organic compounds

2-Aminopyrimidinium hydrogen chloranilate monohydrate

Ping Su, Xue-Ying Huang and Xiang-gao Meng*

Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

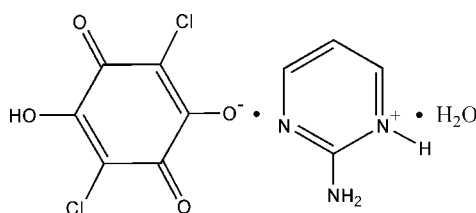Correspondence e-mail: mengxianggao@mail.ccnu.edu.cn

In the title compound, $C_4H_6N_3^+ \cdot C_6HCl_2O_4^- \cdot H_2O$, anions, cations and water molecules are linked by intermolecular O—H⋯O, O—H⋯N and N—H⋯O hydrogen bonds into one-dimensional tapes along [111]. These tapes are further linked by weak Cl⋯Cl interactions [Cl⋯Cl = 3.394 (2) Å], forming sheets parallel to the $(10\bar{1})$ plane.

Related literature

For background information, see: Aakeröy & Salmon (2005); Aakeröy *et al.* (2007); Abrahams *et al.* (2002); Cueto *et al.* (1992); Kawata *et al.* (1994, 1998). For related crystal structures, see: Meng & Qian (2006); Min *et al.* (2006, 2007); Murata *et al.* (2007); Wang & Wei (2005); Yang (2007); Gaballa *et al.* (2008); Gotoh *et al.* (2006, 2007*a*,*b*,*c*); Jia *et al.* (2008). For bond-length data, see: Allen (2002); Allen *et al.* (1987).

Experimental

Crystal data

$C_4H_6N_3^+ \cdot C_6HCl_2O_4^- \cdot H_2O$	$\gamma = 101.925$ (1)°
$M_r = 322.10$	$V = 626.01$ (7) Å³
Triclinic, $P\bar{1}$	$Z = 2$
$a = 6.7969$ (5) Å	Mo $K\alpha$ radiation
$b = 9.4631$ (6) Å	$\mu = 0.54$ mm⁻¹
$c = 11.0604$ (7) Å	$T = 292$ (2) K
$\alpha = 106.074$ (1)°	$0.27 \times 0.10 \times 0.04$ mm
$\beta = 105.892$ (1)°	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5691 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2121 independent reflections
$T_{min} = 0.857$, $T_{max} = 0.979$	1348 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.071$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.078$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.197$	
$S = 0.97$	
2121 reflections	$\Delta\rho_{max} = 0.66$ e Å⁻³
199 parameters	$\Delta\rho_{min} = -0.45$ e Å⁻³
6 restraints	

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O4—H4⋯O3	0.83 (2)	2.16 (6)	2.651 (5)	118 (5)
O4—H4⋯N1ⁱ	0.83 (2)	2.07 (4)	2.795 (6)	146 (6)
O5—H5A⋯O2	0.82 (4)	2.09 (3)	2.872 (5)	156 (5)
O5—H5A⋯O1	0.82 (4)	2.34 (4)	2.859 (5)	121 (4)
O5—H5B⋯O2ⁱⁱ	0.82 (4)	2.09 (4)	2.830 (5)	150 (5)
N3—H3A⋯O5	0.86 (2)	2.02 (3)	2.815 (6)	153 (5)
N2—H2⋯O1	0.84 (5)	1.98 (5)	2.793 (6)	163 (5)
N3—H3B⋯O3ⁱⁱⁱ	0.86 (2)	2.17 (4)	2.953 (6)	151 (5)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT-Plus* (Bruker, 2007); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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supplementary materials

2-Aminopyrimidinium hydrogen chloranilate monohydrate

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Comment

Chloranilic acid (CA) can be regarded as a strong organic acid (pK_{a1}= 1.38; pK_{a2} = 2.98) which can release its two hydroxyl protons easily. For this reason, CA is often used as a bridge ligand in the synthesis of metal coordination complexes (Kawata *et al.*, 1994; Kawata *et al.*, 1998; Abrahams *et al.*, 2002; Cueto *et al.*, 1992; Min *et al.*, 2006; Min *et al.*, 2007) or used as a cocrystal agent in the construction of supramolecular structure based on hydrogen-bonds (Gotoh *et al.*, 2006, 2007*a*, 2007*b* and 2007*c*; Murata *et al.*, 2007; Gaballa *et al.*, 2008; Jia *et al.*, 2008). As part of our continuing studies on the synthesis of co-crystal or organic salts involved CA (Meng & Qian, 2006), we report here the crystal structure of the title compound (I) which was obtained by mixing equivalent amount of CA and 2-aminopyrimidine (2-APy) in 95% methanol solution at room temperature.

In (I), one of the CA hydroxyl protons is transferred to a pyrimidine N atom, forming a 1:1 organic adduct with one water molecule being incorporated into the crystal lattice (Fig. 1). According to the definitions of co-crystal and organic salt proposed by Aakeröy and Salmon (2005), complex (I) can be considered as an organic salt. The bond lengths and bonds angles in the CA⁻ anion are comparable with those from some analogues (Wang & Wei, 2005; Yang, 2007). In the 2-APy⁺ cation, the angles of C7—N1—C8 and C7—N2—C10 [116.5 (1)° and 122.2 (1)°, respectively] are both consistent with the magnitude of C—N—C angles in unprotonated and protonated pyridine molecules [116.3 (16)° and 122.4 (16)°, respectively] (Allen *et al.*, 1987; Allen, 2002). All other geomtric parameters in the structure are as expected.

In the crystal structure, intermolecular O–H⋯O and N–H⋯O hydrogen bonds (Table 1), link the components of (I) into one-dimensional tapes along [111] (Fig.2). In addition, neighbouring tapes are linked by weak Cl⋯Cl interactions [Cl⋯Cl[i] = 3.394 (2) Å, see: Aakeröy *et al.*, 2007); symmetry code: (i) x, y+1, z)] resulting in two-dimensional sheets parallel to the (10-1) plane.

Experimental

All the reagents and solvents were used as obtained without further purification. Equivalent molar amount of chloranilic acid (1 mmol, 210 mg) and 2-aminopyimidine (1 mmol, 9.5 mg) were dissolved in 95% methanol (20 ml). The mixture was stirred for half an hour at ambient temperature and then filtered. The resulting red solution was kept in air for two week. Plate-like crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown at the bottom of the vessel by slow evaporation of the solution.

Refinement

H atoms bonded to C atoms were located in difference maps and subsequently treated as riding modes, with C–H=0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to N and O atoms were also found in difference maps, with the constraints

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of N—H =0.86 (2)Å and O—H =0.82 (2) Å, and the U_{iso}(H) values being set k times of their carrier atoms (k=1.2 for N and 1.5 for O atoms)
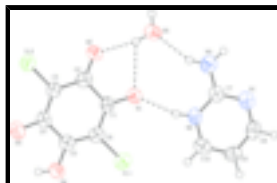
Figures

Fig. 1. Molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H-bonds are shown in dashed lines.
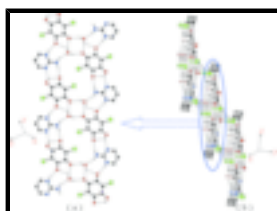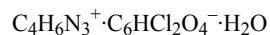

Fig. 2. Part of the crystal structure of (I), showing the formation of the one-dimensional tape (a) linked by intermolecular O-H⋯O and N-H⋯O hydrogen bonds parallel to the [111] direction and the two-dimensional sheet (b) linked by Cl⋯Cl interactin. For the sake of clarity, H atoms not involved in the motif have been omitted from the drawing.

2-Aminopyrimidinium hydrogen chloranilate monohydrate

Crystal data

$C_4H_6N_3{}^+ \cdot C_6HCl_2O_4{}^- \cdot H_2O$	$Z = 2$
$M_r = 322.10$	$F_{000} = 328$
Triclinic, $P\overline{1}$	$D_x = 1.709$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.7969$ (5) Å	Cell parameters from 1004 reflections
$b = 9.4631$ (6) Å	$\theta = 2.2–25.2º$
$c = 11.0604$ (7) Å	$\mu = 0.54$ mm^{-1}
$\alpha = 106.074$ (1)º	$T = 292$ (2) K
$\beta = 105.892$ (1)º	Plate, red
$\gamma = 101.925$ (1)º	$0.27 \times 0.10 \times 0.04$ mm
$V = 626.01$ (7) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2121 independent reflections
Radiation source: fine focus sealed Siemens Mo tube	1348 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.071$
$T = 292(2)$ K	$\theta_{max} = 25.0º$
0.3° wide ω exposures scans	$\theta_{min} = 2.4º$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -7 \rightarrow 8$
$T_{min} = 0.857$, $T_{max} = 0.979$	$k = -11 \rightarrow 11$
5691 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.078$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.197$	$w = 1/[\sigma^2(F_o^2) + (0.1114P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} < 0.001$
2121 reflections	$\Delta\rho_{max} = 0.66$ e Å^{-3}
199 parameters	$\Delta\rho_{min} = -0.45$ e Å^{-3}
6 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

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 $F^2 > 2$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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	−0.1247 (7)	0.1172 (6)	0.1769 (5)	0.0361 (12)
C2	−0.1473 (7)	−0.0408 (6)	0.2001 (5)	0.0425 (13)
C3	−0.2335 (8)	−0.1755 (5)	0.0838 (5)	0.0378 (12)
C4	−0.3014 (7)	−0.1738 (6)	−0.0449 (5)	0.0358 (12)
C5	−0.2867 (7)	−0.0171 (6)	−0.0623 (5)	0.0372 (12)
C6	−0.2029 (7)	0.1163 (6)	0.0438 (5)	0.0363 (12)
Cl1	−0.1870 (2)	0.29304 (15)	0.02393 (13)	0.0479 (5)
Cl2	−0.2558 (2)	−0.35198 (15)	0.10632 (14)	0.0500 (5)
O1	−0.0385 (6)	0.2339 (4)	0.2793 (3)	0.0506 (10)
O2	−0.0871 (6)	−0.0336 (4)	0.3183 (3)	0.0547 (11)
O3	−0.3780 (6)	−0.2884 (4)	−0.1520 (4)	0.0513 (10)
O4	−0.3561 (6)	−0.0196 (4)	−0.1857 (4)	0.0509 (10)
H4	−0.399 (10)	−0.110 (3)	−0.238 (5)	0.076*
C7	0.3286 (7)	0.6009 (6)	0.5065 (5)	0.0365 (12)
C8	0.5278 (8)	0.8089 (6)	0.4821 (6)	0.0462 (14)
H8	0.6301	0.9059	0.5206	0.055*

C9	0.4403 (9)	0.7485 (6)	0.3461 (6)	0.0481 (14)
H9	0.4801	0.8020	0.2933	0.058*
C10	0.2900 (8)	0.6044 (7)	0.2895 (5)	0.0468 (14)
H10	0.2244	0.5573	0.1967	0.056*
N1	0.4796 (6)	0.7413 (5)	0.5644 (4)	0.0447 (11)
N2	0.2407 (6)	0.5338 (5)	0.3717 (4)	0.0378 (11)
H2	0.162 (9)	0.442 (6)	0.329 (5)	0.045*
N3	0.2768 (7)	0.5294 (6)	0.5858 (5)	0.0504 (12)
H3A	0.200 (8)	0.434 (3)	0.548 (5)	0.060*
H3B	0.337 (9)	0.579 (6)	0.671 (2)	0.060*
O5	0.0043 (6)	0.2393 (4)	0.5451 (3)	0.0493 (10)
H5A	−0.050 (10)	0.171 (5)	0.468 (2)	0.074*
H5B	0.021 (10)	0.205 (6)	0.606 (3)	0.074*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.026 (3)	0.037 (3)	0.041 (3)	0.006 (2)	0.012 (2)	0.009 (3)
C2	0.024 (3)	0.053 (4)	0.050 (3)	0.008 (2)	0.011 (2)	0.023 (3)
C3	0.034 (3)	0.034 (3)	0.046 (3)	0.013 (2)	0.015 (2)	0.013 (3)
C4	0.020 (3)	0.042 (3)	0.040 (3)	0.011 (2)	0.010 (2)	0.006 (3)
C5	0.027 (3)	0.047 (3)	0.042 (3)	0.016 (2)	0.016 (2)	0.016 (3)
C6	0.023 (3)	0.045 (3)	0.048 (3)	0.015 (2)	0.015 (2)	0.020 (3)
Cl1	0.0427 (8)	0.0484 (9)	0.0582 (9)	0.0174 (6)	0.0181 (7)	0.0246 (7)
Cl2	0.0507 (9)	0.0413 (8)	0.0540 (9)	0.0113 (6)	0.0153 (7)	0.0161 (7)
O1	0.058 (2)	0.044 (2)	0.040 (2)	0.0055 (19)	0.0164 (19)	0.0100 (19)
O2	0.070 (3)	0.049 (2)	0.034 (2)	0.010 (2)	0.0066 (19)	0.0145 (18)
O3	0.052 (2)	0.046 (2)	0.044 (2)	0.0126 (19)	0.0096 (19)	0.0068 (19)
O4	0.062 (3)	0.046 (2)	0.038 (2)	0.016 (2)	0.0110 (19)	0.0117 (17)
C7	0.024 (3)	0.045 (3)	0.043 (3)	0.018 (2)	0.013 (2)	0.012 (3)
C8	0.026 (3)	0.047 (3)	0.059 (4)	0.006 (2)	0.015 (3)	0.013 (3)
C9	0.044 (3)	0.057 (4)	0.053 (4)	0.019 (3)	0.019 (3)	0.029 (3)
C10	0.040 (3)	0.062 (4)	0.043 (3)	0.021 (3)	0.017 (3)	0.017 (3)
N1	0.031 (2)	0.048 (3)	0.051 (3)	0.016 (2)	0.010 (2)	0.011 (2)
N2	0.024 (2)	0.037 (2)	0.044 (3)	0.0089 (18)	0.0065 (19)	0.007 (2)
N3	0.041 (3)	0.052 (3)	0.058 (3)	0.014 (2)	0.017 (3)	0.020 (3)
O5	0.051 (2)	0.059 (2)	0.040 (2)	0.021 (2)	0.013 (2)	0.0214 (19)

Geometric parameters (Å, °)

C1—O1	1.234 (6)	C7—N2	1.347 (6)
C1—C6	1.419 (7)	C7—N1	1.354 (6)
C1—C2	1.569 (7)	C8—N1	1.321 (6)
C2—O2	1.236 (5)	C8—C9	1.355 (7)
C2—C3	1.412 (7)	C8—H8	0.9300
C3—C4	1.377 (7)	C9—C10	1.377 (7)
C3—Cl2	1.738 (5)	C9—H9	0.9300
C4—O3	1.252 (6)	C10—N2	1.341 (6)
C4—C5	1.533 (7)	C10—H10	0.9300

C5—O4	1.308 (6)	N2—H2	0.84 (5)
C5—C6	1.346 (7)	N3—H3A	0.86 (2)
C6—Cl1	1.732 (5)	N3—H3B	0.86 (2)
O4—H4	0.83 (2)	O5—H5A	0.82 (4)
C7—N3	1.323 (6)	O5—H5B	0.82 (4)
O1—C1—C6	125.3 (5)	N3—C7—N1	118.2 (5)
O1—C1—C2	115.6 (4)	N2—C7—N1	120.6 (4)
C6—C1—C2	119.1 (5)	N1—C8—C9	125.3 (5)
O2—C2—C3	127.1 (5)	N1—C8—H8	117.3
O2—C2—C1	116.4 (5)	C9—C8—H8	117.3
C3—C2—C1	116.5 (4)	C8—C9—C10	117.1 (5)
C4—C3—C2	123.5 (4)	C8—C9—H9	121.4
C4—C3—Cl2	118.9 (4)	C10—C9—H9	121.4
C2—C3—Cl2	117.6 (4)	N2—C10—C9	118.2 (5)
O3—C4—C3	126.8 (5)	N2—C10—H10	120.9
O3—C4—C5	115.2 (4)	C9—C10—H10	120.9
C3—C4—C5	118.1 (5)	C8—N1—C7	116.5 (5)
O4—C5—C6	121.7 (5)	C10—N2—C7	122.2 (5)
O4—C5—C4	116.6 (4)	C10—N2—H2	112 (3)
C6—C5—C4	121.8 (4)	C7—N2—H2	126 (3)
C5—C6—C1	121.0 (5)	C7—N3—H3A	117 (4)
C5—C6—Cl1	121.7 (4)	C7—N3—H3B	117 (4)
C1—C6—Cl1	117.4 (4)	H3A—N3—H3B	126 (5)
C1—O1—H2	135.7 (14)	H3A—O5—H5A	112 (4)
C2—O2—H5A	118.4 (13)	H3A—O5—H5B	126 (4)
C5—O4—H4	109 (4)	H5A—O5—H5B	114 (3)
N3—C7—N2	121.2 (5)		
O1—C1—C2—O2	3.6 (7)	O4—C5—C6—Cl1	1.4 (7)
C6—C1—C2—O2	−176.2 (4)	C4—C5—C6—Cl1	−179.9 (3)
O1—C1—C2—C3	−176.3 (4)	O1—C1—C6—C5	177.2 (5)
C6—C1—C2—C3	3.9 (7)	C2—C1—C6—C5	−3.0 (7)
O2—C2—C3—C4	178.5 (5)	O1—C1—C6—Cl1	−3.0 (7)
C1—C2—C3—C4	−1.7 (7)	C2—C1—C6—Cl1	176.8 (3)
O2—C2—C3—Cl2	−1.0 (7)	C6—C1—O1—H2	−38 (2)
C1—C2—C3—Cl2	178.8 (3)	C2—C1—O1—H2	143 (2)
C2—C3—C4—O3	179.6 (5)	C3—C2—O2—H5A	−163 (2)
Cl2—C3—C4—O3	−0.9 (7)	C1—C2—O2—H5A	17 (2)
C2—C3—C4—C5	−1.4 (7)	N1—C8—C9—C10	−0.4 (8)
Cl2—C3—C4—C5	178.1 (3)	C8—C9—C10—N2	−0.1 (8)
O3—C4—C5—O4	0.4 (6)	C9—C8—N1—C7	−0.7 (8)
C3—C4—C5—O4	−178.8 (4)	N3—C7—N1—C8	179.8 (5)
O3—C4—C5—C6	−178.4 (4)	N2—C7—N1—C8	2.4 (7)
C3—C4—C5—C6	2.5 (7)	C9—C10—N2—C7	1.9 (8)
O4—C5—C6—C1	−178.8 (4)	N3—C7—N2—C10	179.6 (5)
C4—C5—C6—C1	−0.1 (7)	N1—C7—N2—C10	−3.1 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*		*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O4—H4···O3	0.83 (2)	2.16 (6)	2.651 (5)	118 (5)
O4—H4···N1[i]	0.83 (2)	2.07 (4)	2.795 (6)	146 (6)
O5—H5A···O2	0.82 (4)	2.09 (3)	2.872 (5)	156 (6)
O5—H5A···O1	0.82 (4)	2.34 (4)	2.859 (5)	121 (4)
O5—H5B···O2[ii]	0.82 (4)	2.09 (4)	2.830 (5)	150 (5)
N3—H3A···O5	0.86 (2)	2.02 (3)	2.815 (6)	153 (5)
N2—H2···O1	0.84 (5)	1.98 (5)	2.793 (6)	163 (5)
N3—H3B···O3[iii]	0.86 (2)	2.17 (4)	2.953 (6)	151 (5)

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

Fig. 1

Fig. 2