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2-Amino-4,6-dimethylpyrimidinium chloroacetate

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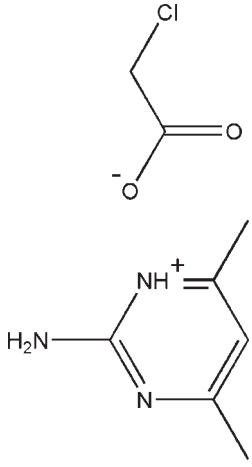
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.195; data-to-parameter ratio = 18.8.

There are two cations and two anions in the asymmetric unit of the title compound, $C_6H_{10}N_3^+\cdot C_2H_2ClO_2^-$. In the crystal, the components are linked by intermolecular N—H···O and N—H···N hydrogen bonds to form a two-dimensional network. Additional stabilization is provided by weak intermolecular C—H···O interactions.

Related literature

For background to pyrimidine derivatives, see: Xue *et al.* (1993); Hemamalini *et al.* (2005).



Experimental

Crystal data

$C_6H_{10}N_3^+\cdot C_2H_2ClO_2^-$
M_r = 217.66
Triclinic, $P\overline{1}$
a = 4.4560 (9) Å
b = 12.302 (3) Å
c = 19.441 (4) Å
α = 92.90 (3)°
β = 96.53 (3)°
γ = 91.15 (3)°
V = 1057.1 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 293 K
0.20 × 0.15 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: none
10303 measured reflections
4761 independent reflections
3452 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.195
S = 1.08
4761 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N3^{i}	0.86	2.14	2.999 (3)	177
N1—H1B···O3^{ii}	0.86	1.98	2.830 (3)	173
N2—H2A···O4^{ii}	0.86	1.74	2.593 (3)	175
N4—H4A···N6^{iii}	0.86	2.19	3.046 (3)	175
N4—H4B···O1^{iv}	0.86	2.00	2.851 (3)	173
N5—H5A···O2^{iv}	0.86	1.75	2.606 (3)	174
C1—H1C···O4^{ii}	0.96	2.56	3.355 (4)	140
C7—H7A···O2^{iv}	0.96	2.57	3.355 (4)	139

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5174).

References

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supporting information

Acta Cryst. (2009). E**65**, o2913 [https://doi.org/10.1107/S1600536809044444]

2-Amino-4,6-dimethylpyrimidinium chloroacetate

Cui-Hua Lin, Nai-Sheng Liu and Fang-Fang Jian

S1. Comment

As useful precursors to potentially bioactive pyrimidine derivatives, methylpyrimidine has attracted considerable attention for many years (Xue *et al.*, 1993). In recent years, new complexes of pyrimidine have been synthesized (Hemamalini *et al.*, 2005). The title compound(I), was synthesized and we report herein its crystal structure (Fig. 1).

There are two 2-amino-4,6-dimethylpyrimidine cations and two chloracetate anions in the asymmetric unit. In the crystal structure, cations and anions are linked by intermolecular N—H···O and N—H···N hydrogen bonds to form a two-dimensional network. Additional stabilization is provided by weak intermolecular C—H···O interactions.

S2. Experimental

A mixture of guanidine hydrochloride (0.1 mol), acetyl acetone (0.2 mol), sodium carbonate (0.03 mol) and 2-chloro-acetic acid (0.1 mol) was stirred with water (30 ml) for 3 h to afford the title compound (yield 67%). Colourless blocks of (I) were obtained by recrystallization of the title compound from water at room temperature.

S3. Refinement

H atoms bonded to C atoms were fixed geometrically and and included in a riding-model approximation with C—H = 0.93–0.96 Å and U_{iso}(H)=1.2–1.5U_{eq}(C).

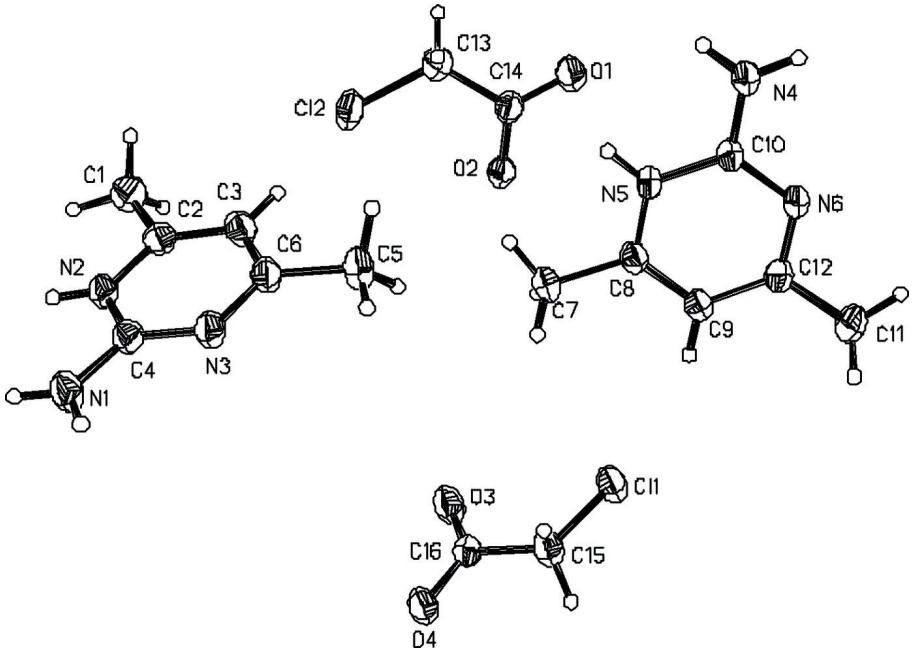

Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids.

2-Amino-4,6-dimethylpyrimidinium chloroacetate

Crystal data

$C_6H_{10}N_3^+ \cdot C_2H_2ClO_2^-$
$M_r = 217.66$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 4.4560\ (9)$ Å
$b = 12.302\ (3)$ Å
$c = 19.441\ (4)$ Å
$\alpha = 92.90\ (3)°$
$\beta = 96.53\ (3)°$
$\gamma = 91.15\ (3)°$
$V = 1057.1\ (4)$ Å^3
$Z = 4$
$F(000) = 456$
$D_x = 1.368$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3452 reflections
$\theta = 3.2–27.5°$
$\mu = 0.34$ mm^{-1}
$T = 293$ K
Block, colourless
0.20 × 0.15 × 0.11 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
10303 measured reflections
4761 independent reflections
3452 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -5 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.195$
$S = 1.08$
4761 reflections
253 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.1056P)^2 + 0.3945P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.42$ e Å^{-3}
	$\Delta\rho_{min} = -0.43$ 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}
Cl1	0.92264 (17)	0.01264 (6)	0.17209 (4)	0.0623 (2)
O4	0.7689 (5)	0.14297 (17)	−0.00572 (10)	0.0681 (6)
C16	0.8811 (6)	0.13347 (19)	0.05672 (13)	0.0463 (5)
O3	1.0794 (5)	0.19170 (18)	0.08873 (11)	0.0742 (7)
C15	0.7353 (7)	0.0407 (2)	0.09016 (14)	0.0616 (7)
H15A	0.7320	−0.0243	0.0596	0.074*
H15B	0.5276	0.0584	0.0954	0.074*
Cl2	0.8148 (2)	0.60659 (7)	0.34169 (5)	0.0862 (3)
O2	0.9854 (5)	0.38470 (15)	0.37047 (10)	0.0594 (5)
C14	0.8160 (6)	0.4192 (2)	0.41493 (13)	0.0497 (6)
O1	0.7445 (6)	0.36870 (18)	0.46320 (12)	0.0798 (7)
C13	0.6862 (8)	0.5308 (2)	0.40795 (16)	0.0632 (7)
H13A	0.7342	0.5722	0.4518	0.076*
H13B	0.4680	0.5230	0.3993	0.076*
N5	0.1724 (4)	0.18552 (15)	0.37450 (10)	0.0418 (4)
H5A	0.1093	0.2511	0.3762	0.050*
N6	0.1954 (5)	0.01175 (16)	0.42234 (10)	0.0467 (5)
C10	0.1065 (6)	0.11536 (19)	0.42261 (12)	0.0436 (5)
C9	0.4323 (6)	0.0461 (2)	0.32177 (13)	0.0502 (6)
H9A	0.5446	0.0210	0.2870	0.060*
C12	0.3572 (6)	−0.02223 (19)	0.37232 (13)	0.0477 (5)
C8	0.3363 (5)	0.15178 (19)	0.32440 (12)	0.0430 (5)
N4	−0.0552 (6)	0.15065 (18)	0.47176 (12)	0.0610 (6)
H4A	−0.1012	0.1075	0.5026	0.073*
H4B	−0.1145	0.2167	0.4729	0.073*
C7	0.4002 (7)	0.2310 (2)	0.27171 (13)	0.0554 (6)
H7A	0.3149	0.2998	0.2829	0.083*
H7B	0.3119	0.2038	0.2266	0.083*
H7C	0.6146	0.2402	0.2718	0.083*
C11	0.4550 (8)	−0.1383 (2)	0.37303 (18)	0.0689 (8)

H11A	0.3841	−0.1721	0.4118	0.103*
H11B	0.6715	−0.1400	0.3770	0.103*
H11C	0.3719	−0.1768	0.3308	0.103*
N2	0.0615 (5)	0.69331 (16)	0.07225 (10)	0.0457 (5)
H2A	0.1088	0.7470	0.0486	0.055*
N3	−0.2359 (5)	0.53279 (17)	0.07940 (11)	0.0489 (5)
C6	−0.0956 (6)	0.5215 (2)	0.14272 (13)	0.0493 (6)
N1	−0.2951 (5)	0.63311 (18)	−0.01745 (11)	0.0566 (6)
H1A	−0.4349	0.5876	−0.0354	0.068*
H1B	−0.2464	0.6878	−0.0401	0.068*
C4	−0.1547 (5)	0.61899 (19)	0.04524 (12)	0.0443 (5)
C2	0.2013 (5)	0.6821 (2)	0.13654 (13)	0.0472 (5)
C3	0.1249 (6)	0.5956 (2)	0.17351 (14)	0.0520 (6)
H3B	0.2183	0.5868	0.2181	0.062*
C1	0.4302 (6)	0.7682 (2)	0.16441 (15)	0.0594 (7)
H1C	0.4485	0.8204	0.1300	0.089*
H1D	0.6220	0.7355	0.1759	0.089*
H1E	0.3673	0.8039	0.2052	0.089*
C5	−0.1883 (8)	0.4234 (2)	0.17923 (16)	0.0657 (8)
H5B	−0.3422	0.3821	0.1499	0.099*
H5C	−0.2654	0.4466	0.2216	0.099*
H5D	−0.0162	0.3788	0.1896	0.099*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0689 (4)	0.0673 (4)	0.0516 (4)	−0.0052 (3)	0.0041 (3)	0.0202 (3)
O4	0.0883 (15)	0.0633 (12)	0.0497 (11)	−0.0230 (11)	−0.0076 (10)	0.0170 (9)
C16	0.0500 (13)	0.0415 (12)	0.0478 (13)	−0.0017 (10)	0.0065 (10)	0.0057 (10)
O3	0.0887 (15)	0.0727 (14)	0.0573 (12)	−0.0334 (12)	−0.0100 (11)	0.0213 (10)
C15	0.0666 (17)	0.0649 (17)	0.0515 (15)	−0.0184 (14)	−0.0035 (12)	0.0182 (13)
Cl2	0.1195 (7)	0.0527 (4)	0.0972 (7)	0.0286 (4)	0.0432 (5)	0.0302 (4)
O2	0.0773 (13)	0.0450 (10)	0.0609 (11)	0.0132 (9)	0.0229 (10)	0.0130 (8)
C14	0.0569 (14)	0.0407 (12)	0.0512 (14)	0.0017 (11)	0.0031 (11)	0.0057 (10)
O1	0.1139 (19)	0.0612 (13)	0.0750 (14)	0.0228 (12)	0.0437 (13)	0.0261 (11)
C13	0.0779 (19)	0.0520 (15)	0.0638 (17)	0.0163 (14)	0.0193 (14)	0.0105 (13)
N5	0.0532 (11)	0.0323 (9)	0.0405 (10)	0.0009 (8)	0.0054 (8)	0.0097 (7)
N6	0.0617 (12)	0.0356 (10)	0.0449 (10)	0.0052 (9)	0.0101 (9)	0.0118 (8)
C10	0.0554 (13)	0.0375 (11)	0.0387 (11)	0.0014 (10)	0.0054 (9)	0.0096 (9)
C9	0.0628 (15)	0.0461 (13)	0.0436 (12)	0.0069 (11)	0.0116 (11)	0.0071 (10)
C12	0.0581 (14)	0.0393 (12)	0.0463 (13)	0.0068 (10)	0.0044 (10)	0.0076 (9)
C8	0.0476 (12)	0.0429 (12)	0.0383 (11)	−0.0006 (9)	0.0008 (9)	0.0096 (9)
N4	0.0932 (17)	0.0420 (11)	0.0545 (13)	0.0128 (11)	0.0300 (12)	0.0158 (9)
C7	0.0702 (16)	0.0512 (14)	0.0475 (13)	−0.0013 (12)	0.0140 (12)	0.0159 (11)
C11	0.094 (2)	0.0426 (14)	0.074 (2)	0.0197 (14)	0.0196 (17)	0.0118 (13)
N2	0.0515 (11)	0.0420 (10)	0.0458 (11)	−0.0001 (9)	0.0120 (8)	0.0094 (8)
N3	0.0563 (12)	0.0423 (10)	0.0505 (12)	0.0016 (9)	0.0129 (9)	0.0112 (9)
C6	0.0574 (14)	0.0451 (12)	0.0490 (13)	0.0119 (11)	0.0147 (11)	0.0138 (10)

N1	0.0679 (14)	0.0504 (12)	0.0507 (12)	−0.0145 (11)	0.0014 (10)	0.0147 (9)
C4	0.0480 (12)	0.0426 (12)	0.0443 (12)	0.0013 (10)	0.0116 (10)	0.0070 (9)
C2	0.0444 (12)	0.0497 (13)	0.0494 (13)	0.0098 (10)	0.0111 (10)	0.0051 (10)
C3	0.0547 (14)	0.0561 (14)	0.0472 (13)	0.0110 (12)	0.0089 (11)	0.0118 (11)
C1	0.0571 (15)	0.0599 (16)	0.0599 (16)	0.0006 (13)	0.0025 (12)	0.0015 (13)
C5	0.085 (2)	0.0530 (15)	0.0628 (17)	0.0037 (14)	0.0126 (15)	0.0231 (13)

Geometric parameters (Å, º)

Cl1—C15	1.766 (3)	C7—H7A	0.9600
O4—C16	1.271 (3)	C7—H7B	0.9600
C16—O3	1.219 (3)	C7—H7C	0.9600
C16—C15	1.512 (3)	C11—H11A	0.9600
C15—H15A	0.9700	C11—H11B	0.9600
C15—H15B	0.9700	C11—H11C	0.9600
Cl2—C13	1.767 (3)	N2—C2	1.347 (3)
O2—C14	1.273 (3)	N2—C4	1.357 (3)
C14—O1	1.220 (3)	N2—H2A	0.8600
C14—C13	1.507 (4)	N3—C6	1.331 (3)
C13—H13A	0.9700	N3—C4	1.344 (3)
C13—H13B	0.9700	C6—C3	1.389 (4)
N5—C8	1.337 (3)	C6—C5	1.505 (3)
N5—C10	1.356 (3)	N1—C4	1.326 (3)
N5—H5A	0.8600	N1—H1A	0.8600
N6—C12	1.331 (3)	N1—H1B	0.8600
N6—C10	1.342 (3)	C2—C3	1.372 (4)
C10—N4	1.322 (3)	C2—C1	1.493 (4)
C9—C8	1.378 (4)	C3—H3B	0.9300
C9—C12	1.389 (3)	C1—H1C	0.9600
C9—H9A	0.9300	C1—H1D	0.9600
C12—C11	1.501 (4)	C1—H1E	0.9600
C8—C7	1.495 (3)	C5—H5B	0.9600
N4—H4A	0.8600	C5—H5C	0.9600
N4—H4B	0.8600	C5—H5D	0.9600
O3—C16—O4	126.0 (2)	C8—C7—H7C	109.5
O3—C16—C15	121.5 (2)	H7A—C7—H7C	109.5
O4—C16—C15	112.5 (2)	H7B—C7—H7C	109.5
C16—C15—Cl1	113.42 (19)	C12—C11—H11A	109.5
C16—C15—H15A	108.9	C12—C11—H11B	109.5
Cl1—C15—H15A	108.9	H11A—C11—H11B	109.5
C16—C15—H15B	108.9	C12—C11—H11C	109.5
Cl1—C15—H15B	108.9	H11A—C11—H11C	109.5
H15A—C15—H15B	107.7	H11B—C11—H11C	109.5
O1—C14—O2	125.4 (2)	C2—N2—C4	119.3 (2)
O1—C14—C13	116.1 (2)	C2—N2—H2A	120.4
O2—C14—C13	118.5 (2)	C4—N2—H2A	120.4
C14—C13—Cl2	115.3 (2)	C6—N3—C4	117.5 (2)

C14—C13—H13A	108.5	N3—C6—C3	122.1 (2)
Cl2—C13—H13A	108.5	N3—C6—C5	116.2 (2)
C14—C13—H13B	108.5	C3—C6—C5	121.7 (2)
Cl2—C13—H13B	108.5	C4—N1—H1A	120.0
H13A—C13—H13B	107.5	C4—N1—H1B	120.0
C8—N5—C10	119.4 (2)	H1A—N1—H1B	120.0
C8—N5—H5A	120.3	N1—C4—N3	118.6 (2)
C10—N5—H5A	120.3	N1—C4—N2	118.3 (2)
C12—N6—C10	117.6 (2)	N3—C4—N2	123.1 (2)
N4—C10—N6	118.5 (2)	N2—C2—C3	119.7 (2)
N4—C10—N5	118.3 (2)	N2—C2—C1	116.9 (2)
N6—C10—N5	123.2 (2)	C3—C2—C1	123.4 (2)
C8—C9—C12	118.4 (2)	C2—C3—C6	118.4 (2)
C8—C9—H9A	120.8	C2—C3—H3B	120.8
C12—C9—H9A	120.8	C6—C3—H3B	120.8
N6—C12—C9	121.8 (2)	C2—C1—H1C	109.5
N6—C12—C11	116.7 (2)	C2—C1—H1D	109.5
C9—C12—C11	121.5 (2)	H1C—C1—H1D	109.5
N5—C8—C9	119.7 (2)	C2—C1—H1E	109.5
N5—C8—C7	117.8 (2)	H1C—C1—H1E	109.5
C9—C8—C7	122.5 (2)	H1D—C1—H1E	109.5
C10—N4—H4A	120.0	C6—C5—H5B	109.5
C10—N4—H4B	120.0	C6—C5—H5C	109.5
H4A—N4—H4B	120.0	H5B—C5—H5C	109.5
C8—C7—H7A	109.5	C6—C5—H5D	109.5
C8—C7—H7B	109.5	H5B—C5—H5D	109.5
H7A—C7—H7B	109.5	H5C—C5—H5D	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N3^{i}	0.86	2.14	2.999 (3)	177
N1—H1*B*···O3^{ii}	0.86	1.98	2.830 (3)	173
N2—H2*A*···O4^{ii}	0.86	1.74	2.593 (3)	175
N4—H4*A*···N6^{iii}	0.86	2.19	3.046 (3)	175
N4—H4*B*···O1^{iv}	0.86	2.00	2.851 (3)	173
N5—H5*A*···O2^{iv}	0.86	1.75	2.606 (3)	174
C1—H1*C*···O4^{ii}	0.96	2.56	3.355 (4)	140
C7—H7*A*···O2^{iv}	0.96	2.57	3.355 (4)	139

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