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## Key indicators

Single-crystal X-ray study

T = 298 K

Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

R factor = 0.060

wR factor = 0.141

Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Benzimidazolium chloranilate monohydrate

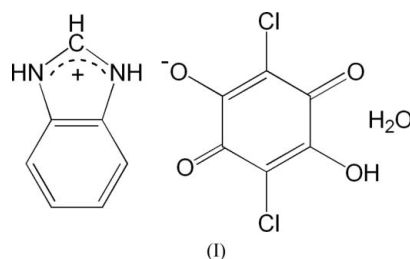
In the title compound,  $\text{C}_7\text{H}_7\text{N}_2^+ \cdot \text{C}_6\text{HCl}_2\text{O}_4^- \cdot \text{H}_2\text{O}$ , the components are linked by hydrogen bonds into layers running parallel to  $(\bar{2}04)$ , built from a sequence of  $R_{10}^{10}(38)$ ,  $R_4^4(18)$  and  $R_3^2(10)$  rings. These layers are further linked into a three-dimensional network by means of an  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bond and  $\pi-\pi$  stacking interactions.

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## Comment

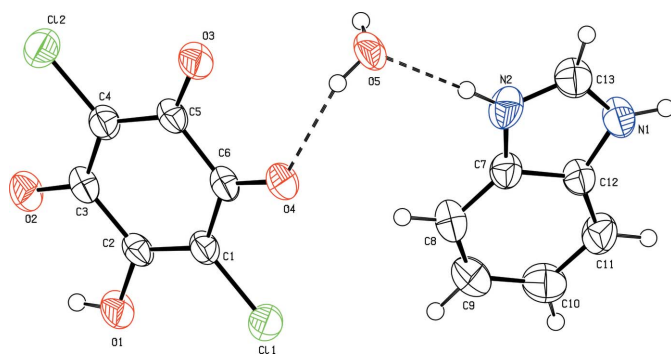
The X-ray crystal structures of a series of chloranilate complexes with imidazole and benzotriazole have been reported recently (Meng & Qian, 2006; Wang & Wei, 2005; Ishida & Kashino, 2001). In order to study further how molecules interact in the solid state, we have prepared the title compound, (I), and report here details of its crystal structure.



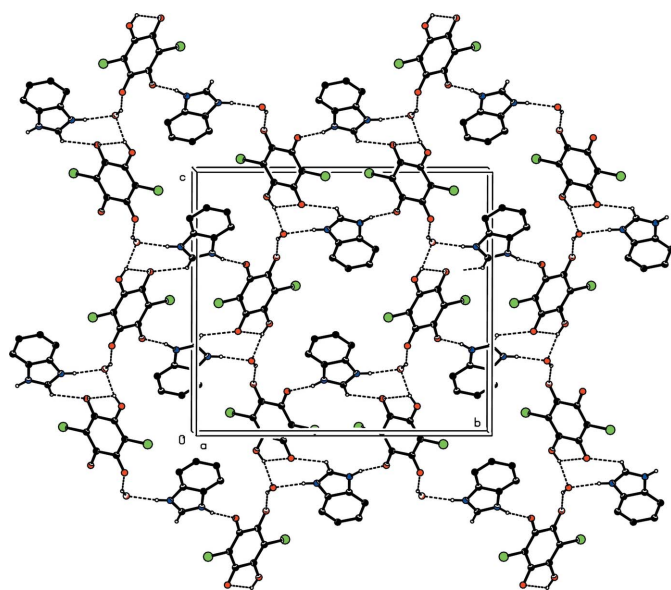
The asymmetric unit of (I) consists of a benzimidazolium cation, one chloranilate anion and a water molecule (Fig. 1). As expected, (I) exists as an organic salt, with one of the chloranilic hydroxyl H atoms transferred to the benzimidazole N atom. Bond lengths and angles are unremarkable.

The supramolecular structure of (I) contains both N (or O)–H  $\cdots$  O and C–H  $\cdots$  O hydrogen bonds (Table 1), as well as  $\pi-\pi$  stacking interactions. As a result, the crystal structure is three-dimensional, similar to recently reported structures (Meng & Qian, 2006; Wang & Wei, 2005). The formation of the three-dimensional supramolecular network can be described in term of layers running parallel to  $(\bar{2}04)$  and chains along the [100] direction. Hydrogen bonds with atoms N1, O1, N2 and O5 as donors (Table 1) form centrosymmetric  $R_{10}^{10}(38)$  rings centred at  $(-\frac{1}{2}, 1, 0)$  (Batten & Robson, 1998) (Fig. 2). In a similar way, another centrosymmetric  $R_4^4(18)$  ring centred at  $(-\frac{1}{2}, \frac{1}{2}, 0)$  is formed by means of an N–H  $\cdots$  O hydrogen bond and a C–H  $\cdots$  O interaction, forming the only non-classical hydrogen bond in the crystal structure. In addition, hydrogen bonds with atoms C13, N2 and O1 as donors form an  $R_3^2(10)$  ring. Propagation of these three ring types generates a layer running parallel to  $(\bar{2}04)$ .

Analysis using *PLATON* (Spek, 2003) shows that the only possible direction-specific interaction between adjacent layers

**Figure 1**

The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

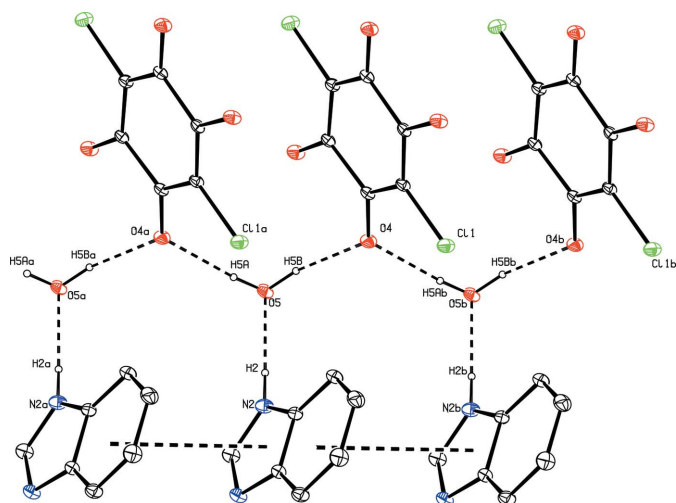
**Figure 2**

Part of the crystal structure of (I), showing the formation of a  $(\bar{2}04)$  sheet of  $R_{10}^{10}(38)$ ,  $R_4^4(18)$  and  $R_3^2(10)$  rings generated by N—H...O, O—H...O and C—H...O hydrogen bonds (dashed lines). For the sake of clarity, H atoms not involved in these motifs have been omitted.

is from an O5—H5A...O4 hydrogen bond and a  $\pi$ – $\pi$  stacking interaction between the imidazole and benzene rings, which propagate along the [100] direction (Fig. 3). The imidazole ring at  $(x, y, z)$  and the benzene ring at  $(-1 + x, y, z)$  are almost parallel, with a dihedral angle of  $1.2(1)^\circ$ , an interplanar spacing of  $3.451(1) \text{ \AA}$  and a centroid separation of  $3.655(2) \text{ \AA}$ . The effect of this interaction is to consolidate the adjacent  $(\bar{2}04)$  layers, forming a three-dimensional network.

## Experimental

All reagents and solvents were used as obtained without further purification. Chloranilic acid (1 mmol, 0.209 g) and benzimidazole (1 mmol, 0.106 g) were dissolved in methanol (20 ml). The mixture was stirred for half an hour at ambient temperature and then filtered. The resulting clear red solution was kept in air for two weeks. Crystals of (I) suitable for single-crystal X-ray diffraction analysis were grown by slow evaporation of the solution at the bottom of the vessel.

**Figure 3**

Part of the crystal structure of (I), viewed along the [100] direction, showing  $\pi$ – $\pi$  interactions and hydrogen bonds as dashed lines. For the sake of clarity, H atoms not involved in the motifs have been omitted. Atoms marked with the suffixes a and b are at the symmetry positions  $(-1 + x, y, z)$  and  $(1 + x, y, z)$ , respectively.

## Crystal data

$C_7H_7N_2^+ \cdot C_6HCl_2O_4^- \cdot H_2O$   
 $M_r = 345.13$   
 Monoclinic,  $P2_1/c$   
 $a = 4.5087(8) \text{ \AA}$   
 $b = 18.886(3) \text{ \AA}$   
 $c = 16.825(3) \text{ \AA}$   
 $\beta = 91.896(3)^\circ$   
 $V = 1431.9(4) \text{ \AA}^3$

$Z = 4$   
 $D_x = 1.601 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.48 \text{ mm}^{-1}$   
 $T = 298(2) \text{ K}$   
 Block, red  
 $0.20 \times 0.15 \times 0.13 \text{ mm}$

## Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 16576 measured reflections

3453 independent reflections  
 2378 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.091$   
 $\theta_{max} = 28.3^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.060$   
 $wR(F^2) = 0.142$   
 $S = 1.02$   
 3453 reflections  
 214 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0696P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.68 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.24 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1...O3 <sup>i</sup>	0.86 (1)	1.84 (1)	2.688 (3)	166 (3)
O1—H1C...O5 <sup>ii</sup>	0.82 (1)	1.91 (1)	2.667 (2)	154 (3)
O5—H5A...O4 <sup>iii</sup>	0.82 (1)	1.96 (1)	2.786 (3)	175 (3)
C13—H13...O2 <sup>iv</sup>	0.93	2.42	3.045 (3)	124
O1—H1C...O2	0.82 (1)	2.22 (3)	2.664 (3)	114 (3)
N2—H2...O5	0.86 (1)	1.97 (1)	2.818 (3)	173 (3)
O5—H5B...O4	0.82 (1)	2.06 (1)	2.824 (2)	155 (3)

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

The aromatic H atoms were placed in ideal geometric positions with C–H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The imidazole, hydroxyl and water H atoms were located in difference maps and refined with the restraints N–H = 0.86 (1) Å and  $U_{\text{iso}}(\text{H}) = 0.054 \text{ \AA}^2$ , and O–H = 0.82 (1) Å and  $U_{\text{iso}}(\text{H}) = 0.067 \text{ \AA}^2$ .

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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