	0.056*
N3	0.25965 (11)	−0.0223 (2)	1.02128 (16)	0.0480 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0469 (4)	0.0883 (5)	0.0535 (4)	0.0071 (3)	0.0131 (3)	0.0016 (3)
C1	0.0433 (12)	0.0489 (13)	0.0451 (14)	−0.0002 (11)	0.0144 (11)	−0.0052 (11)
C2	0.0516 (13)	0.0483 (13)	0.0459 (13)	−0.0037 (11)	0.0193 (11)	−0.0071 (11)
C3	0.0415 (12)	0.0603 (15)	0.0579 (16)	−0.0074 (11)	0.0190 (11)	−0.0044 (13)
C4	0.0447 (13)	0.0536 (14)	0.0469 (14)	0.0019 (11)	0.0117 (11)	−0.0066 (11)
C5	0.0717 (16)	0.0674 (16)	0.0581 (16)	−0.0057 (14)	0.0280 (13)	0.0069 (14)
C6	0.0487 (13)	0.0823 (19)	0.0663 (19)	0.0064 (14)	0.0073 (13)	0.0103 (15)
N1	0.0407 (11)	0.0734 (15)	0.0629 (15)	−0.0037 (10)	0.0129 (10)	0.0083 (10)
N2	0.0434 (10)	0.0530 (11)	0.0428 (11)	0.0034 (9)	0.0107 (8)	0.0017 (9)
N3	0.0425 (10)	0.0528 (12)	0.0467 (12)	0.0015 (9)	0.0110 (9)	0.0027 (9)

Geometric parameters (Å, º)

C1—N1	1.325 (3)	C5—H5A	0.9600
C1—N3	1.331 (3)	C5—H5B	0.9600
C1—N2	1.356 (3)	C5—H5C	0.9600
C2—N2	1.356 (3)	C6—H6A	0.9600
C2—C3	1.359 (3)	C6—H6B	0.9600
C2—C5	1.486 (3)	C6—H6C	0.9600
C3—C4	1.395 (3)	N1—H1A	0.8600
C3—H3A	0.9300	N1—H1B	0.8600
C4—N3	1.333 (3)	N2—H2N	0.8600
C4—C6	1.494 (3)		
N1—C1—N3	119.3 (2)	H5A—C5—H5C	109.5
N1—C1—N2	118.9 (2)	H5B—C5—H5C	109.5
N3—C1—N2	121.8 (2)	C4—C6—H6A	109.5
N2—C2—C3	117.2 (2)	C4—C6—H6B	109.5
N2—C2—C5	117.3 (2)	H6A—C6—H6B	109.5
C3—C2—C5	125.4 (2)	C4—C6—H6C	109.5
C2—C3—C4	119.0 (2)	H6A—C6—H6C	109.5
C2—C3—H3A	120.5	H6B—C6—H6C	109.5
C4—C3—H3A	120.5	C1—N1—H1A	120.0
N3—C4—C3	122.7 (2)	C1—N1—H1B	120.0
N3—C4—C6	116.7 (2)	H1A—N1—H1B	120.0
C3—C4—C6	120.6 (2)	C2—N2—C1	121.99 (18)
C2—C5—H5A	109.5	C2—N2—H2N	119.0
C2—C5—H5B	109.5	C1—N2—H2N	119.0
H5A—C5—H5B	109.5	C1—N3—C4	117.2 (2)
C2—C5—H5C	109.5		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C4/N2/N3 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl^{i}	0.86	2.42	3.260 (2)	167
N1—H1*B*···Cl^{ii}	0.86	2.57	3.262 (2)	138
N2—H2*N*···Cl	0.86	2.22	3.042 (2)	161
C5—H5*A*···*Cg*1^{iii}	0.96	3.00	3.446 (3)	110

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