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# 2-Carboxypyridinium hydrogen chloranilate

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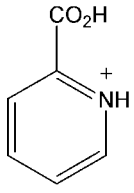
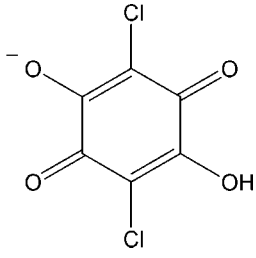
Key indicators: single-crystal X-ray study; $T$ = 103 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.045; $wR$ factor = 0.144; data-to-parameter ratio = 17.0.

In the crystal structure of the title salt, $C_6H_6NO_2^+\cdot C_6HCl_2O_4^-$, the pyridine ring and the mean plane of the hydrogen chloranilate anion form a dihedral angle of 77.40 (8)°. The ionic components are held together by N—H···O and O—H···O hydrogen bonds, forming a supramolecular ladder. C—H···O interactions are also present.

## Related literature

For the structures of related carboxypyridinium hydrogen chloranilates, see: Gotoh *et al.* (2006); Tabuchi *et al.* (2005); Ishida (2009).




## Experimental

### Crystal data

$C_6H_6NO_2^+\cdot C_6HCl_2O_4^-$
$M_r$ = 332.10
Monoclinic, $P2_1/c$
$a$ = 9.4166 (8) Å
$b$ = 19.6900 (16) Å
$c$ = 6.7089 (6) Å
$\beta$ = 99.043 (3)°
$V$ = 1228.45 (18) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.56 mm$^{-1}$
$T$ = 103 K
0.30 × 0.30 × 0.23 mm

### Data collection

Rigaku R-AXIS RAPID-II diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.847, $T_{max}$ = 0.880
9710 measured reflections
3433 independent reflections
2228 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.047

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.144
$S$ = 1.10
3433 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.92 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1 | 0.92 (4) | 2.11 (3) | 2.932 (2) | 147 (3) |
| O2—H2···O5$^{i}$ | 0.79 (3) | 2.05 (3) | 2.746 (2) | 148 (3) |
| O6—H6···O4$^{ii}$ | 0.90 (3) | 1.63 (3) | 2.528 (2) | 177.1 (15) |
| C8—H8···O4$^{iii}$ | 0.95 | 2.50 | 3.338 (3) | 147 |
| C9—H9···O3$^{iv}$ | 0.95 | 2.33 | 3.227 (3) | 156 |
| C11—H11···O1$^{v}$ | 0.95 | 2.46 | 3.374 (3) | 162 |

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

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2376).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o614 [ **doi:10.1107/S1600536809006412** ]

# 2-Carboxypyridinium hydrogen chloranilate

**K. Gotoh, H. Nagoshi and H. Ishida**

## Comment

The title salt, (I), was prepared in order to extend our study on D—H···A hydrogen bonding (D = N, O or C; A = N, O or Cl) in chloranilic acid – substituted-pyridine systems (Gotoh *et al.*, 2006; Tabuchi *et al.*, 2005).

Compound (I) comprises 2-carboxypyridinium cations and hydrogen chloranilate anions in the ratio 1:1. Ions directly connected by an N—H···O hydrogen bond, Fig. 1, form a dihedral angle between their respective mean planes of 77.40 (8)°. In the cation, the carboxy O5/O6/C12 plane forms a dihedral angle of 11.44 (6)° with the pyridine ring, which is similar to those of 2.74 (6) and 10.01 (3)° observed in 3-carboxypyridinium hydrogen chloranilate and 4-carboxypyridinium hydrogen chloranilate monohydrate, respectively (Ishida, 2009). The ions are further connected by O—H···O hydrogen bonds (Table 1) to afford a supramolecular ladder running along the *c* axis (Fig. 2). The ladders are linked by weaker N—H···O hydrogen bonds and C—H···O contacts to form a 3-D network (Table 1).

## Experimental

Crystals were obtained by slow evaporation from a methanol solution (*ca* 30 ml) containing a 1:1 molar ratio of chloranilic acid (0.302 g) and picolinic acid (0.179 g).

## Refinement

The H atoms attached to O and N were located from a difference Fourier map and refined isotropically to O—H = 0.79 (3) & 0.90 (3) Å and N—H = 0.92 (4) Å. The remaining H atoms were included in the riding approximation with C—H = 0.95 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C).

## Figures

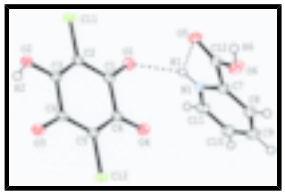

Fig. 1. Molecular components of (I) showing the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Intra- and inter-molecular N—H···O hydrogen bonds are indicated by dashed lines.

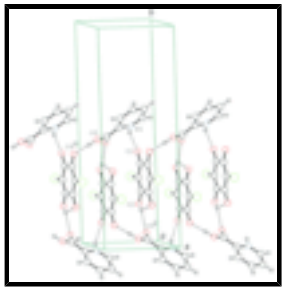

Fig. 2. A partial packing diagram, viewed approximately along the *a* axis, showing the hydrogen-bonded supramolecular ladder. Dashed lines show N—H···O and O—H···O hydrogen bonds (symmetry codes as given in Table 1).

**2-Carboxypyridinium hydrogen chloranilate**

*Crystal data*

| | |
|---|---|
| $C_6H_6NO_2^+ \cdot C_6HCl_2O_4^-$ | $F_{000}$ = 672.00 |
| $M_r$ = 332.10 | $D_x$ = 1.795 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71075 Å |
| Hall symbol: -P 2ybc | Cell parameters from 7392 reflections |
| $a$ = 9.4166 (8) Å | θ = 3.0–30.0º |
| $b$ = 19.6900 (16) Å | μ = 0.56 mm$^{-1}$ |
| $c$ = 6.7089 (6) Å | $T$ = 103 K |
| β = 99.043 (3)º | Platelet, dark purple |
| $V$ = 1228.45 (18) Å$^3$ | 0.30 × 0.30 × 0.23 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Rigaku R-AXIS RAPID-II diffractometer | 2228 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.00 pixels mm$^{-1}$ | $R_{int}$ = 0.047 |
| ω scans | $\theta_{max}$ = 30.0º |
| Absorption correction: Multi-scan (*ABSCOR*; Higashi, 1995) | $h$ = −13→13 |
| $T_{min}$ = 0.847, $T_{max}$ = 0.880 | $k$ = −27→27 |
| 9710 measured reflections | $l$ = −8→9 |
| 3433 independent reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.045 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.144 | $w = 1/[\sigma^2(F_o^2) + (0.0659P)^2 + 0.8975P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.10 | $(\Delta/\sigma)_{max} < 0.001$ |
| 3433 reflections | $\Delta\rho_{max}$ = 0.47 e Å$^{-3}$ |

| | |
|---|---|
| 202 parameters | $\Delta\rho_{min} = -0.92$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |
| Secondary atom site location: difference Fourier map | |

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | −0.17894 (6) | 0.28996 (3) | 0.27912 (9) | 0.02060 (16) |
| Cl2 | 0.46528 (6) | 0.29140 (3) | 0.10812 (9) | 0.02077 (16) |
| O1 | 0.00723 (19) | 0.40867 (8) | 0.2367 (3) | 0.0218 (4) |
| O2 | 0.01147 (19) | 0.17042 (9) | 0.2397 (3) | 0.0184 (3) |
| O3 | 0.27117 (18) | 0.17271 (8) | 0.1488 (3) | 0.0196 (4) |
| O4 | 0.27772 (19) | 0.41277 (8) | 0.1577 (3) | 0.0209 (4) |
| O5 | 0.12383 (18) | 0.45615 (9) | 0.6917 (3) | 0.0215 (4) |
| O6 | 0.3466 (2) | 0.47658 (10) | 0.8601 (3) | 0.0265 (4) |
| N1 | 0.1860 (2) | 0.52690 (11) | 0.3720 (3) | 0.0199 (4) |
| C1 | 0.0667 (2) | 0.35416 (11) | 0.2174 (3) | 0.0164 (4) |
| C2 | −0.0036 (2) | 0.28950 (11) | 0.2347 (3) | 0.0160 (4) |
| C3 | 0.0678 (2) | 0.23079 (11) | 0.2188 (3) | 0.0154 (4) |
| C4 | 0.2206 (2) | 0.22965 (11) | 0.1715 (3) | 0.0155 (4) |
| C5 | 0.2899 (2) | 0.29272 (11) | 0.1544 (4) | 0.0170 (4) |
| C6 | 0.2232 (2) | 0.35480 (12) | 0.1732 (3) | 0.0165 (4) |
| C7 | 0.2794 (3) | 0.52837 (12) | 0.5464 (4) | 0.0198 (5) |
| C8 | 0.3984 (3) | 0.56970 (13) | 0.5626 (4) | 0.0229 (5) |
| H8 | 0.4656 | 0.5708 | 0.6840 | 0.027* |
| C9 | 0.4194 (3) | 0.60996 (13) | 0.3987 (4) | 0.0262 (5) |
| H9 | 0.5010 | 0.6388 | 0.4077 | 0.031* |
| C10 | 0.3206 (3) | 0.60759 (13) | 0.2230 (4) | 0.0268 (5) |
| H10 | 0.3332 | 0.6352 | 0.1109 | 0.032* |
| C11 | 0.2035 (3) | 0.56488 (13) | 0.2118 (4) | 0.0239 (5) |
| H11 | 0.1357 | 0.5624 | 0.0913 | 0.029* |
| C12 | 0.2418 (3) | 0.48289 (12) | 0.7090 (4) | 0.0195 (5) |
| H1 | 0.109 (5) | 0.498 (2) | 0.363 (6) | 0.053 (11)* |
| H2 | 0.071 (4) | 0.1437 (17) | 0.227 (5) | 0.032 (9)* |
| H6 | 0.319 (4) | 0.4534 (18) | 0.964 (6) | 0.043 (10)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0146 (3) | 0.0253 (3) | 0.0233 (3) | 0.0013 (2) | 0.0076 (2) | −0.0006 (2) |
| Cl2 | 0.0151 (3) | 0.0258 (3) | 0.0230 (3) | −0.0018 (2) | 0.0080 (2) | −0.0011 (2) |
| O1 | 0.0207 (8) | 0.0196 (8) | 0.0256 (9) | 0.0020 (7) | 0.0051 (7) | −0.0022 (7) |
| O2 | 0.0163 (8) | 0.0164 (7) | 0.0238 (9) | 0.0013 (7) | 0.0074 (7) | −0.0008 (7) |
| O3 | 0.0176 (8) | 0.0201 (8) | 0.0220 (8) | 0.0016 (7) | 0.0063 (7) | −0.0008 (7) |
| O4 | 0.0232 (9) | 0.0200 (8) | 0.0210 (9) | −0.0027 (7) | 0.0083 (7) | 0.0019 (6) |
| O5 | 0.0177 (8) | 0.0212 (8) | 0.0274 (9) | −0.0017 (7) | 0.0094 (7) | 0.0018 (7) |
| O6 | 0.0221 (9) | 0.0336 (10) | 0.0235 (9) | −0.0063 (8) | 0.0024 (7) | 0.0050 (8) |
| N1 | 0.0145 (9) | 0.0229 (10) | 0.0229 (10) | −0.0018 (8) | 0.0050 (8) | 0.0000 (8) |
| C1 | 0.0182 (10) | 0.0180 (10) | 0.0130 (10) | 0.0007 (9) | 0.0020 (8) | 0.0001 (8) |
| C2 | 0.0130 (10) | 0.0197 (10) | 0.0152 (10) | 0.0009 (8) | 0.0023 (8) | −0.0019 (8) |
| C3 | 0.0154 (10) | 0.0183 (10) | 0.0132 (10) | −0.0002 (8) | 0.0048 (8) | 0.0005 (8) |
| C4 | 0.0149 (10) | 0.0193 (10) | 0.0132 (10) | 0.0009 (8) | 0.0048 (8) | 0.0003 (8) |
| C5 | 0.0132 (10) | 0.0207 (10) | 0.0176 (10) | −0.0013 (9) | 0.0041 (8) | −0.0006 (9) |
| C6 | 0.0165 (10) | 0.0204 (10) | 0.0133 (10) | −0.0014 (9) | 0.0039 (8) | −0.0011 (8) |
| C7 | 0.0179 (11) | 0.0184 (11) | 0.0241 (12) | 0.0001 (9) | 0.0067 (9) | −0.0006 (9) |
| C8 | 0.0188 (11) | 0.0236 (12) | 0.0272 (13) | 0.0000 (10) | 0.0066 (10) | −0.0018 (10) |
| C9 | 0.0223 (12) | 0.0231 (12) | 0.0355 (14) | −0.0031 (10) | 0.0118 (11) | 0.0023 (11) |
| C10 | 0.0292 (13) | 0.0248 (12) | 0.0291 (13) | 0.0006 (11) | 0.0129 (11) | 0.0049 (10) |
| C11 | 0.0229 (12) | 0.0270 (12) | 0.0221 (12) | 0.0049 (10) | 0.0051 (10) | 0.0028 (10) |
| C12 | 0.0210 (11) | 0.0193 (10) | 0.0197 (11) | −0.0002 (9) | 0.0076 (9) | −0.0021 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Cl1—C2 | 1.723 (2) | C1—C6 | 1.548 (3) |
| Cl2—C5 | 1.727 (2) | C2—C3 | 1.350 (3) |
| O1—C1 | 1.227 (3) | C3—C4 | 1.521 (3) |
| O2—C3 | 1.318 (3) | C4—C5 | 1.416 (3) |
| O2—H2 | 0.79 (3) | C5—C6 | 1.389 (3) |
| O3—C4 | 1.237 (3) | C7—C8 | 1.375 (3) |
| O4—C6 | 1.263 (3) | C7—C12 | 1.497 (3) |
| O5—C12 | 1.218 (3) | C8—C9 | 1.394 (4) |
| O6—C12 | 1.305 (3) | C8—H8 | 0.9500 |
| O6—H6 | 0.90 (4) | C9—C10 | 1.383 (4) |
| N1—C11 | 1.340 (3) | C9—H9 | 0.9500 |
| N1—C7 | 1.349 (3) | C10—C11 | 1.379 (4) |
| N1—H1 | 0.92 (4) | C10—H10 | 0.9500 |
| C1—C2 | 1.448 (3) | C11—H11 | 0.9500 |
| C3—O2—H2 | 107 (3) | O4—C6—C1 | 115.8 (2) |
| C12—O6—H6 | 112 (2) | C5—C6—C1 | 117.90 (19) |
| C11—N1—C7 | 122.5 (2) | N1—C7—C8 | 119.6 (2) |
| C11—N1—H1 | 119 (2) | N1—C7—C12 | 115.0 (2) |
| C7—N1—H1 | 118 (2) | C8—C7—C12 | 125.4 (2) |
| O1—C1—C2 | 122.6 (2) | C7—C8—C9 | 119.3 (2) |

| | | | |
|---|---|---|---|
| O1—C1—C6 | 118.5 (2) | C7—C8—H8 | 120.4 |
| C2—C1—C6 | 118.91 (19) | C9—C8—H8 | 120.4 |
| C3—C2—C1 | 120.4 (2) | C10—C9—C8 | 119.5 (2) |
| C3—C2—Cl1 | 121.40 (18) | C10—C9—H9 | 120.2 |
| C1—C2—Cl1 | 118.15 (17) | C8—C9—H9 | 120.2 |
| O2—C3—C2 | 123.3 (2) | C11—C10—C9 | 119.5 (2) |
| O2—C3—C4 | 114.75 (19) | C11—C10—H10 | 120.3 |
| C2—C3—C4 | 121.9 (2) | C9—C10—H10 | 120.3 |
| O3—C4—C5 | 126.4 (2) | N1—C11—C10 | 119.7 (2) |
| O3—C4—C3 | 115.7 (2) | N1—C11—H11 | 120.2 |
| C5—C4—C3 | 117.85 (19) | C10—C11—H11 | 120.2 |
| C6—C5—C4 | 122.9 (2) | O5—C12—O6 | 126.9 (2) |
| C6—C5—Cl2 | 119.23 (17) | O5—C12—C7 | 120.4 (2) |
| C4—C5—Cl2 | 117.86 (17) | O6—C12—C7 | 112.7 (2) |
| O4—C6—C5 | 126.3 (2) | | |
| O1—C1—C2—C3 | −177.9 (2) | C4—C5—C6—C1 | 0.7 (3) |
| C6—C1—C2—C3 | 2.1 (3) | Cl2—C5—C6—C1 | −179.21 (16) |
| O1—C1—C2—Cl1 | 1.3 (3) | O1—C1—C6—O4 | −0.9 (3) |
| C6—C1—C2—Cl1 | −178.77 (16) | C2—C1—C6—O4 | 179.2 (2) |
| C1—C2—C3—O2 | 177.7 (2) | O1—C1—C6—C5 | 179.2 (2) |
| Cl1—C2—C3—O2 | −1.4 (3) | C2—C1—C6—C5 | −0.7 (3) |
| C1—C2—C3—C4 | −3.3 (3) | C11—N1—C7—C8 | −0.6 (4) |
| Cl1—C2—C3—C4 | 177.58 (16) | C11—N1—C7—C12 | 179.6 (2) |
| O2—C3—C4—O3 | 3.3 (3) | N1—C7—C8—C9 | 0.7 (4) |
| C2—C3—C4—O3 | −175.8 (2) | C12—C7—C8—C9 | −179.5 (2) |
| O2—C3—C4—C5 | −177.73 (19) | C7—C8—C9—C10 | −0.1 (4) |
| C2—C3—C4—C5 | 3.2 (3) | C8—C9—C10—C11 | −0.7 (4) |
| O3—C4—C5—C6 | 177.0 (2) | C7—N1—C11—C10 | −0.2 (4) |
| C3—C4—C5—C6 | −1.8 (3) | C9—C10—C11—N1 | 0.8 (4) |
| O3—C4—C5—Cl2 | −3.0 (3) | N1—C7—C12—O5 | −11.4 (3) |
| C3—C4—C5—Cl2 | 178.11 (16) | C8—C7—C12—O5 | 168.8 (2) |
| C4—C5—C6—O4 | −179.2 (2) | N1—C7—C12—O6 | 168.4 (2) |
| Cl2—C5—C6—O4 | 0.8 (3) | C8—C7—C12—O6 | −11.4 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1 | 0.92 (4) | 2.11 (3) | 2.932 (2) | 147 (3) |
| N1—H1···O5 | 0.92 (4) | 2.33 (4) | 2.698 (2) | 103 (2) |
| N1—H1···O5$^{i}$ | 0.92 (4) | 2.34 (4) | 2.900 (2) | 119 (3) |
| O2—H2···O3 | 0.79 (3) | 2.11 (3) | 2.612 (2) | 122 (3) |
| O2—H2···O5$^{ii}$ | 0.79 (3) | 2.05 (3) | 2.746 (2) | 148 (3) |
| O6—H6···O4$^{iii}$ | 0.90 (3) | 1.63 (3) | 2.528 (2) | 177.1 (15) |
| C8—H8···O4$^{iv}$ | 0.95 | 2.50 | 3.338 (3) | 147 |
| C9—H9···O3$^{v}$ | 0.95 | 2.33 | 3.227 (3) | 156 |
| C11—H11···O1$^{vi}$ | 0.95 | 2.46 | 3.374 (3) | 162 |

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

**Fig. 1**

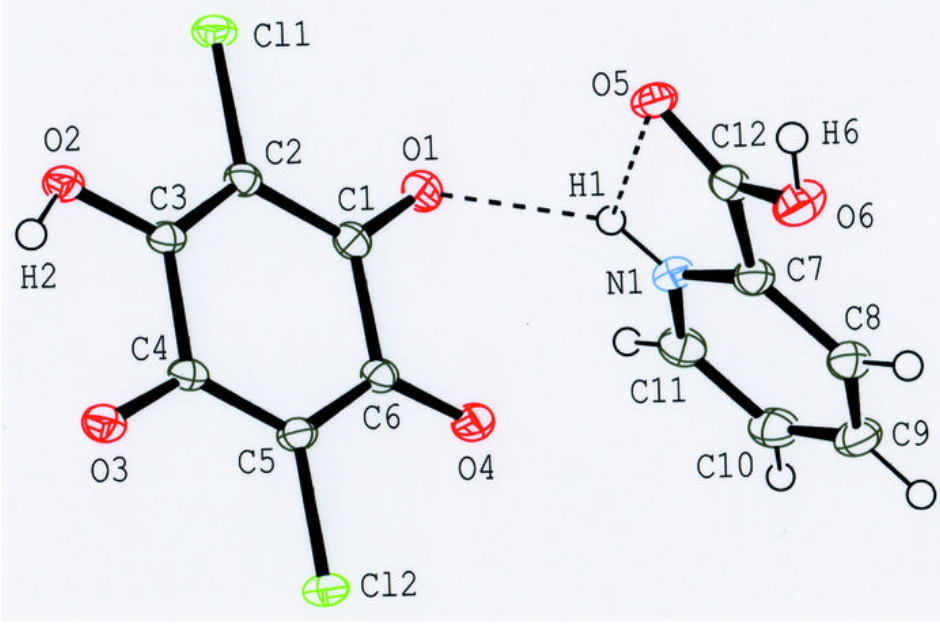
Cl1
O2
C2
O1
O5
C12
H6
C3
C1
H1
O6
H2
N1
C7
C4
C8
C11
C6
C9
O3
C5
O4
C10
C12

**Fig. 2**