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# Triethylammonium tetrachlorido(pyrazine-2-carboxylato-$\kappa^2N^1,O$)stannate(IV)

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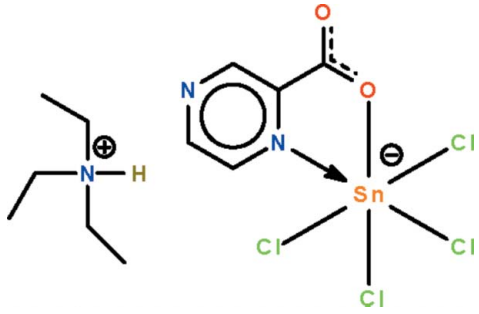
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.022; $wR$ factor = 0.052; data-to-parameter ratio = 21.1.

The $Sn^{IV}$ atom in the title ammonium stannate, $(Et_3NH)[Sn(C_5H_3N_2O_2)Cl_4]$, is chelated by an pyrazine-2-carboxylate ligand and exists in a *cis*-$SnCl_4NO$ octahedral geometry. The cation and the anion are linked by an N—H···N hydrogen bond.

## Related literature

For triethylammonium tetrachlorido(pyridine-2-carboxylato)stannate(IV), see: Najafi *et al.* (2011).




## Experimental

### Crystal data

$(C_6H_{16}N)[Sn(C_5H_3N_2O_2)Cl_4]$
$M_r$ = 485.78
Triclinic, $P\overline{1}$
$a$ = 7.4497 (2) Å
$b$ = 9.9752 (3) Å
$c$ = 12.3728 (4) Å
$\alpha$ = 86.491 (2)°
$\beta$ = 80.125 (3)°
$\gamma$ = 83.817 (2)°
$V$ = 899.70 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 2.02 mm$^{-1}$
$T$ = 100 K
0.35 × 0.30 × 0.25 mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.538, $T_{max}$ = 0.632
15321 measured reflections
4094 independent reflections
3800 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.030

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.052
$S$ = 1.02
4094 reflections
194 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H1···N2 | 0.91 (3) | 2.10 (3) | 2.999 (2) | 167 (2) |

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QK2007).

## References

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m711 [ **doi:10.1107/S1600536811016473** ]

# Triethylammonium tetrachlorido(pyrazine-2-carboxylato-$\kappa^2N^1,O$)stannate(IV)

**E. Najafi, M. M. Amini and S. W. Ng**

## Comment

We have recently reported the crystal structure of triethylammonium tetrachlorido(pyridine-2-carboxylato)stannate, which was synthesized by the reaction of triethylammonium pyridine-2-carboxylate and stannic chloride. The $Sn^{IV}$ atom in the anion is *N*,*O*-chelated by the pyridine-2-carboxylate in a *cis*-$SnCl_4NO$ octahedral geometry (Najafi *et al.*, 2011). In our previous studies, we have reacted aromatic carboxylic acid with stannic chloride, with/without a proton-abstraction agent. In the present study, replacing pyrdine-2-carboxylic acid by pyrazine-2-carboxylic acid affords a similar salt, $(Et_3NH)^+$ $[SnCl_4(C_5H_3N_2O_2)]^-$ (Scheme I, Fig. 1). The tin atom in the stannate is chelated by the pyrazine-2-carboxylate group in a *cis*-$SnCl_4NO$ octahedral geometry. The cation forms an N–H···N hydrogen bond with the anion. Of the four Sn–Cl bonds, the ones that are *trans* to the Sn–O/Sn–N bonds are somewhat shorter than the other two. No Cl···Cl interactions are present.

## Experimental

The reaction was carried out under a nitrogen atmosphere. Pyrazine-2-carboxylic acid (1.0 mmol, 0.12 g) and the triethylamine (1.0 mmol, 0.10 g) were dissolved in dry methanol (20 ml). Stannic chloride (1.0 mmol, 0.35 g) was added to the mixture and stirred for 12 h. Suitable crystals were obtained by slow evaporation of the solvent.

## Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 to 1.5*U*(C). The ammonium H-atom was located in a difference Fourier map, and was freely refined.

## Figures

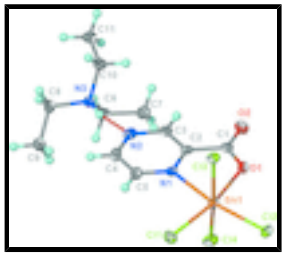

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $(Et_3NH)^+$ $[SnCl_4(C_5H_3N_2O_2)]^-$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The hydrogen bond is denoted by a dashed bond.

## Triethylammonium tetrachlorido(pyrazine-2-carboxylato-$\kappa^2N^1,O$)stannate(IV)

*Crystal data*

| | |
|---|---|
| $(C_6H_{16}N)[Sn(C_5H_3N_2O_2)Cl_4]$ | $Z = 2$ |
| $M_r = 485.78$ | $F(000) = 480$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.793$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.4497$ (2) Å | Cell parameters from 10335 reflections |
| $b = 9.9752$ (3) Å | $\theta = 2.6$–$29.2°$ |
| $c = 12.3728$ (4) Å | $\mu = 2.02$ mm$^{-1}$ |
| $\alpha = 86.491$ (2)° | $T = 100$ K |
| $\beta = 80.125$ (3)° | Irregular block, colorless |
| $\gamma = 83.817$ (2)° | 0.35 × 0.30 × 0.25 mm |
| $V = 899.70$ (5) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Agilent SuperNova Dual diffractometer with an Atlas detector | 4094 independent reflections |
| Radiation source: SuperNova (Mo) X-ray Source | 3800 reflections with $I > 2\sigma(I)$ |
| Mirror | $R_{int} = 0.030$ |
| Detector resolution: 10.4041 pixels mm$^{-1}$ | $\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$ |
| ω scans | $h = -9 \rightarrow 9$ |
| Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010) | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.538$, $T_{max} = 0.632$ | $l = -15 \rightarrow 16$ |
| 15321 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.022$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.052$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.02$ | $w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 0.2896P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4094 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 194 parameters | $\Delta\rho_{max} = 0.35$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.65$ e Å$^{-3}$ |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn1 | 0.310753 (18) | 0.248889 (13) | 0.740250 (10) | 0.01198 (5) |
| Cl1 | 0.46068 (7) | 0.34171 (5) | 0.86858 (4) | 0.01988 (11) |
| Cl2 | 0.00680 (7) | 0.26586 (5) | 0.83792 (4) | 0.01703 (11) |
| Cl3 | 0.39067 (7) | 0.02423 (5) | 0.80641 (4) | 0.01605 (11) |
| Cl4 | 0.26028 (7) | 0.46373 (5) | 0.64356 (4) | 0.02064 (11) |
| O1 | 0.22917 (19) | 0.16094 (14) | 0.60971 (11) | 0.0149 (3) |
| O2 | 0.3047 (2) | 0.10363 (15) | 0.43513 (11) | 0.0194 (3) |
| N1 | 0.5661 (2) | 0.22659 (16) | 0.61249 (13) | 0.0128 (3) |
| N2 | 0.8334 (2) | 0.21721 (17) | 0.42643 (14) | 0.0171 (4) |
| N3 | 1.0881 (2) | 0.24246 (17) | 0.21208 (14) | 0.0142 (3) |
| C1 | 0.3419 (3) | 0.14663 (19) | 0.51771 (16) | 0.0134 (4) |
| C2 | 0.5317 (3) | 0.18609 (19) | 0.51747 (16) | 0.0128 (4) |
| C3 | 0.6667 (3) | 0.18070 (19) | 0.42525 (16) | 0.0155 (4) |
| H3A | 0.6397 | 0.1501 | 0.3592 | 0.019* |
| C4 | 0.8662 (3) | 0.2544 (2) | 0.52239 (17) | 0.0179 (4) |
| H4A | 0.9846 | 0.2789 | 0.5264 | 0.021* |
| C5 | 0.7345 (3) | 0.2587 (2) | 0.61660 (17) | 0.0168 (4) |
| H5A | 0.7638 | 0.2844 | 0.6837 | 0.020* |
| C6 | 0.9980 (3) | 0.3321 (2) | 0.13009 (16) | 0.0161 (4) |
| H6A | 1.0734 | 0.3221 | 0.0564 | 0.019* |
| H6B | 0.9943 | 0.4272 | 0.1495 | 0.019* |
| C7 | 0.8062 (3) | 0.3011 (2) | 0.12490 (18) | 0.0201 (5) |
| H7A | 0.7565 | 0.3610 | 0.0691 | 0.030* |
| H7B | 0.7288 | 0.3151 | 0.1966 | 0.030* |
| H7C | 0.8084 | 0.2070 | 0.1057 | 0.030* |
| C8 | 1.2722 (3) | 0.2874 (2) | 0.22036 (17) | 0.0173 (4) |
| H8A | 1.3358 | 0.3118 | 0.1459 | 0.021* |
| H8B | 1.3477 | 0.2116 | 0.2511 | 0.021* |
| C9 | 1.2544 (3) | 0.4075 (2) | 0.29232 (19) | 0.0220 (5) |
| H9A | 1.3763 | 0.4344 | 0.2947 | 0.033* |
| H9B | 1.1952 | 0.3827 | 0.3668 | 0.033* |
| H9C | 1.1801 | 0.4829 | 0.2620 | 0.033* |
| C10 | 1.1019 (3) | 0.0937 (2) | 0.19176 (16) | 0.0168 (4) |
| H10A | 1.1673 | 0.0429 | 0.2470 | 0.020* |
| H10B | 0.9769 | 0.0646 | 0.2021 | 0.020* |
| C11 | 1.2003 (3) | 0.0582 (2) | 0.07822 (17) | 0.0189 (4) |
| H11A | 1.2039 | −0.0392 | 0.0701 | 0.028* |
| H11B | 1.3255 | 0.0840 | 0.0681 | 0.028* |
| H11C | 1.1352 | 0.1067 | 0.0230 | 0.028* |
| H1 | 1.015 (3) | 0.249 (2) | 0.279 (2) | 0.027 (7)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| Sn1 | 0.01291 (8) | 0.01297 (8) | 0.00947 (8) | 0.00012 (5) | −0.00092 (5) | −0.00091 (5) |
| Cl1 | 0.0232 (3) | 0.0225 (3) | 0.0154 (2) | −0.0057 (2) | −0.0037 (2) | −0.0045 (2) |
| Cl2 | 0.0141 (2) | 0.0218 (3) | 0.0137 (2) | 0.00087 (19) | 0.00009 (19) | −0.00038 (19) |
| Cl3 | 0.0189 (3) | 0.0141 (2) | 0.0142 (2) | 0.00126 (19) | −0.00218 (19) | 0.00034 (18) |
| Cl4 | 0.0249 (3) | 0.0158 (2) | 0.0181 (2) | 0.0031 (2) | 0.0002 (2) | 0.00323 (19) |
| O1 | 0.0143 (7) | 0.0201 (7) | 0.0107 (7) | −0.0020 (6) | −0.0023 (6) | −0.0023 (6) |
| O2 | 0.0241 (8) | 0.0229 (8) | 0.0123 (7) | −0.0054 (6) | −0.0030 (6) | −0.0027 (6) |
| N1 | 0.0154 (9) | 0.0120 (8) | 0.0104 (8) | 0.0013 (7) | −0.0017 (7) | −0.0008 (6) |
| N2 | 0.0182 (9) | 0.0166 (9) | 0.0150 (9) | 0.0021 (7) | −0.0011 (7) | 0.0008 (7) |
| N3 | 0.0151 (9) | 0.0164 (9) | 0.0103 (8) | −0.0020 (7) | 0.0002 (7) | −0.0004 (7) |
| C1 | 0.0183 (10) | 0.0092 (9) | 0.0121 (9) | 0.0000 (8) | −0.0028 (8) | 0.0015 (7) |
| C2 | 0.0167 (10) | 0.0088 (9) | 0.0116 (9) | 0.0016 (7) | −0.0011 (8) | 0.0006 (7) |
| C3 | 0.0201 (11) | 0.0130 (10) | 0.0126 (10) | 0.0001 (8) | −0.0023 (8) | 0.0004 (8) |
| C4 | 0.0133 (10) | 0.0222 (11) | 0.0180 (10) | −0.0011 (8) | −0.0038 (8) | 0.0028 (8) |
| C5 | 0.0157 (10) | 0.0189 (10) | 0.0161 (10) | −0.0010 (8) | −0.0040 (8) | −0.0005 (8) |
| C6 | 0.0195 (11) | 0.0144 (10) | 0.0139 (10) | 0.0010 (8) | −0.0035 (8) | 0.0002 (8) |
| C7 | 0.0199 (11) | 0.0211 (11) | 0.0190 (10) | 0.0015 (9) | −0.0046 (9) | −0.0012 (9) |
| C8 | 0.0140 (10) | 0.0213 (11) | 0.0164 (10) | −0.0028 (8) | −0.0017 (8) | 0.0005 (8) |
| C9 | 0.0199 (11) | 0.0191 (11) | 0.0283 (12) | −0.0030 (9) | −0.0062 (10) | −0.0019 (9) |
| C10 | 0.0207 (11) | 0.0135 (10) | 0.0158 (10) | −0.0022 (8) | −0.0022 (9) | 0.0009 (8) |
| C11 | 0.0215 (11) | 0.0176 (11) | 0.0169 (10) | 0.0008 (9) | −0.0018 (9) | −0.0031 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Sn1—O1 | 2.0911 (13) | C4—H4A | 0.9500 |
| Sn1—N1 | 2.2558 (16) | C5—H5A | 0.9500 |
| Sn1—Cl2 | 2.3707 (5) | C6—C7 | 1.507 (3) |
| Sn1—Cl1 | 2.3742 (5) | C6—H6A | 0.9900 |
| Sn1—Cl3 | 2.3879 (5) | C6—H6B | 0.9900 |
| Sn1—Cl4 | 2.4150 (5) | C7—H7A | 0.9800 |
| O1—C1 | 1.299 (2) | C7—H7B | 0.9800 |
| O2—C1 | 1.217 (2) | C7—H7C | 0.9800 |
| N1—C5 | 1.337 (3) | C8—C9 | 1.517 (3) |
| N1—C2 | 1.340 (2) | C8—H8A | 0.9900 |
| N2—C3 | 1.334 (3) | C8—H8B | 0.9900 |
| N2—C4 | 1.334 (3) | C9—H9A | 0.9800 |
| N3—C6 | 1.508 (3) | C9—H9B | 0.9800 |
| N3—C8 | 1.509 (3) | C9—H9C | 0.9800 |
| N3—C10 | 1.510 (3) | C10—C11 | 1.513 (3) |
| N3—H1 | 0.91 (3) | C10—H10A | 0.9900 |
| C1—C2 | 1.508 (3) | C10—H10B | 0.9900 |
| C2—C3 | 1.385 (3) | C11—H11A | 0.9800 |
| C3—H3A | 0.9500 | C11—H11B | 0.9800 |
| C4—C5 | 1.389 (3) | C11—H11C | 0.9800 |
| O1—Sn1—N1 | 75.62 (6) | N1—C5—H5A | 120.1 |
| O1—Sn1—Cl2 | 91.17 (4) | C4—C5—H5A | 120.1 |
| N1—Sn1—Cl2 | 166.13 (4) | C7—C6—N3 | 113.48 (17) |
| O1—Sn1—Cl1 | 168.99 (4) | C7—C6—H6A | 108.9 |
| N1—Sn1—Cl1 | 93.47 (4) | N3—C6—H6A | 108.9 |

| | | | |
|---|---|---|---|
| Cl2—Sn1—Cl1 | 99.813 (18) | C7—C6—H6B | 108.9 |
| O1—Sn1—Cl3 | 86.56 (4) | N3—C6—H6B | 108.9 |
| N1—Sn1—Cl3 | 88.14 (4) | H6A—C6—H6B | 107.7 |
| Cl2—Sn1—Cl3 | 95.397 (18) | C6—C7—H7A | 109.5 |
| Cl1—Sn1—Cl3 | 91.748 (18) | C6—C7—H7B | 109.5 |
| O1—Sn1—Cl4 | 87.08 (4) | H7A—C7—H7B | 109.5 |
| N1—Sn1—Cl4 | 82.96 (4) | C6—C7—H7C | 109.5 |
| Cl2—Sn1—Cl4 | 92.285 (18) | H7A—C7—H7C | 109.5 |
| Cl1—Sn1—Cl4 | 93.058 (19) | H7B—C7—H7C | 109.5 |
| Cl3—Sn1—Cl4 | 170.120 (17) | N3—C8—C9 | 111.95 (17) |
| C1—O1—Sn1 | 119.66 (12) | N3—C8—H8A | 109.2 |
| C5—N1—C2 | 118.45 (17) | C9—C8—H8A | 109.2 |
| C5—N1—Sn1 | 129.40 (13) | N3—C8—H8B | 109.2 |
| C2—N1—Sn1 | 111.85 (13) | C9—C8—H8B | 109.2 |
| C3—N2—C4 | 116.56 (18) | H8A—C8—H8B | 107.9 |
| C6—N3—C8 | 110.51 (15) | C8—C9—H9A | 109.5 |
| C6—N3—C10 | 114.20 (15) | C8—C9—H9B | 109.5 |
| C8—N3—C10 | 111.59 (16) | H9A—C9—H9B | 109.5 |
| C6—N3—H1 | 108.5 (15) | C8—C9—H9C | 109.5 |
| C8—N3—H1 | 108.8 (15) | H9A—C9—H9C | 109.5 |
| C10—N3—H1 | 102.8 (15) | H9B—C9—H9C | 109.5 |
| O2—C1—O1 | 124.81 (19) | N3—C10—C11 | 113.47 (16) |
| O2—C1—C2 | 119.63 (17) | N3—C10—H10A | 108.9 |
| O1—C1—C2 | 115.56 (16) | C11—C10—H10A | 108.9 |
| N1—C2—C3 | 120.55 (18) | N3—C10—H10B | 108.9 |
| N1—C2—C1 | 116.58 (17) | C11—C10—H10B | 108.9 |
| C3—C2—C1 | 122.87 (17) | H10A—C10—H10B | 107.7 |
| N2—C3—C2 | 121.97 (18) | C10—C11—H11A | 109.5 |
| N2—C3—H3A | 119.0 | C10—C11—H11B | 109.5 |
| C2—C3—H3A | 119.0 | H11A—C11—H11B | 109.5 |
| N2—C4—C5 | 122.67 (19) | C10—C11—H11C | 109.5 |
| N2—C4—H4A | 118.7 | H11A—C11—H11C | 109.5 |
| C5—C4—H4A | 118.7 | H11B—C11—H11C | 109.5 |
| N1—C5—C4 | 119.72 (18) | | |
| N1—Sn1—O1—C1 | −6.70 (13) | C5—N1—C2—C1 | 178.09 (16) |
| Cl2—Sn1—O1—C1 | 169.01 (13) | Sn1—N1—C2—C1 | −7.6 (2) |
| Cl1—Sn1—O1—C1 | −14.2 (3) | O2—C1—C2—N1 | −176.95 (18) |
| Cl3—Sn1—O1—C1 | −95.65 (13) | O1—C1—C2—N1 | 2.4 (3) |
| Cl4—Sn1—O1—C1 | 76.78 (13) | O2—C1—C2—C3 | 2.6 (3) |
| O1—Sn1—N1—C5 | −178.97 (18) | O1—C1—C2—C3 | −178.07 (18) |
| Cl2—Sn1—N1—C5 | 162.83 (14) | C4—N2—C3—C2 | 2.5 (3) |
| Cl1—Sn1—N1—C5 | −0.41 (17) | N1—C2—C3—N2 | −1.1 (3) |
| Cl3—Sn1—N1—C5 | −92.05 (17) | C1—C2—C3—N2 | 179.39 (18) |
| Cl4—Sn1—N1—C5 | 92.25 (17) | C3—N2—C4—C5 | −1.5 (3) |
| O1—Sn1—N1—C2 | 7.47 (12) | C2—N1—C5—C4 | 2.4 (3) |
| Cl2—Sn1—N1—C2 | −10.7 (3) | Sn1—N1—C5—C4 | −170.79 (14) |
| Cl1—Sn1—N1—C2 | −173.97 (12) | N2—C4—C5—N1 | −1.0 (3) |
| Cl3—Sn1—N1—C2 | 94.39 (13) | C8—N3—C6—C7 | −174.78 (16) |
| Cl4—Sn1—N1—C2 | −81.31 (12) | C10—N3—C6—C7 | 58.4 (2) |

| | | | |
|---|---|---|---|
| Sn1—O1—C1—O2 | −175.82 (15) | C6—N3—C8—C9 | 79.8 (2) |
| Sn1—O1—C1—C2 | 4.8 (2) | C10—N3—C8—C9 | −151.96 (17) |
| C5—N1—C2—C3 | −1.4 (3) | C6—N3—C10—C11 | 56.1 (2) |
| Sn1—N1—C2—C3 | 172.92 (15) | C8—N3—C10—C11 | −70.1 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H1···N2 | 0.91 (3) | 2.10 (3) | 2.999 (2) | 167 (2) |

**Fig. 1**