ARTICLE IN PRESS – IUCrData

IUCrData

ISSN 2414-3146

Bis(diisobutylammonium) tetrachloridobis[3-(trifluoromethyl)phenyl]stannate

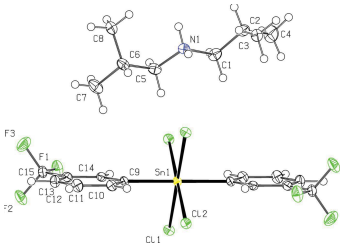
Proof instructions

Proof corrections should be returned by **22 October 2023**. After this period, the Editors reserve the right to publish your data article with only the Managing Editor's corrections.

Please
(1) Read these proofs and assess whether any corrections are necessary.
(2) Check that any technical editing queries highlighted in **bold underlined** text have been answered.
(3) Send corrections by email to **checkin@iucr.org**. Please describe corrections using plain text, where possible, giving the line numbers indicated in the proof. Please do not make corrections to the pdf file electronically and please do not return the pdf file. If no corrections are required please let us know.

To arrange payment for **open access**, please visit **https://scripts.iucr.org/openaccess/?code=tk4096**.

Please check the following details for your article:



Article thumbnail

Synopsis: The title salt comprises di-*iso*butylammonium cations and centrosymmetric tetrachlorobis-(3-trifuoromethylphenyl)stannate(IV) anions, which are connected in the crystal by N—H···Cl and C—H···F interactions.

Abbreviated author list: Song, X.; Li, W.

Keywords: stannate, ammonium cation, crystal structure, hydrogen bonding, salt

How to cite your IUCrData article

Your data article may be cited as follows:

X. Song and W. Li (2023). *IUCrData* **8**, https://doi.org/10.1107/S2414314623009136.

When the final version of your article is published, you will be given instructions on how to download an electronic reprint.

IUCrData

ISSN 2414-3146

Bis(diisobutylammonium) tetrachloridobis[3-(trifluoromethyl)phenyl]stannate

Xueqing Song* and William Li

University of the District of Columbia, Chemistry, 4200 Connecticut Avenue, NW, Washington DC, 20008, USA. *Correspondence e-mail: xsong@udc.edu

Received 29 August 2023
Accepted 17 October 2023

Edited by E. R. T. Tiekink, Sunway University, Malaysia

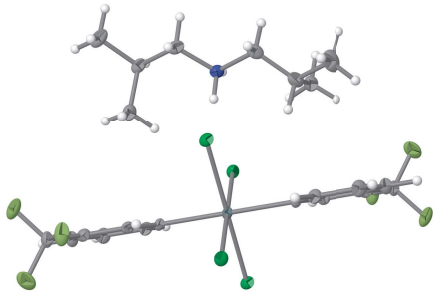
Keywords: stannate; ammonium cation; crystal structure; hydrogen bonding; salt.

CCDC reference: 2301782

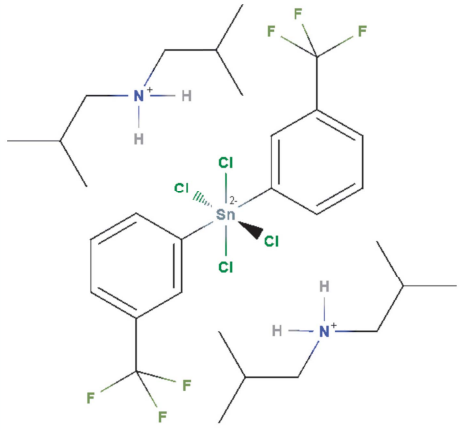
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit in the title salt, $(C_8H_{20}N)_2[SnCl_4(C_7H_4Cl_2F_3)_2]$, features a di-*iso*butylammonium cation in a general position and a diorganotin tetrachloride dianion, *i.e.* tetrachloridobis(3-trifuoromethylphenyl)stannate(IV), located on a centre of inversion; the Sn^{IV} atom is octahedrally coordinated. In the crystal, charge-assisted N^+—H···Cl hydrogen bonds along with C—H···F contacts occur within supramolecular layers that interdigitate along the *a*-axis direction.

3D view



Chemical scheme



Structure description

The title salt, bis(di-*iso*butylammonium) tetrachloridobis(3-trifluoromethylphenyl)stannate, was obtained as a by-product in a reaction of tris(3-trifluoromethylphenyl)tin chloride with acetic acid in the presence of di-*iso*butylamine. An interesting Sn—C cleavage occurred during this reaction.

The crystal comprises di-*iso*butylammonium cations and tetrachloridobis-(3-trifluoromethylphenyl)stannate(IV) anions, with the Sn^{IV} atom of the latter located on a centre of inversion, Fig. 1. The coordination geometry about the Sn^{IV} atom is based on an octahedron, Table 1. This observation resembles literature precedents, *e.g.* Teoh *et al.* (1992) and Hazell *et al.* (1998).

In the crystal, charge-assisted N^+—H···Cl hydrogen bonds along with C—H···F contacts link molecules into a supramolecular layer parallel to (011). As noted from Table 2, the Cl1 atom accepts two N^+—H···Cl hydrogen bonds, each of which is significantly shorter than the N^+—H···Cl hydrogen bond involving the Cl2 atom. This observation accounts for the disparity in the Sn—Cl bond lengths, Table 1. The supramolecular layers interdigitate along [100], Fig. 2.

Table 1
Selected geometric parameters (Å, °).

Sn1—Cl1	2.5845 (4)	Sn1—C9	2.147 (2)
Sn1—Cl2	2.5719 (4)		
C9—Sn1—Cl1	89.36 (6)	Cl1—Sn1—Cl2	90.308 (14)
C9—Sn1—Cl2	90.11 (5)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···Cl1^{i}	0.91	2.31	3.1877 (17)	161
N1—H1*D*···Cl1	0.91	2.44	3.1771 (17)	138
N1—H1*D*···Cl2	0.91	2.75	3.4094 (17)	130
C7—H7*A*···F1^{ii}	0.98	2.56	3.227 (3)	125

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

Synthesis and crystallization

The crystal was obtained as a by-product in an attempt to poduce tris(3-trifluoromethylphenyl)tin acetate in a reaction involving tris(3-trifluoromethylphenyl)tin chloride and acetic acid in the presence of di-isobutylamine. The anticipated tris(3-trifluoromethylphenyl)tin acetate was isolated as the major product along with a few smaller crystals of the title compound in the mother liquid, comprising a mixture of dichloromethane and hexane.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Table 3
Experimental details.

Crystal data	
Chemical formula	$(C_8H_{20}N)_2[SnCl_4(C_7H_4Cl_2F_3)_2]$
M_r	811.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	12.2614 (1), 10.8318 (1), 14.6297 (1)
β (°)	108.523 (1)
V (Å^3)	1842.36 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	8.64
Crystal size (mm)	0.1 × 0.07 × 0.03
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.293, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18706, 3822, 3652
R_{int}	0.057
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.634
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.027, 0.075, 1.08
No. of reflections	3822
No. of parameters	200
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.66, −0.90

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Funding information

Financial assistance from the National Science Foundation (NSF grants Nos. 2117621, 1622811 and 1833656) and the University of the District of Columbia (UDC) is gratefully acknowledged.

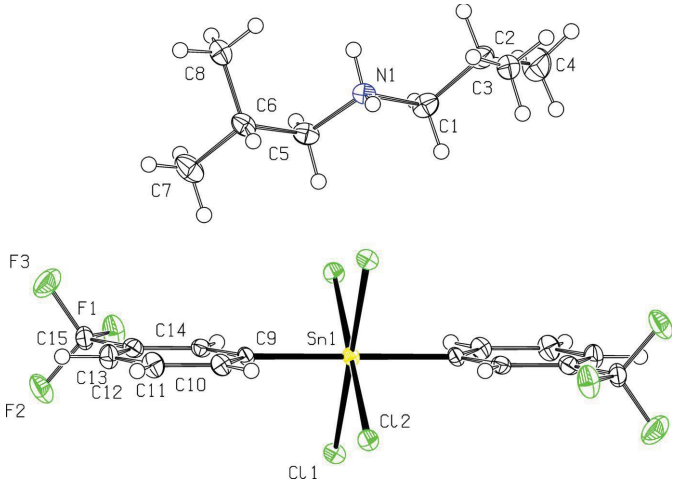


Figure 1
A view of the molecular structures of the di-*iso*butylammonium cation and the tetrachloridobis-(3-trifuoromethylphenyl)stannate(IV) anion, showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. The unlabelled atoms for the anion are related by $1-x, 1-y, 1-z$.

References

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.

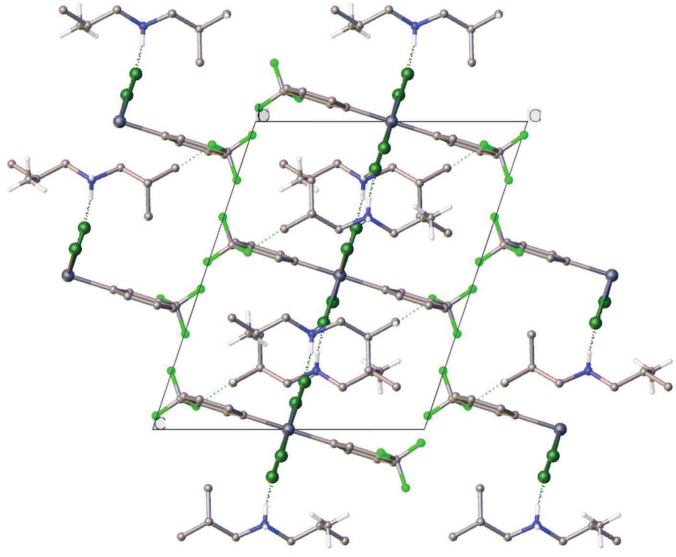


Figure 2
A packing diagram viewed along [010] with intermolecular hydrogen bonding shown as dashed lines.

Hazell, A., Khoo, L. E., Ouyang, J., Rausch, B. J. & Tavares, Z. M. (1998). *Acta Cryst.* C**54**, 728–732.
Rigaku OD (2023). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Teoh, S. G., Teo, S. B., Yeap, G. Y. & Declercq, J. P. (1992). *Polyhedron*, **11**, 2351–2356.

full crystallographic data

Bis(diisobutylammonium) tetrachloridobis[3-(trifluromethyl)phenyl]stannate

Xueqing Song* and William Li

Bis(diisobutylammonium) tetrachloridobis[3-(trifluromethyl)phenyl]stannate

Crystal data

$(C_8H_{20}N)_2[SnCl_4(C_7H_4Cl_2F_3)_2]$
M_r = 811.19
Monoclinic, $P2_1/c$
a = 12.2614 (1) Å
b = 10.8318 (1) Å
c = 14.6297 (1) Å
β = 108.523 (1)°
V = 1842.36 (3) Å^3
Z = 2
$F(000)$ = 828
D_x = 1.462 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 14287 reflections
θ = 3.8–77.8°
μ = 8.64 mm^{-1}
T = 100 K
Block, clear brown-orange
0.1 × 0.07 × 0.03 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix diffractometer
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min} = 0.293, T_{max} = 1.000
18706 measured reflections
3822 independent reflections
3652 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 78.0°, θ_{min} = 3.8°
h = −15→15
k = −13→11
l = −18→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.075
S = 1.08
3822 reflections
200 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.7503P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.66 e Å^{-3}
$\Delta\rho_{min}$ = −0.90 e Å^{-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.

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

	x	y	z	U_{iso}*/U_{eq}
C1	0.35270 (19)	0.5478 (2)	0.13703 (15)	0.0239 (4)

H1A	0.358554	0.457309	0.130324	0.029*
H1B	0.326308	0.583776	0.071441	0.029*
C2	0.26367 (19)	0.5751 (2)	0.18694 (15)	0.0260 (5)
H2	0.295430	0.546221	0.255225	0.031*
C3	0.23739 (19)	0.7127 (2)	0.18845 (16)	0.0275 (5)
H3A	0.306651	0.756553	0.226965	0.041*
H3B	0.175849	0.724982	0.216927	0.041*
H3C	0.212799	0.744875	0.122425	0.041*
C4	0.1551 (3)	0.5004 (2)	0.1380 (3)	0.0411 (8)
H4A	0.121094	0.528525	0.071310	0.062*
H4B	0.099624	0.511991	0.172948	0.062*
H4C	0.174867	0.412669	0.138369	0.062*
C5	0.56054 (19)	0.55525 (19)	0.14964 (15)	0.0222 (4)
H5A	0.537390	0.577720	0.080518	0.027*
H5B	0.565458	0.464099	0.154047	0.027*
C6	0.67905 (19)	0.60917 (19)	0.20024 (15)	0.0218 (4)
H6	0.674857	0.700698	0.190829	0.026*
C7	0.7618 (2)	0.5571 (2)	0.15105 (19)	0.0328 (5)
H7A	0.765195	0.467094	0.157844	0.049*
H7B	0.838600	0.591970	0.181228	0.049*
H7C	0.734647	0.578953	0.082497	0.049*
C8	0.72259 (19)	0.5828 (2)	0.30827 (16)	0.0274 (5)
H8A	0.669735	0.619158	0.338881	0.041*
H8B	0.799278	0.618867	0.336388	0.041*
H8C	0.726737	0.493329	0.318920	0.041*
N1	0.46944 (15)	0.59824 (15)	0.19037 (12)	0.0177 (3)
H1C	0.466464	0.682178	0.188412	0.021*
H1D	0.488962	0.574815	0.253256	0.021*
C9	0.68457 (19)	0.50380 (16)	0.54647 (16)	0.0146 (4)
C10	0.74444 (18)	0.6150 (2)	0.56702 (15)	0.0178 (4)
H10	0.702813	0.690201	0.560520	0.021*
C11	0.86397 (19)	0.6180 (2)	0.59687 (16)	0.0220 (4)
H11	0.903295	0.694773	0.610510	0.026*
C12	0.9258 (2)	0.50866 (18)	0.60672 (18)	0.0215 (5)
H12	1.007476	0.509922	0.627119	0.026*
C13	0.86647 (18)	0.3971 (2)	0.58629 (14)	0.0180 (4)
C14	0.74712 (18)	0.39424 (19)	0.55628 (14)	0.0157 (4)
H14	0.707913	0.317433	0.542374	0.019*
C15	0.93450 (17)	0.2801 (2)	0.59848 (15)	0.0205 (4)
Cl1	0.50101 (4)	0.38477 (4)	0.34558 (3)	0.01643 (11)
Cl2	0.49391 (4)	0.70843 (4)	0.41432 (3)	0.01725 (11)
F1	0.86867 (11)	0.17902 (12)	0.57535 (11)	0.0291 (3)
F2	1.00453 (12)	0.27762 (13)	0.54416 (10)	0.0306 (3)
F3	1.00321 (13)	0.26451 (14)	0.69011 (10)	0.0364 (3)
Sn1	0.500000	0.500000	0.500000	0.01258 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0260 (11)	0.0198 (11)	0.0220 (9)	−0.0067 (9)	0.0021 (8)	−0.0019 (8)
C2	0.0229 (10)	0.0294 (11)	0.0233 (10)	−0.0069 (9)	0.0038 (8)	0.0065 (9)
C3	0.0221 (11)	0.0338 (13)	0.0268 (10)	0.0007 (9)	0.0080 (8)	0.0042 (9)
C4	0.0291 (15)	0.0419 (19)	0.0480 (18)	−0.0161 (10)	0.0061 (13)	0.0051 (10)
C5	0.0301 (11)	0.0173 (10)	0.0218 (9)	0.0001 (8)	0.0118 (8)	−0.0026 (8)
C6	0.0270 (10)	0.0160 (9)	0.0269 (10)	0.0026 (8)	0.0151 (8)	0.0001 (8)
C7	0.0383 (13)	0.0285 (13)	0.0404 (13)	0.0049 (10)	0.0249 (11)	−0.0024 (10)
C8	0.0212 (10)	0.0331 (12)	0.0300 (11)	−0.0014 (9)	0.0112 (8)	0.0022 (10)
N1	0.0220 (8)	0.0135 (8)	0.0181 (7)	−0.0022 (6)	0.0071 (6)	−0.0008 (6)
C9	0.0117 (10)	0.0175 (11)	0.0161 (10)	−0.0006 (6)	0.0063 (8)	−0.0003 (6)
C10	0.0190 (10)	0.0152 (10)	0.0204 (9)	0.0002 (8)	0.0081 (7)	−0.0026 (8)
C11	0.0199 (10)	0.0188 (11)	0.0275 (10)	−0.0063 (8)	0.0077 (8)	−0.0041 (8)
C12	0.0155 (11)	0.0232 (12)	0.0254 (11)	−0.0015 (7)	0.0057 (9)	0.0001 (7)
C13	0.0189 (9)	0.0194 (10)	0.0176 (9)	0.0016 (8)	0.0086 (7)	0.0013 (8)
C14	0.0170 (9)	0.0158 (10)	0.0155 (8)	0.0007 (7)	0.0070 (7)	0.0017 (7)
C15	0.0136 (9)	0.0234 (10)	0.0250 (9)	0.0015 (8)	0.0068 (7)	0.0033 (8)
Cl1	0.0205 (2)	0.0118 (2)	0.0188 (2)	−0.00014 (15)	0.00893 (16)	−0.00113 (15)
Cl2	0.0188 (2)	0.0129 (2)	0.0212 (2)	0.00085 (15)	0.00785 (16)	0.00294 (16)
F1	0.0222 (6)	0.0172 (6)	0.0500 (8)	0.0021 (5)	0.0143 (6)	0.0042 (6)
F2	0.0271 (7)	0.0289 (7)	0.0442 (8)	0.0067 (5)	0.0235 (6)	0.0043 (6)
F3	0.0351 (8)	0.0389 (8)	0.0284 (6)	0.0168 (6)	0.0005 (6)	0.0061 (6)
Sn1	0.01231 (11)	0.01048 (12)	0.01599 (11)	0.00097 (5)	0.00599 (8)	0.00084 (5)

Geometric parameters (Å, º)

C1—C2	1.523 (3)	C11—C12	1.389 (3)
C1—N1	1.499 (3)	C12—C13	1.393 (3)
C2—C3	1.527 (3)	C13—C14	1.388 (3)
C2—C4	1.528 (3)	C13—C15	1.497 (3)
C5—C6	1.522 (3)	C15—F1	1.338 (3)
C5—N1	1.497 (3)	C15—F2	1.343 (2)
C6—C7	1.526 (3)	C15—F3	1.348 (2)
C6—C8	1.526 (3)	Sn1—Cl1	2.5845 (4)
C9—C10	1.393 (3)	Sn1—Cl2	2.5719 (4)
C9—C14	1.396 (3)	Sn1—C9	2.147 (2)
C10—C11	1.390 (3)		
N1—C1—C2	113.03 (17)	F1—C15—F2	106.35 (17)
C1—C2—C3	112.52 (18)	F1—C15—F3	106.55 (17)
C1—C2—C4	108.9 (2)	F2—C15—C13	112.55 (17)
C3—C2—C4	111.5 (2)	F2—C15—F3	105.72 (16)
N1—C5—C6	113.87 (16)	F3—C15—C13	111.92 (17)
C5—C6—C7	107.69 (18)	C9—Sn1—C9^{i}	180.0
C5—C6—C8	113.43 (18)	C9^{i}—Sn1—Cl1^{i}	89.36 (6)
C7—C6—C8	110.67 (19)	C9—Sn1—Cl1	89.36 (6)

C5—N1—C1	112.90 (16)	C9—Sn1—Cl1^{i}	90.64 (6)
C10—C9—C14	118.6 (2)	C9^{i}—Sn1—Cl1	90.64 (6)
C10—C9—Sn1	121.02 (14)	C9—Sn1—Cl2^{i}	89.89 (5)
C14—C9—Sn1	120.40 (14)	C9^{i}—Sn1—Cl2^{i}	90.11 (5)
C11—C10—C9	121.3 (2)	C9^{i}—Sn1—Cl2	89.89 (5)
C12—C11—C10	119.9 (2)	C9—Sn1—Cl2	90.11 (5)
C11—C12—C13	119.1 (2)	Cl1^{i}—Sn1—Cl1	180.0
C12—C13—C15	118.4 (2)	Cl1—Sn1—Cl2	90.308 (14)
C14—C13—C12	120.9 (2)	Cl2^{i}—Sn1—Cl1^{i}	90.308 (14)
C14—C13—C15	120.68 (19)	Cl2^{i}—Sn1—Cl1	89.692 (14)
C13—C14—C9	120.20 (19)	Cl2—Sn1—Cl1^{i}	89.693 (14)
F1—C15—C13	113.22 (17)	Cl2^{i}—Sn1—Cl2	180.00 (3)
C2—C1—N1—C5	171.26 (17)	C12—C13—C14—C9	−0.3 (3)
C6—C5—N1—C1	177.79 (17)	C12—C13—C15—F1	−178.98 (19)
N1—C1—C2—C3	66.3 (2)	C12—C13—C15—F2	−58.3 (3)
N1—C1—C2—C4	−169.55 (19)	C12—C13—C15—F3	60.6 (3)
N1—C5—C6—C7	179.98 (17)	C14—C9—C10—C11	−0.1 (3)
N1—C5—C6—C8	57.2 (2)	C14—C13—C15—F1	1.7 (3)
C9—C10—C11—C12	−0.1 (3)	C14—C13—C15—F2	122.3 (2)
C10—C9—C14—C13	0.2 (3)	C14—C13—C15—F3	−118.8 (2)
C10—C11—C12—C13	0.0 (4)	C15—C13—C14—C9	179.09 (19)
C11—C12—C13—C14	0.1 (4)	Sn1—C9—C10—C11	−179.81 (16)
C11—C12—C13—C15	−179.2 (2)	Sn1—C9—C14—C13	179.96 (15)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···Cl1^{ii}	0.91	2.31	3.1877 (17)	161
N1—H1*D*···Cl1	0.91	2.44	3.1771 (17)	138
N1—H1*D*···Cl2	0.91	2.75	3.4094 (17)	130
C7—H7*A*···F1^{iii}	0.98	2.56	3.227 (3)	125

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

other supporting information

The following files will be made available to readers when your article is published. Unless otherwise stated, these files will be the same as those submitted during the review process.

Crystal structure: contains datablock I. tk4096sup1.cif

Structure factors: contains datablock I. tk4096Isup2.hkl

IUCrData

ORDER FORM

ISSN: 2414-3146

YOU WILL AUTOMATICALLY BE SENT DETAILS OF HOW TO DOWNLOAD
AN ELECTRONIC REPRINT OF YOUR PAPER, FREE OF CHARGE.
PRINTED REPRINTS MAY BE PURCHASED USING THIS FORM.

Please scan your order and send to checkin@iucr.org

INTERNATIONAL UNION OF CRYSTALLOGRAPHY
5 Abbey Square
Chester CH1 2HU, England.

VAT No. GB 161 9034 76

Article No.: X230913-TK4096

Title of article Bis(diisobutylammonium) tetrachloridobis[3-(trifluoromethyl)phenyl]stannate

Name Xueqing Song

Address University of DC, 4200 Connecticut Avenue NW, Washington, DC 2008, USA,

E-mail address (for electronic reprints) xsong@udc.edu

DIGITAL PRINTED REPRINTS

I wish to order . . . . . paid reprints

These reprints will be sent to the address given above. If the above address or e-mail address is not correct, please indicate an alternative:

PAYMENT

☐ An official purchase order made out to **INTERNATIONAL UNION OF CRYSTALLOGRAPHY** ☐ is enclosed ☐ will follow

Purchase order No.

☐ Please invoice me

☐ I wish to pay by credit card

EU authors only: VAT No:

Date | Signature

DIGITAL PRINTED REPRINTS

An electronic reprint is supplied free of charge.

Printed reprints without limit of number may be purchased at the prices given in the table below. The requirements of all joint authors, if any, and of their laboratories should be included in a single order, specifically ordered on the form overleaf. All orders for reprints must be submitted promptly.

Prices for reprints are given below in **United States dollars** and include postage.

	Size of paper (in printed pages)				
Number of reprints required	1–2	3–4	5–8	9–16	Additional 8's
50	184	268	372	560	246
100	278	402	556	842	370
150	368	534	740	1122	490
200	456	664	920	1400	610
Additional 50's	86	128	178	276	116

PAYMENT AND ORDERING

Official purchase orders should be made out to **INTERNATIONAL UNION OF CRYSTALLOGRAPHY**.

Orders should be returned by email to checkin@iucr.org

ENQUIRIES

Enquiries concerning reprints should be sent to support@iucr.org.