

Diisonicotinium pentachlorido-antimonate(III) monohydrate

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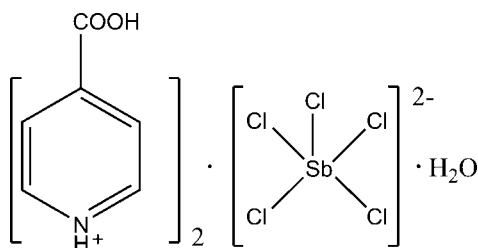
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.057; wR factor = 0.085; data-to-parameter ratio = 20.6.

In the title compound, $(\text{C}_6\text{H}_6\text{NO}_2)_2[\text{SbCl}_5]\cdot\text{H}_2\text{O}$, the Sb^{III} atom exhibits a distorted square-pyramidal coordination geometry. The crystal structure is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{Cl}$, $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds, forming an extended three-dimensional network.

Related literature

For related structures, see: Bujak & Zaleski (1999); Feng *et al.* (2007); Shen-Tu *et al.* (2008).



Experimental

Crystal data

$(\text{C}_6\text{H}_6\text{NO}_2)_2[\text{SbCl}_5]\cdot\text{H}_2\text{O}$
 $M_r = 565.25$
Monoclinic, $P2_1/c$

$a = 10.334$ (2) Å
 $b = 8.7319$ (17) Å
 $c = 23.615$ (7) Å

$\beta = 106.98$ (3)°
 $V = 2038.0$ (9) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 2.03$ mm⁻¹
 $T = 291$ K
 $0.25 \times 0.20 \times 0.20$ mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2005)
 $T_{\text{min}} = 0.61$, $T_{\text{max}} = 0.67$

19258 measured reflections
4675 independent reflections
4071 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.085$
 $S = 1.19$
4675 reflections

227 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.76$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.76$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{O1}-\text{H1C}\cdots\text{O1W}^{\text{i}}$ | 0.85 | 1.67 | 2.520 (5) | 175 |
| $\text{N1}-\text{H1B}\cdots\text{O4}^{\text{ii}}$ | 0.86 | 2.45 | 3.031 (6) | 126 |
| $\text{O1W}-\text{H1WA}\cdots\text{Cl3}^{\text{iii}}$ | 0.85 | 2.71 | 3.378 (7) | 136 |
| $\text{O1W}-\text{H1WB}\cdots\text{Cl5}^{\text{iii}}$ | 0.85 | 2.54 | 3.241 (4) | 140 |
| $\text{O3}-\text{H3A}\cdots\text{Cl5}^{\text{iv}}$ | 0.85 | 2.19 | 3.034 (4) | 175 |
| $\text{N2}-\text{H2A}\cdots\text{O2}^{\text{v}}$ | 0.86 | 2.41 | 2.988 (5) | 125 |
| $\text{N2}-\text{H2A}\cdots\text{Cl2}^{\text{v}}$ | 0.86 | 2.49 | 3.224 (4) | 144 |
| $\text{N1}-\text{H1B}\cdots\text{Cl5}$ | 0.86 | 2.42 | 3.147 (4) | 143 |

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2323).

References

- Bujak, M. & Zaleski, J. (1999). *Acta Cryst.* **C55**, 1775–1778.
Feng, W.-J., Wang, H.-B., Ma, X.-J., Li, H.-Y. & Jin, Z.-M. (2007). *Acta Cryst.* **E63**, m1786–m1787.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Shen-Tu, C., Li, H. Y., Ma, X. J., Huang, W. & Jin, Z. M. (2008). *Acta Cryst.* **E64**, m146.

supporting information

Acta Cryst. (2009). E65, m683 [doi:10.1107/S1600536809019072]

Diisonicotinium pentachloridoantimonate(III) monohydrate

Li-Zhuang Chen

S1. Comment

Recently, the crystal structure of some halogenoantimonate salts has been reported (Feng *et al.*, 2007; Bujak & Zaleski, 1999; Shen-Tu *et al.* 2008). As a contribution to this field, the synthesis and crystal structure of the title compound is reported herein.

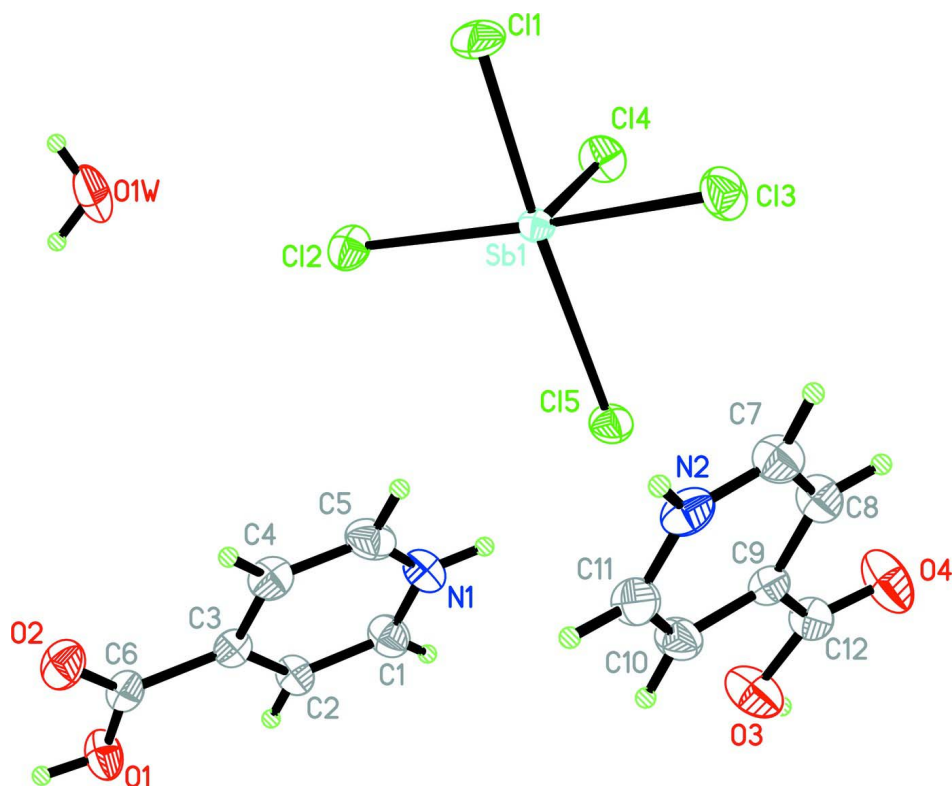
The asymmetric unit of the title compound (Fig. 1) contains two protonated isonicotinic acid cations, a pentachloridoantimonate anion and a water molecule. The antimony(III) ion is in a distorted square-pyramidal coordination geometry, with the Sb—Cl distances ranging from 2.3642 (12) to 2.9002 (14) Å. This range of values is in agreement with that observed in N-methylpiperazinediium pentachloridoantimonate(III) monohydrate (2.4110 (10)–2.9112 (11) Å; Shen-Tu *et al.*, 2008) and slightly larger than that reported for bis(ethylidimethylammonium) pentachloroantimonate(III) (2.499 (4)–2.768 (4) Å; Bujak & Zaleski, 1999). The crystal structure is stabilized by intermolecular N—H···Cl, N—H···O, O—H···Cl and O—H···O hydrogen bonds (Table 1), forming an extended three-dimensional network (Fig. 2).

S2. Experimental

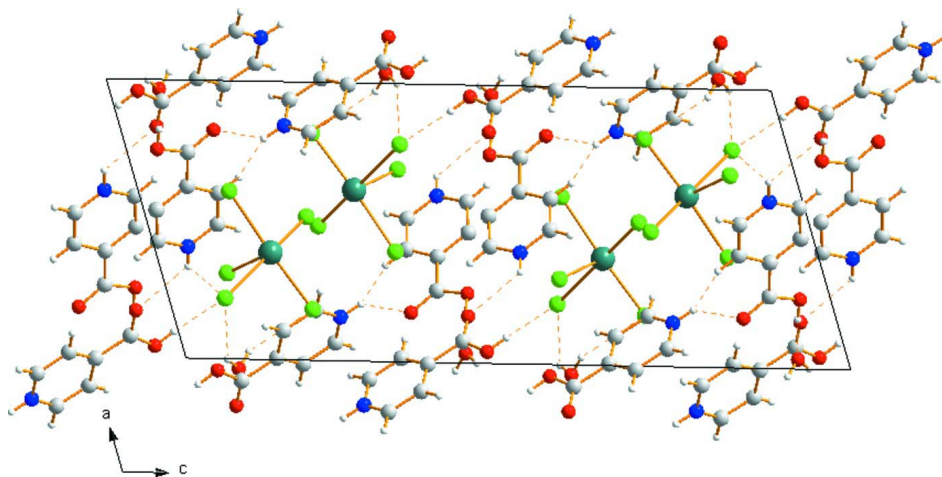
SbCl₃, isonicotinic acid and 20% aqueous HCl in a molar ratio of 1:1:3 were mixed and dissolved in water by heating to 373 K forming a clear solution. The reaction mixture was cooled slowly to room temperature, crystals of the title compound were formed, collected and washed with dilute aqueous HCl.

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.93 Å, O—H = 0.85 Å and N—H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ or $1.5U_{\text{eq}}(\text{O})$. The deepest residual electron density hole is located 1.47 Å from atom H5A.

**Figure 1**

A view of the title compound with the atom-numbering scheme. Displacement ellipsoids were drawn at the 30% probability level.

**Figure 2**

The crystal packing of the title compound viewed approximately along the *b* axis. Hydrogen bonds are drawn as dashed lines.

Diisonicotinium pentachloridoantimonate(III) monohydrate

Crystal data

 $(C_6H_6NO_2)_2[SbCl_5] \cdot H_2O$ $M_r = 565.25$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 10.334 (2) \text{ \AA}$ $b = 8.7319 (17) \text{ \AA}$ $c = 23.615 (7) \text{ \AA}$ $\beta = 106.98 (3)^\circ$ $V = 2038.0 (9) \text{ \AA}^3$ $Z = 4$ $F(000) = 1104$ $D_x = 1.842 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 4071 reflections

 $\theta = 3.1\text{--}27.5^\circ$ $\mu = 2.03 \text{ mm}^{-1}$ $T = 291 \text{ K}$

Block, colourless

 $0.25 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Rigaku SCXmini

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 13.6612 pixels mm^{-1} ω scans

Absorption correction: multi-scan

(CrystalClear; Rigaku, 2005)

 $T_{\min} = 0.61$, $T_{\max} = 0.67$

19258 measured reflections

4675 independent reflections

4071 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.061$ $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.1^\circ$ $h = -13 \rightarrow 12$ $k = -11 \rightarrow 11$ $l = -30 \rightarrow 30$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.057$ $wR(F^2) = 0.085$ $S = 1.19$

4675 reflections

227 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

 $w = 1/[\sigma^2(F_o^2) + (0.0112P)^2 + 1.8681P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.76 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -1.76 \text{ e \AA}^{-3}$ Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0094 (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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|------------|--------------|----------------------------------|
| O1 | 0.7498 (3) | 0.9688 (4) | 0.04677 (14) | 0.0569 (9) |
| H1C | 0.8214 | 1.0222 | 0.0583 | 0.085* |

| | | | | |
|------|--------------|---------------|---------------|--------------|
| O2 | 0.8222 (3) | 0.8846 (4) | 0.14010 (14) | 0.0583 (10) |
| N1 | 0.4007 (4) | 0.6022 (5) | 0.0507 (2) | 0.0561 (11) |
| H1B | 0.3308 | 0.5436 | 0.0427 | 0.067* |
| C1 | 0.4199 (5) | 0.6891 (5) | 0.0081 (2) | 0.0527 (13) |
| H1A | 0.3586 | 0.6866 | -0.0296 | 0.063* |
| C6 | 0.7409 (5) | 0.8855 (5) | 0.0914 (2) | 0.0419 (11) |
| C2 | 0.5301 (5) | 0.7820 (5) | 0.01973 (19) | 0.0425 (11) |
| H2B | 0.5451 | 0.8430 | -0.0100 | 0.051* |
| C5 | 0.4841 (6) | 0.6009 (6) | 0.1054 (2) | 0.0586 (14) |
| H5A | 0.4668 | 0.5372 | 0.1338 | 0.070* |
| C4 | 0.5956 (5) | 0.6935 (6) | 0.1197 (2) | 0.0489 (12) |
| H4A | 0.6541 | 0.6947 | 0.1580 | 0.059* |
| C3 | 0.6198 (4) | 0.7850 (5) | 0.07631 (18) | 0.0376 (10) |
| Cl5 | 0.21814 (12) | 0.35116 (14) | 0.08488 (5) | 0.0501 (3) |
| O1W | 0.9650 (5) | 0.1234 (6) | 0.0754 (3) | 0.195 (4) |
| H1WA | 1.0285 | 0.0715 | 0.0984 | 0.292* |
| H1WB | 0.9982 | 0.2007 | 0.0627 | 0.292* |
| Sb1 | 0.38449 (3) | 0.14611 (3) | 0.173118 (11) | 0.03103 (11) |
| Cl1 | 0.51635 (14) | -0.04608 (16) | 0.24298 (6) | 0.0646 (4) |
| Cl3 | 0.18317 (14) | 0.09286 (16) | 0.21279 (7) | 0.0642 (4) |
| Cl2 | 0.60393 (12) | 0.19468 (15) | 0.13735 (5) | 0.0521 (3) |
| Cl4 | 0.30831 (13) | -0.04201 (14) | 0.09880 (6) | 0.0554 (3) |
| O3 | -0.0419 (4) | 0.6811 (4) | 0.04218 (15) | 0.0734 (12) |
| H3A | -0.0944 | 0.6770 | 0.0070 | 0.110* |
| O4 | -0.1684 (4) | 0.4904 (5) | 0.05540 (16) | 0.0797 (13) |
| N2 | 0.1577 (4) | 0.5697 (5) | 0.25122 (17) | 0.0513 (11) |
| H2A | 0.2057 | 0.5670 | 0.2877 | 0.062* |
| C12 | -0.0780 (5) | 0.5765 (6) | 0.0741 (2) | 0.0474 (12) |
| C9 | 0.0065 (4) | 0.5778 (5) | 0.13730 (19) | 0.0388 (10) |
| C8 | -0.0139 (5) | 0.4684 (6) | 0.1746 (2) | 0.0497 (12) |
| H8A | -0.0816 | 0.3958 | 0.1610 | 0.060* |
| C11 | 0.1813 (5) | 0.6798 (6) | 0.2169 (2) | 0.0565 (14) |
| H11A | 0.2490 | 0.7516 | 0.2321 | 0.068* |
| C10 | 0.1047 (5) | 0.6868 (5) | 0.1585 (2) | 0.0528 (13) |
| H10A | 0.1190 | 0.7639 | 0.1339 | 0.063* |
| C7 | 0.0648 (5) | 0.4649 (6) | 0.2321 (2) | 0.0533 (13) |
| H7A | 0.0525 | 0.3886 | 0.2576 | 0.064* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|----|-----------|-----------|-------------|--------------|--------------|--------------|
| O1 | 0.051 (2) | 0.072 (3) | 0.046 (2) | -0.0181 (18) | 0.0115 (17) | 0.0049 (18) |
| O2 | 0.052 (2) | 0.071 (3) | 0.0415 (19) | 0.0017 (18) | -0.0026 (17) | -0.0019 (17) |
| N1 | 0.060 (3) | 0.047 (3) | 0.062 (3) | -0.012 (2) | 0.019 (2) | -0.002 (2) |
| C1 | 0.058 (3) | 0.051 (3) | 0.044 (3) | -0.010 (3) | 0.007 (3) | -0.004 (2) |
| C6 | 0.039 (3) | 0.050 (3) | 0.036 (2) | 0.003 (2) | 0.009 (2) | -0.006 (2) |
| C2 | 0.048 (3) | 0.047 (3) | 0.031 (2) | -0.007 (2) | 0.009 (2) | 0.000 (2) |
| C5 | 0.077 (4) | 0.050 (3) | 0.058 (3) | 0.001 (3) | 0.033 (3) | 0.014 (3) |

| | | | | | | |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| C4 | 0.055 (3) | 0.058 (3) | 0.036 (3) | 0.006 (3) | 0.016 (2) | 0.007 (2) |
| C3 | 0.040 (3) | 0.044 (3) | 0.032 (2) | 0.004 (2) | 0.015 (2) | -0.002 (2) |
| Cl5 | 0.0542 (7) | 0.0498 (7) | 0.0434 (6) | 0.0001 (6) | 0.0096 (6) | 0.0118 (6) |
| O1W | 0.074 (4) | 0.146 (5) | 0.316 (9) | -0.059 (4) | -0.017 (5) | 0.112 (6) |
| Sb1 | 0.03618 (18) | 0.02999 (17) | 0.02550 (15) | 0.00013 (12) | 0.00678 (12) | 0.00076 (12) |
| Cl1 | 0.0674 (9) | 0.0654 (9) | 0.0561 (8) | 0.0156 (7) | 0.0105 (7) | 0.0324 (7) |
| Cl3 | 0.0663 (9) | 0.0638 (9) | 0.0750 (10) | -0.0064 (7) | 0.0401 (8) | -0.0022 (7) |
| Cl2 | 0.0472 (7) | 0.0707 (9) | 0.0378 (6) | 0.0062 (6) | 0.0115 (6) | 0.0107 (6) |
| Cl4 | 0.0676 (9) | 0.0479 (7) | 0.0506 (7) | -0.0077 (6) | 0.0169 (7) | -0.0207 (6) |
| O3 | 0.094 (3) | 0.070 (3) | 0.041 (2) | -0.026 (2) | -0.005 (2) | 0.0129 (18) |
| O4 | 0.079 (3) | 0.102 (3) | 0.043 (2) | -0.046 (3) | -0.006 (2) | 0.007 (2) |
| N2 | 0.053 (3) | 0.058 (3) | 0.034 (2) | 0.012 (2) | -0.0022 (19) | -0.002 (2) |
| C12 | 0.051 (3) | 0.049 (3) | 0.037 (3) | -0.002 (2) | 0.006 (2) | -0.002 (2) |
| C9 | 0.039 (3) | 0.039 (3) | 0.035 (2) | 0.004 (2) | 0.005 (2) | -0.005 (2) |
| C8 | 0.053 (3) | 0.053 (3) | 0.039 (3) | -0.008 (2) | 0.008 (2) | -0.003 (2) |
| C11 | 0.049 (3) | 0.049 (3) | 0.057 (3) | -0.004 (2) | -0.006 (3) | -0.006 (3) |
| C10 | 0.055 (3) | 0.046 (3) | 0.050 (3) | -0.005 (2) | 0.002 (3) | 0.007 (2) |
| C7 | 0.060 (3) | 0.057 (3) | 0.039 (3) | -0.001 (3) | 0.008 (3) | 0.007 (2) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|-------------|-------------|
| O1—C6 | 1.306 (5) | Sb1—Cl1 | 2.4661 (13) |
| O1—H1C | 0.8500 | Sb1—Cl3 | 2.5613 (15) |
| O2—C6 | 1.210 (5) | Sb1—Cl2 | 2.6748 (14) |
| N1—C1 | 1.322 (6) | O3—C12 | 1.306 (6) |
| N1—C5 | 1.325 (6) | O3—H3A | 0.8500 |
| N1—H1B | 0.8600 | O4—C12 | 1.180 (5) |
| C1—C2 | 1.359 (6) | N2—C7 | 1.307 (6) |
| C1—H1A | 0.9300 | N2—C11 | 1.326 (6) |
| C6—C3 | 1.484 (6) | N2—H2A | 0.8600 |
| C2—C3 | 1.386 (6) | C12—C9 | 1.493 (6) |
| C2—H2B | 0.9300 | C9—C8 | 1.357 (6) |
| C5—C4 | 1.366 (7) | C9—C10 | 1.375 (6) |
| C5—H5A | 0.9300 | C8—C7 | 1.365 (6) |
| C4—C3 | 1.379 (6) | C8—H8A | 0.9300 |
| C4—H4A | 0.9300 | C11—C10 | 1.375 (6) |
| O1W—H1WA | 0.8500 | C11—H11A | 0.9300 |
| O1W—H1WB | 0.8499 | C10—H10A | 0.9300 |
| Sb1—Cl5 | 2.9002 (14) | C7—H7A | 0.9300 |
| Sb1—Cl4 | 2.3646 (12) | | |
| C6—O1—H1C | 107.9 | Cl4—Sb1—Cl3 | 90.89 (5) |
| C1—N1—C5 | 123.2 (5) | Cl1—Sb1—Cl3 | 88.91 (5) |
| C1—N1—H1B | 118.4 | Cl4—Sb1—Cl2 | 90.28 (5) |
| C5—N1—H1B | 118.4 | Cl1—Sb1—Cl2 | 88.01 (5) |
| N1—C1—C2 | 119.4 (5) | Cl3—Sb1—Cl2 | 176.73 (4) |
| N1—C1—H1A | 120.3 | C12—O3—H3A | 109.1 |
| C2—C1—H1A | 120.3 | C7—N2—C11 | 123.0 (4) |

| | | | |
|---------------|------------|--------------|-----------|
| O2—C6—O1 | 125.3 (5) | C7—N2—H2A | 118.5 |
| O2—C6—C3 | 121.8 (4) | C11—N2—H2A | 118.5 |
| O1—C6—C3 | 112.8 (4) | O4—C12—O3 | 123.9 (5) |
| C1—C2—C3 | 119.4 (5) | O4—C12—C9 | 123.2 (5) |
| C1—C2—H2B | 120.3 | O3—C12—C9 | 112.9 (4) |
| C3—C2—H2B | 120.3 | C8—C9—C10 | 119.2 (4) |
| N1—C5—C4 | 119.9 (5) | C8—C9—C12 | 119.2 (4) |
| N1—C5—H5A | 120.1 | C10—C9—C12 | 121.6 (4) |
| C4—C5—H5A | 120.1 | C9—C8—C7 | 120.1 (5) |
| C5—C4—C3 | 118.7 (5) | C9—C8—H8A | 119.9 |
| C5—C4—H4A | 120.6 | C7—C8—H8A | 119.9 |
| C3—C4—H4A | 120.6 | N2—C11—C10 | 119.3 (5) |
| C4—C3—C2 | 119.3 (4) | N2—C11—H11A | 120.3 |
| C4—C3—C6 | 119.2 (4) | C10—C11—H11A | 120.3 |
| C2—C3—C6 | 121.5 (4) | C9—C10—C11 | 118.8 (5) |
| H1WA—O1W—H1WB | 109.5 | C9—C10—H10A | 120.6 |
| Cl5—Sb1—Cl11 | 175.24 (4) | C11—C10—H10A | 120.6 |
| Cl5—Sb1—Cl13 | 90.03 (4) | N2—C7—C8 | 119.4 (5) |
| Cl5—Sb1—Cl12 | 93.12 (4) | N2—C7—H7A | 120.3 |
| Cl5—Sb1—Cl14 | 84.06 (4) | C8—C7—H7A | 120.3 |
| Cl4—Sb1—Cl11 | 91.32 (6) | | |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| O1—H1C \cdots O1W ⁱ | 0.85 | 1.67 | 2.520 (5) | 175 |
| N1—H1B \cdots O4 ⁱⁱ | 0.86 | 2.45 | 3.031 (6) | 126 |
| O1W—H1WA \cdots Cl3 ⁱⁱⁱ | 0.85 | 2.71 | 3.378 (7) | 136 |
| O1W—H1WB \cdots Cl5 ⁱⁱⁱ | 0.85 | 2.54 | 3.241 (4) | 140 |
| O3—H3A \cdots Cl5 ⁱⁱ | 0.85 | 2.19 | 3.034 (4) | 175 |
| N2—H2A \cdots O2 ^{iv} | 0.86 | 2.41 | 2.988 (5) | 125 |
| N2—H2A \cdots Cl2 ^v | 0.86 | 2.49 | 3.224 (4) | 144 |
| N1—H1B \cdots Cl5 | 0.86 | 2.42 | 3.147 (4) | 143 |

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