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2,2'-Iminodipyridinium(1+) dichlorotriphenylstannate and 2,2'-iminodipyridinium(1+) tricyclohexylbis(trifluoroacetato)stannate

S. W. Ng

Abstract

The Sn atom in 2,2'-iminodipyridinium(1+) dichlorotriphenylstannate shows *trans*-C_3SnCl_2 trigonal bipyramidal coordination. The anion is linked to adjacent anions through the counter-ion to form a chain that runs diagonally on the a-c face of the unit cell; the 2,2'-iminodipyridinium(1+) cation, which is disordered over a twofold axis, uses the amino and pyridinium N-atoms to link to the chlorine atoms; $N_{amino}\cdots Cl$ = 3.32 (2) Å; $N_{pyridinium}\cdots Cl$ = 3.62 (2) and 3.69 (2) Å. 2,2'-Iminodipyridinium(1+) bis(trifluoroacetato)tricyclohexylstannate adopts a similar hydrogen bonded [$N_{amino}\cdots O$ = 2.72 (1) Å, $N_{pyridinium}\cdots O$ = 3.14 (2) and 3.14 (2) Å] chain structure.

Comment

Triaryltin halides when treated with 1,10-phenanthroline afford 1/1 complexes containing a molecule of water. The N-heterocycle is not bonded directly the Lewis acid; instead, the water molecule is linked to the Lewis acid by a coordinate bond and to the N-heterocycle by two hydrogen bonds (Ng, 1996; Ng & Kumar Das, 1996; Ng *et al.*, 1997). An analogous `outer-sphere coordination' complex (Gabe *et al.*, 1984) is expected of 2,2'-dipyridylamine; however, its reaction with triphenyltin chloride yielded the ammonium stannate (I). The isolation of the 2,2'-iminodipyridinium cation suggests that the di-2-pyridylamino entity would be thermodynamically more stable in the protonated form; in this form, the pyridinium moiety interacts with the pyridyl moiety through a hydrogen bond. The hydrogen-bonded 2,2'-iminodipyridinium cation has also been authenticated in other organostannates (Ng, 1998*a*,b; Ng & Hook, 1999). In the dichlorotriphenystannate, nitrogen$\cdots$chlorine hydrogen bonds [$N\cdots Cl$ = 3.32 (2) Å, 3.62 (2) Å, 3.69 (2) Å] link the amino/pyridinium groups with the Cl atoms of the anion to form chains. The hydrogen bonds are somewhat longer than those [$N\cdots Cl$ = 3.145 (2) Å, 3.176 (2) Å] found in dicyclohexylammonium chloride (Ng, 1995*b*) as well as that [$N\cdots Cl$ = 3.18 (3) Å] found in quinolinium trichlorodimethylstannate (Buttenshaw *et al.*, 1975). 2,2'-Iminodipyridinium chloride crystallizes as a monohydrate, but there is no interaction between the N atoms and the Cl atom (Gluth, 1993).

The Sn atom, which lies on a twofold axis, shows *trans*-C_3SnCl_2 trigonal bipyramidal geometry in the 2,2'-iminodipyridinium salt [Sn—Cl = 2.622 (2) Å], as does the Sn atom in tetramethylammonium dichlorotriphenylstannate [Sn—Cl = 2.598 (1) Å], which also lies on a twofold axis (Ng, 1995*a*).

Tricyclohexyltin trifluoroacetate exists as monomeric molecule centring four-coordinate Sn; adjacent molecules are linked into a chain by a weak tin-oxygen interaction [Sn—O = 2.08 (4) Å, $Sn\cdots O$ = 3.11 Å] (Calogero *et al.*, 1980). A second trifluoroacetato group increases the tin-oxygen bond distance to 2.313 (5) Å in (II), whose Sn atom lies on a twofold axis. The bond distance exceeds those [Sn—O = 2.200 (5) Å, 2.252 (5) =Å] found in 2,2'-iminodipyridinium bis(trifluoroacetato)triphenylstannate (Ng, 1998*b*); the long covalent bond is probably compensated by a shorter

N_{amino}···$O_{carbonyl}$ hydrogen bond [N···O = 2.72 (2) Å in (I), N···O = 2.843 (3) Å in $[C_{10}H_{10}N_3]$ $[(C_6H_5)_3Sn(O_2CCF_3)_2]$ (Ng, 1998*b*)].

Experimental

In an attempt to synthesize chlorotriphenyltin·water·2,2'-dipyridylamine, equimolar quantities of triphenyltin chloride and 2,2'-dipyridylamine were heated in a small volume of 95% ethanol until the reactants dissolved completely. The ammonium stannate (I) precipitated out of solution as large colorless crystals when the solution was cooled.

To prepare (II), equimolar quantities of tricyclohexyltin hydroxide and trifluoroacetic acid was reacted in ethanol to yield tricyclohexyltin trifluoroacetate *in situ*. To the solution was added an ethanol solution of 2,2'-iminodipyridinium trifluoroacetate, prepared by neutralizing trifluoroacetic acid with di-2-pyridylamine. Slow cooling of the filtered mixture yielded colorless crystals of (II).

Refinement

Both structures are disordered. For (I), the 2,2'-iminodipyridinium cation is disordered over a twofold axis, and was refined as a FLAT 0.02 C11/C12/C13/C14/C15—N1—C11'/C12'/C13'/C14'/C15'/N2' entity whose atoms have 1/2 site occupancy. The pyridyl rings were refined as hexagons by an AFIX 66 instruction, and the atoms of each ring were given the same temperature factors by an EADP instruction. The N—C distances were restrained to be the same by a SADI 0.02 instruction.

Only one of the two pyridyl N atoms is protonated; the amino N atom [N_{amino}···Cl = 3.32 (1) Å] as well as the protonated pyridinium N atom would then form hydrogen bonds to the Cl atoms of adjacent anions. Owing to the disorder, the N2 atom was arbitrarily designated the pyridinium N atom; the N2' atom is equally as likely to be linked [$N_{pyridinium}$···Cl = 3.62 (2) Å, 3.69 (2) Å].

The final difference map had a peak larger than 2 e $Å^{-3}$ at 1 Å from the Sn1 atom and 1.5 Å from the Cl1 atom; other peaks are less than 1 e $Å^{-3}$.

For (II), the 2,2'-iminodipyridinium cation is also disordered over a twofold axis, and was refined as a FLAT 0.02 C13/C14/C15/C16/C17—N1—C13'/C14'/C15'/C16'/C17'/N2'; the pyridyl rings were refined as hexagons, and the atoms of each ring were given the same temperature factors. The N—C distances were restrained to be a SADI 0.02 instruction.

Only one of the two pyridyl N atoms is protonated; the amino N atom [N_{amino}···O = 2.72 (2) Å] as well as the protonated pyridinium N atom would then form hydrogen bonds to the double-bond O atom of adjacent anions. The N2 atom was arbitrarily designated the pyridinium N atom; both the N2···O2 and N2'···O2 distances are 3.14 (2) Å. Evidence for this type of hydrogen bonding scheme is furnished by the 2,2'-iminodipyridinium salts of bis(trihaloacetato)triphenylstannates (Ng, 1998*b*; Ng & Hook, 1999). The N···O hydrogen bond involving the amino N-atom is shorter than that involving the pyridinium N-atom in these structures, which are not disordered.

The cyclohexyl ring lying on the twofold axis is also disordered; the pairs of C8/C8' and C9/C9' were give the same temperature factors by an EADP instruction. The C8, C9, C8', C9' atoms were given 1/2 site occupancies. A SIMU 0.02

instruction was also imposed on the set of C7, C8 C9, C10 atoms. For the two cyclohexyl rings, C—C, C···C and C···C···C distances were DFIXed at 1.54±0.01 Å, 2.51±0.02 Å and 2.95± Å. If this cyclohexyl ring is generated by applying the appropriate symmetry transformation to the C7/C8/C9/C10 set of atoms only, the ring has a twist boat conformation.

The $–CF_3$ group was refined as two half-site occupancy $–CF_3$ groups sharing a common C atom, subject to C—F = 1.36±0.01 Å, F···F = 2.22±0.02 Å and C···C···F = 2.37±0.02 Å. Each set of three F atoms were constrained to have the same temperature factors.

Computing details

For both compounds, data collection: *CAD-4-PC* (Kretschmar, 1994); cell refinement: *CELDIM* (Enraf-Nonius, 1988); data reduction: *XCAD4* (Harms, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*

2,2'-Iminodipyridinium(1+) dichlorotriphenylstannate

Crystal data

$(C_{10}H_{10}N_3)[SnCl_2(C_6H_5)_3]$	V = 2617.7 (5) Å^3
M_r = 593.10	Z = 4
Monoclinic, $C2/c$	Mo $K\alpha$
a = 16.283 (1) Å	μ = 1.20 mm^{-1}
b = 10.694 (1) Å	T = 298 (2) K
c = 15.038 (2) Å	0.57 × 0.50 × 0.43 mm
β = 91.443 (9)°	

Data collection

Enraf-Nonius CAD-4 diffractometer	2150 reflections with $I > 2\sigma(I)$
Absorption correction: ψ scan (North et al., 1968) in WinGX (Farrugia, 1998)	R_{int} = 0.024
T_{min} = 0.500, T_{max} = 0.597	3 standard reflections
4787 measured reflections	every 60 min
2302 independent reflections	intensity decay: 2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048	11 restraints
$wR(F^2)$ = 0.145	Constrained, U(H) = 1.5U_{eq}(C,N)
S = 1.14	$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 17.8556P]$ where $P = (F_o^2 + 2F_c^2)/3$
2302 reflections	$\Delta\rho_{max}$ = 2.12 e Å^{-3}
130 parameters	$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected geometric parameters (Å, °)

Sn1—C1	2.127 (5)	Sn1—Cl1	2.622 (2)
Sn1—C1^{i}	2.127 (5)	Sn1—Cl1^{i}	2.622 (2)
Sn1—C7	2.164 (8)		
C1—Sn1—C1^{i}	121.9 (3)	C1^{i}—Sn1—Cl1	88.8 (2)
C1—Sn1—C7	119.0 (2)	C1^{i}—Sn1—Cl1^{i}	87.5 (2)
C1—Sn1—Cl1	87.5 (2)	C7—Sn1—Cl1	93.8 (1)
C1—Sn1—Cl1^{i}	88.8 (2)	C7—Sn1—Cl1^{i}	93.8 (1)
C1^{i}—Sn1—C7	119.0 (2)	Cl1—Sn1—Cl1^{i}	172.3 (1)

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

2,2'-Iminodipyridinium(1+) bis(trifluoroacetato)tricyclohexylstannate

Crystal data

$(C_{10}H_{10}N_3)[Sn(C_2F_3O_2)(C_6H_{11})_3]$	V = 3565.8 (4) Å^3
M_r = 766.38	Z = 4
Monoclinic, *C*2/*c*	Mo *K*α
a = 18.8548 (8) Å	μ = 0.79 mm^{-1}
b = 10.9063 (7) Å	*T* = 298 (2) K
c = 17.591 (2) Å	0.58 × 0.54 × 0.50 mm
β = 99.678 (5)°	

Data collection

Enraf-Nonius CAD-4 diffractometer	2685 reflections with $I > 2\sigma(I)$
Absorption correction: ψ scan (North et al., 1968) in WinGX (Farrugia, 1998)	R_{int} = 0.026
T_{min} = 0.621, T_{max} = 0.675	3 standard reflections
6439 measured reflections	every 60 min
3121 independent reflections	intensity decay: 3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059	77 restraints
$wR(F^2)$ = 0.173	Constrained, U(H) = 1.5U$_{eq}$(C,N).
S = 1.08	$\Delta\rho_{max}$ = 0.73 e Å^{-3}
3121 reflections	$\Delta\rho_{min}$ = −0.85 e Å^{-3}
192 parameters	

Table 2

Selected geometric parameters (Å, °)

Sn1—C1	2.143 (5)	Sn1—O1	2.313 (5)
Sn1—C1^{i}	2.143 (5)	Sn1—O1^{i}	2.313 (5)
Sn1—C7	2.117 (9)		
C1—Sn1—C7	121.3 (2)	C1^{i}—Sn1—O1	93.7 (2)
C1—Sn1—C1^{i}	117.4 (3)	C1^{i}—Sn1—O1^{i}	87.5 (2)
C1—Sn1—O1	87.5 (2)	C7—Sn1—O1	88.8 (1)
C1—Sn1—O1^{i}	93.7 (2)	C7—Sn1—O1^{i}	88.8 (1)
C1^{i}—Sn1—C7	121.3 (2)	O1—Sn1—O1^{i}	177.5 (3)

Symmetry codes: (i) $-x+1, y, -z+1/2$.

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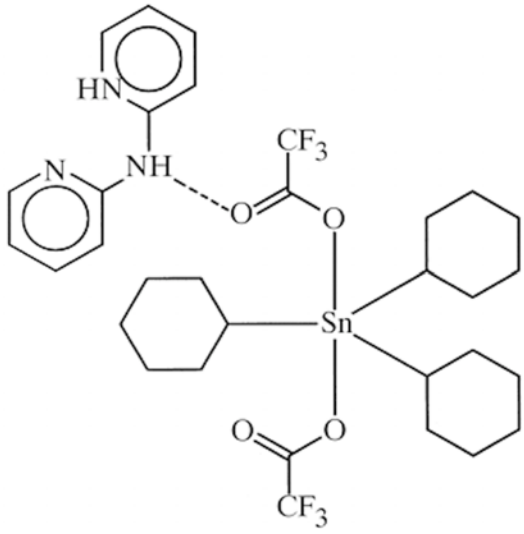
CIF access

Scheme 1



supplementary materials

2,2'-Iminodipyridinium(1+) dichlorotriphenylstannate

Crystal data

$(C_{10}H_{10}N_3)[SnCl_2(C_6H_5)_3]$	F_{000} = 1192
M_r = 593.10	D_x = 1.505 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 16.283 (1) Å	Cell parameters from 25 reflections
b = 10.694 (1) Å	θ = 12.0–13.0º
c = 15.038 (2) Å	μ = 1.20 mm^{-1}
β = 91.443 (9)º	*T* = 298 (2) K
V = 2617.7 (5) Å^3	Triangular block, colourless
Z = 4	0.57 × 0.50 × 0.43 mm

Data collection

Enraf-Nonius CAD-4 diffractometer	R_{int} = 0.024
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.3º
T = 298(2) K	*h* = −19→19
ω scans	*k* = 0→12
Absorption correction: ψ scan (North et al., 1968) in WinGX (Farrugia, 1998)	*l* = −17→17
T_{min} = 0.500, T_{max} = 0.597	3 standard reflections
4787 measured reflections	every 60 min
2302 independent reflections	intensity decay: 2%
2150 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.048	Constrained, U(H) = 1.5U_{eq}(C,N)
$wR(F^2)$ = 0.145	$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 17.8556P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.14	$(\Delta/\sigma)_{max}$ = 0.001
2302 reflections	$\Delta\rho_{max}$ = 2.12 e Å^{-3}
130 parameters	$\Delta\rho_{min}$ = −0.76 e Å^{-3}
11 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.5000	0.15646 (5)	0.2500	0.0348 (2)	
Cl1	0.4908 (1)	0.1728 (2)	0.4235 (1)	0.0537 (4)	
N1	0.3146 (7)	0.2314 (9)	0.4920 (5)	0.053 (3)	0.50
N2	0.1941 (9)	0.139 (1)	0.5342 (7)	0.072 (5)	0.50
N2'	0.2116 (8)	0.378 (1)	0.4897 (7)	0.056 (3)	0.50
C1	0.6139 (3)	0.2530 (5)	0.2618 (4)	0.038 (1)	
C2	0.6238 (5)	0.3622 (6)	0.3126 (5)	0.056 (2)	
C3	0.7001 (5)	0.4168 (8)	0.3228 (5)	0.069 (2)	
C4	0.7667 (5)	0.3675 (8)	0.2823 (6)	0.071 (2)	
C5	0.7596 (4)	0.2599 (7)	0.2354 (5)	0.061 (2)	
C6	0.6829 (4)	0.2037 (7)	0.2242 (4)	0.049 (1)	
C7	0.5000	−0.0459 (8)	0.2500	0.041 (2)	
C8	0.4962 (4)	−0.1108 (7)	0.1714 (4)	0.049 (1)	
C9	0.4968 (5)	−0.2412 (7)	0.1715 (5)	0.063 (2)	
C10	0.5000	−0.307 (1)	0.2500	0.066 (3)	
C11	0.2776 (9)	0.130 (1)	0.5179 (6)	0.072 (5)	0.50
C12	0.3182 (6)	0.017 (2)	0.5294 (7)	0.072 (5)	0.50
C13	0.2753 (9)	−0.088 (1)	0.5573 (7)	0.072 (5)	0.50
C14	0.1918 (9)	−0.079 (1)	0.5736 (8)	0.072 (5)	0.50
C15	0.1513 (6)	0.034 (2)	0.5621 (8)	0.072 (5)	0.50
C11'	0.2935 (8)	0.3472 (7)	0.4776 (7)	0.056 (3)	0.50
C12'	0.3481 (6)	0.437 (1)	0.4483 (7)	0.056 (3)	0.50
C13'	0.3208 (7)	0.558 (1)	0.4312 (6)	0.056 (3)	0.50
C14'	0.2389 (8)	0.5891 (8)	0.4433 (7)	0.056 (3)	0.50
C15'	0.1843 (6)	0.499 (1)	0.4725 (7)	0.056 (3)	0.50
H2	0.5787	0.3980	0.3395	0.083*	
H3	0.7062	0.4880	0.3578	0.104*	
H4	0.8172	0.4080	0.2869	0.107*	
H5	0.8057	0.2236	0.2108	0.091*	
H6	0.6782	0.1310	0.1904	0.073*	
H8	0.4932	−0.0676	0.1177	0.074*	
H9	0.4949	−0.2843	0.1178	0.094*	
H10	0.5000	−0.3937	0.2500	0.100*	
H1	0.3657	0.2185	0.4819	0.080*	0.50
H12	0.3740	0.0108	0.5185	0.107*	0.50
H13	0.3024	−0.1640	0.5650	0.107*	0.50
H14	0.1631	−0.1494	0.5923	0.107*	0.50
H15	0.0954	0.0399	0.5731	0.107*	0.50
H2a	0.1690	0.2089	0.5271	0.107*	0.50
H12'	0.4029	0.4167	0.4402	0.084*	0.50
H13'	0.3573	0.6187	0.4117	0.084*	0.50
H14'	0.2206	0.6701	0.4319	0.084*	0.50
H15'	0.1295	0.5196	0.4806	0.084*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0253 (3)	0.0365 (3)	0.0427 (3)	0.000	0.0017 (2)	0.000
Cl1	0.0573 (9)	0.068 (1)	0.0362 (8)	0.0090 (7)	0.0081 (6)	0.0010 (6)
N1	0.044 (6)	0.066 (7)	0.051 (6)	0.008 (5)	0.010 (5)	0.004 (5)
N2	0.076 (7)	0.070 (7)	0.069 (7)	0.006 (4)	−0.004 (4)	0.014 (4)
N2'	0.072 (6)	0.044 (5)	0.051 (5)	0.002 (3)	0.000 (3)	0.006 (3)
C1	0.033 (3)	0.036 (3)	0.043 (3)	−0.002 (2)	0.000 (2)	0.004 (2)
C2	0.057 (4)	0.052 (4)	0.057 (4)	−0.003 (3)	0.006 (3)	−0.005 (3)
C3	0.078 (5)	0.058 (4)	0.071 (5)	−0.021 (4)	−0.004 (4)	−0.009 (4)
C4	0.049 (4)	0.078 (5)	0.086 (5)	−0.024 (4)	−0.009 (4)	0.016 (4)
C5	0.033 (3)	0.070 (5)	0.079 (5)	−0.002 (3)	0.005 (3)	0.010 (4)
C6	0.038 (3)	0.055 (4)	0.053 (3)	0.000 (3)	0.005 (3)	0.001 (3)
C7	0.032 (4)	0.040 (4)	0.050 (5)	0.000	0.002 (3)	0.000
C8	0.047 (3)	0.049 (3)	0.051 (4)	0.004 (3)	0.002 (3)	−0.003 (3)
C9	0.067 (5)	0.052 (4)	0.070 (5)	0.001 (3)	−0.005 (4)	−0.013 (3)
C10	0.074 (7)	0.038 (5)	0.087 (8)	0.000	−0.009 (6)	0.000
C11	0.076 (7)	0.070 (7)	0.069 (7)	0.006 (4)	−0.004 (4)	0.014 (4)
C12	0.076 (7)	0.070 (7)	0.069 (7)	0.006 (4)	−0.004 (4)	0.014 (4)
C13	0.076 (7)	0.070 (7)	0.069 (7)	0.006 (4)	−0.004 (4)	0.014 (4)
C14	0.076 (7)	0.070 (7)	0.069 (7)	0.006 (4)	−0.004 (4)	0.014 (4)
C15	0.076 (7)	0.070 (7)	0.069 (7)	0.006 (4)	−0.004 (4)	0.014 (4)
C11'	0.072 (6)	0.044 (5)	0.051 (5)	0.002 (3)	0.000 (3)	0.006 (3)
C12'	0.072 (6)	0.044 (5)	0.051 (5)	0.002 (3)	0.000 (3)	0.006 (3)
C13'	0.072 (6)	0.044 (5)	0.051 (5)	0.002 (3)	0.000 (3)	0.006 (3)
C14'	0.072 (6)	0.044 (5)	0.051 (5)	0.002 (3)	0.000 (3)	0.006 (3)
C15'	0.072 (6)	0.044 (5)	0.051 (5)	0.002 (3)	0.000 (3)	0.006 (3)

Geometric parameters (Å, °)

Sn1—C1	2.127 (5)	C10—C9^{i}	1.373 (9)
Sn1—C1^{i}	2.127 (5)	N1—C11'	1.30 (1)
Sn1—C7	2.164 (8)	N1—C11	1.31 (1)
Sn1—Cl1	2.622 (2)	C11—C12	1.3900
Sn1—Cl1^{i}	2.622 (2)	C11—N2	1.3900
C1—C6	1.375 (8)	C12—C13	1.3900
C1—C2	1.403 (9)	C13—C14	1.3900
C2—C3	1.38 (1)	C14—C15	1.3900
C3—C4	1.36 (1)	C15—N2	1.3900
C4—C5	1.35 (1)	C11'—C12'	1.3900
C5—C6	1.392 (9)	C11'—N2'	1.3900
C7—C8	1.371 (8)	C12'—C13'	1.3900
C7—C8^{i}	1.371 (8)	C13'—C14'	1.3900
C8—C9	1.40 (1)	C14'—C15'	1.3900
C9—C10	1.373 (9)	C15'—N2'	1.3900
C1—Sn1—C1^{i}	121.9 (3)	C7—C8—C9	120.3 (7)

C1—Sn1—C7	119.0 (2)	C10—C9—C8	120.8 (7)
C1—Sn1—Cl1	87.5 (2)	C9^{i}—C10—C9	119 (1)
C1—Sn1—Cl1^{i}	88.8 (2)	C11'—N1—C11	136 (1)
C1^{i}—Sn1—C7	119.0 (2)	N1—C11—C12	123 (1)
C1^{i}—Sn1—Cl1	88.8 (2)	N1—C11—N2	117 (1)
C1^{i}—Sn1—Cl1^{i}	87.5 (2)	C12—C11—N2	120.0
C7—Sn1—Cl1	93.8 (1)	C11—C12—C13	120.0
C7—Sn1—Cl1^{i}	93.8 (1)	C12—C13—C14	120.0
Cl1—Sn1—Cl1^{i}	172.3 (1)	C15—C14—C13	120.0
C6—C1—C2	117.4 (6)	C14—C15—N2	120.0
C6—C1—Sn1	119.9 (4)	C15—N2—C11	120.0
C2—C1—Sn1	122.5 (4)	N1—C11'—C12'	123 (1)
C3—C2—C1	120.3 (7)	N1—C11'—N2'	117 (1)
C4—C3—C2	120.8 (7)	C12'—C11'—N2'	120.0
C5—C4—C3	120.2 (7)	C11'—C12'—C13'	120.0
C4—C5—C6	119.7 (7)	C12'—C13'—C14'	120.0
C5—C6—C1	121.6 (7)	C15'—C14'—C13'	120.0
C8—C7—C8^{i}	119.2 (8)	C14'—C15'—N2'	120.0
C8—C7—Sn1	120.4 (4)	C15'—N2'—C11'	120.0
C8^{i}—C7—Sn1	120.4 (4)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1	0.86	2.29	3.32 (1)	167

2,2'-Iminodipyridinium(1+) bis(trifluoroacetato)tricyclohexylstannate

Crystal data

$(C_{10}H_{10}N_3)[Sn(C_2F_3O_2)(C_6H_{11})_3]$	F_{000} = 1568
M_r = 766.38	D_x = 1.428 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
a = 18.8548 (8) Å	Cell parameters from 25 reflections
b = 10.9063 (7) Å	θ = 12.0–13.0º
c = 17.591 (2) Å	μ = 0.79 mm^{-1}
β = 99.678 (5)º	*T* = 298 (2) K
V = 3565.8 (4) Å^3	Block, colourless
Z = 4	0.58 × 0.54 × 0.50 mm

Data collection

Enraf-Nonius CAD-4 diffractometer	R_{int} = 0.026
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º

Monochromator: graphite
T = 298(2) K
ω scans
Absorption correction: ψ scan (North et al., 1968) in WinGX (Farrugia, 1998)
T_{min} = 0.621, T_{max} = 0.675
6439 measured reflections
3121 independent reflections
2685 reflections with $I > 2\sigma(I)$

θ_{min} = 2.2º
h = −22→22
k = −12→0
l = −20→20
3 standard reflections
every 60 min
intensity decay: 3%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.173
S = 1.08
3121 reflections
192 parameters
77 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
Constrained, U(H) = 1.5U_{eq}(C,N).
$w = 1/[\sigma^2(F_o^2) + (0.1148P)^2 + 5.3386P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.85 e Å^{-3}
Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.5000	0.19190 (4)	0.2500	0.0578 (3)	
F1	0.5290 (7)	0.185 (1)	−0.0611 (7)	0.124 (2)	0.50
F2	0.4192 (5)	0.179 (1)	−0.0296 (6)	0.124 (2)	0.50
F3	0.4756 (6)	0.347 (1)	−0.0262 (6)	0.124 (2)	0.50
F1'	0.534 (1)	0.234 (2)	−0.0598 (9)	0.202 (5)	0.50
F2'	0.469 (1)	0.091 (1)	−0.0286 (8)	0.202 (5)	0.50
F3'	0.4221 (8)	0.264 (2)	−0.0392 (9)	0.202 (5)	0.50
O1	0.4771 (3)	0.1964 (5)	0.1167 (3)	0.092 (2)	
O2	0.5830 (3)	0.2377 (9)	0.0854 (4)	0.115 (2)	
N1	0.7007 (5)	0.244 (1)	0.0153 (6)	0.076 (3)	0.50
N2	0.8062 (8)	0.142 (1)	0.0069 (6)	0.098 (4)	0.50
N2'	0.7806 (7)	0.376 (1)	−0.0318 (7)	0.092 (4)	0.50
C1	0.4022 (3)	0.0898 (5)	0.2450 (4)	0.072 (2)	
C2	0.3352 (3)	0.1665 (6)	0.2183 (7)	0.106 (3)	
C3	0.2660 (4)	0.0936 (8)	0.2178 (8)	0.139 (4)	
C4	0.2660 (4)	−0.0257 (9)	0.1768 (6)	0.121 (3)	
C5	0.3309 (4)	−0.1015 (7)	0.2106 (9)	0.170 (6)	
C6	0.4002 (4)	−0.0292 (7)	0.2037 (9)	0.157 (6)	
C7	0.5000	0.3860 (8)	0.2500	0.119 (5)	
C8	0.4419 (9)	0.456 (1)	0.281 (1)	0.136 (6)	0.50

C9	0.4302 (6)	0.581 (1)	0.237 (2)	0.159 (6)	0.50
C10	0.5000	0.654 (1)	0.2500	0.170 (7)	
C9'	0.5578 (9)	0.581 (1)	0.219 (1)	0.159 (6)	0.50
C8'	0.5706 (5)	0.457 (1)	0.264 (2)	0.136 (6)	0.50
C11	0.5185 (4)	0.2153 (6)	0.0717 (4)	0.079 (2)*	
C12'	0.4868 (5)	0.218 (1)	−0.0108 (6)	0.141 (5)	0.50
C12	0.4868 (5)	0.218 (1)	−0.0108 (6)	0.141 (5)	0.50
C13	0.7370 (7)	0.146 (1)	0.0244 (6)	0.098 (4)	0.50
C14	0.7071 (6)	0.043 (2)	0.0524 (7)	0.098 (4)	0.50
C15	0.7464 (8)	−0.066 (1)	0.0628 (7)	0.098 (4)	0.50
C16	0.8155 (8)	−0.070 (1)	0.0453 (7)	0.098 (4)	0.50
C17	0.8454 (6)	0.033 (1)	0.0173 (7)	0.098 (4)	0.50
C13'	0.7141 (8)	0.3548 (9)	−0.0101 (6)	0.092 (4)	0.50
C14'	0.6637 (6)	0.449 (1)	−0.0146 (7)	0.092 (4)	0.50
C15'	0.6798 (7)	0.564 (1)	−0.0407 (7)	0.092 (4)	0.50
C16'	0.7463 (8)	0.5854 (8)	−0.0624 (6)	0.092 (4)	0.50
C17'	0.7967 (6)	0.492 (1)	−0.0580 (6)	0.092 (4)	0.50
H1	0.4000	0.0684	0.2987	0.107*	
H2A	0.3353	0.2367	0.2522	0.159*	
H2B	0.3364	0.1969	0.1667	0.159*	
H3A	0.2596	0.0785	0.2706	0.209*	
H3B	0.2254	0.1422	0.1932	0.209*	
H4A	0.2666	−0.0110	0.1225	0.182*	
H4B	0.2224	−0.0706	0.1811	0.182*	
H5A	0.3305	−0.1786	0.1830	0.254*	
H5B	0.3295	−0.1193	0.2643	0.254*	
H6A	0.4420	−0.0776	0.2253	0.236*	
H6B	0.4023	−0.0146	0.1498	0.236*	
H7	0.4852	0.4012	0.1947	0.179*	0.50
H8A	0.4563	0.4709	0.3357	0.204*	0.50
H8B	0.3976	0.4095	0.2732	0.204*	0.50
H9A	0.4151	0.5664	0.1821	0.238*	0.50
H9B	0.3927	0.6278	0.2554	0.238*	0.50
H10A	0.5150	0.6684	0.3047	0.255*	0.50
H10B	0.4929	0.7322	0.2241	0.255*	0.50
H9'1	0.6022	0.6278	0.2247	0.238*	0.50
H9'2	0.5425	0.5649	0.1640	0.238*	0.50
H8'1	0.6081	0.4100	0.2457	0.204*	0.50
H8'2	0.5854	0.4726	0.3185	0.204*	0.50
H1A	0.6588	0.2373	0.0281	0.114*	0.50
H14	0.6609	0.0458	0.0641	0.148*	0.50
H15	0.7264	−0.1350	0.0815	0.148*	0.50
H16	0.8418	−0.1428	0.0522	0.148*	0.50
H17	0.8917	0.0303	0.0056	0.148*	0.50
H2	0.8247	0.2059	−0.0105	0.148*	0.50
H14'	0.6193	0.4344	0.0000	0.137*	0.50
H15'	0.6461	0.6268	−0.0437	0.137*	0.50
H16'	0.7570	0.6626	−0.0799	0.137*	0.50
H17'	0.8411	0.5059	−0.0725	0.137*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0450 (3)	0.0490 (3)	0.0839 (4)	0.000	0.0237 (2)	0.000
F1	0.104 (5)	0.175 (7)	0.095 (4)	0.010 (4)	0.022 (3)	0.006 (4)
F2	0.104 (5)	0.175 (7)	0.095 (4)	0.010 (4)	0.022 (3)	0.006 (4)
F3	0.104 (5)	0.175 (7)	0.095 (4)	0.010 (4)	0.022 (3)	0.006 (4)
F1'	0.22 (1)	0.25 (2)	0.127 (7)	−0.03 (1)	0.015 (7)	−0.017 (8)
F2'	0.22 (1)	0.25 (2)	0.127 (7)	−0.03 (1)	0.015 (7)	−0.017 (8)
F3'	0.22 (1)	0.25 (2)	0.127 (7)	−0.03 (1)	0.015 (7)	−0.017 (8)
O1	0.067 (3)	0.133 (5)	0.084 (3)	−0.007 (2)	0.034 (2)	0.016 (3)
O2	0.071 (3)	0.175 (6)	0.105 (4)	−0.011 (4)	0.035 (3)	0.012 (4)
N1	0.051 (5)	0.093 (7)	0.089 (7)	0.000 (6)	0.029 (5)	−0.002 (7)
N2	0.100 (6)	0.087 (6)	0.109 (8)	0.018 (4)	0.020 (5)	0.013 (5)
N2'	0.098 (6)	0.080 (5)	0.095 (7)	0.012 (4)	0.009 (4)	0.001 (4)
C1	0.055 (3)	0.068 (4)	0.094 (4)	−0.009 (3)	0.019 (3)	0.008 (3)
C2	0.051 (4)	0.084 (5)	0.182 (9)	−0.001 (3)	0.017 (5)	0.002 (5)
C3	0.057 (4)	0.128 (8)	0.23 (1)	−0.006 (5)	0.025 (6)	−0.015 (9)
C4	0.077 (5)	0.139 (8)	0.147 (8)	−0.030 (5)	0.014 (5)	−0.016 (7)
C5	0.085 (6)	0.072 (5)	0.35 (2)	−0.027 (5)	0.017 (9)	−0.014 (8)
C6	0.069 (5)	0.074 (5)	0.33 (2)	−0.013 (4)	0.037 (7)	−0.043 (8)
C7	0.087 (7)	0.058 (6)	0.22 (1)	0.02 (2)	0.051 (8)	0.01 (2)
C8	0.099 (7)	0.067 (5)	0.25 (2)	0.015 (8)	0.05 (1)	0.012 (9)
C9	0.120 (9)	0.076 (6)	0.28 (2)	0.011 (10)	0.02 (1)	0.02 (1)
C10	0.17 (1)	0.073 (8)	0.26 (2)	0.00 (2)	0.01 (1)	0.03 (2)
C9'	0.120 (9)	0.076 (6)	0.28 (2)	0.01 (1)	0.02 (1)	0.02 (1)
C8'	0.099 (7)	0.067 (5)	0.25 (2)	0.015 (8)	0.05 (1)	0.012 (9)
C12	0.099 (8)	0.21 (2)	0.120 (9)	−0.012 (9)	0.035 (7)	0.022 (9)
C12'	0.099 (8)	0.21 (2)	0.120 (9)	−0.012 (9)	0.035 (7)	0.022 (9)
C13	0.100 (6)	0.087 (6)	0.109 (8)	0.018 (4)	0.020 (5)	0.013 (5)
C14	0.100 (6)	0.087 (6)	0.109 (8)	0.018 (4)	0.020 (5)	0.013 (5)
C15	0.100 (6)	0.087 (6)	0.109 (8)	0.018 (4)	0.020 (5)	0.013 (5)
C16	0.100 (6)	0.087 (6)	0.109 (8)	0.018 (4)	0.020 (5)	0.013 (5)
C17	0.100 (6)	0.087 (6)	0.109 (8)	0.018 (4)	0.020 (5)	0.013 (5)
C13'	0.098 (6)	0.080 (5)	0.095 (7)	0.012 (4)	0.009 (4)	0.001 (4)
C14'	0.098 (6)	0.080 (5)	0.095 (7)	0.012 (4)	0.009 (4)	0.001 (4)
C15'	0.098 (6)	0.080 (5)	0.095 (7)	0.012 (4)	0.009 (4)	0.001 (4)
C16'	0.098 (6)	0.080 (5)	0.095 (7)	0.012 (4)	0.009 (4)	0.001 (4)
C17'	0.098 (6)	0.080 (5)	0.095 (7)	0.012 (4)	0.009 (4)	0.001 (4)

Geometric parameters (Å, °)

Sn1—C1	2.143 (5)	C8—C9	1.56 (1)
Sn1—C1^{i}	2.143 (5)	C9—C10	1.52 (1)
Sn1—C7	2.117 (9)	C10—C9'	1.53 (1)
Sn1—O1	2.313 (5)	C9'—C8'	1.57 (1)
Sn1—O1^{i}	2.313 (5)	N1—C13	1.26 (1)

C12—F1	1.334 (9)	N1—C13'	1.33 (1)
C12—F2	1.331 (9)	C13—C14	1.3900
C12—F3	1.440 (9)	C13—N2	1.3900
C12—C11	1.48 (1)	C14—C15	1.3900
O1—C11	1.219 (9)	C15—C16	1.3900
O2—C11	1.223 (9)	C16—C17	1.3900
C1—C6	1.486 (8)	C17—N2	1.3900
C1—C2	1.523 (7)	C13'—C14'	1.3900
C2—C3	1.527 (8)	C13'—N2'	1.3900
C3—C4	1.488 (8)	C14'—C15'	1.3900
C4—C5	1.514 (8)	C15'—C16'	1.3900
C5—C6	1.548 (8)	C16'—C17'	1.3900
C7—C8	1.51 (1)	C17'—N2'	1.3900
C7—C8'	1.52 (1)		
C1—Sn1—C7	121.3 (2)	C8'—C7—Sn1	120.5 (5)
C1—Sn1—C1^{i}	117.4 (3)	C7—C8—C9	108 (1)
C1—Sn1—O1	87.5 (2)	C10—C9—C8	109 (1)
C1—Sn1—O1^{i}	93.7 (2)	C9—C10—C9'	109 (1)
C1^{i}—Sn1—C7	121.3 (2)	C10—C9'—C8'	109 (1)
C1^{i}—Sn1—O1	93.7 (2)	C7—C8'—C9'	108 (1)
C1^{i}—Sn1—O1^{i}	87.5 (2)	O1—C11—O2	129.1 (7)
C7—Sn1—O1	88.8 (1)	O1—C11—C12	116.3 (7)
C7—Sn1—O1^{i}	88.8 (1)	O2—C11—C12	114.5 (7)
O1—Sn1—O1^{i}	177.5 (3)	C13—N1—C13'	133 (1)
F2—C12—F1	114 (1)	N1—C13—C14	119 (1)
F2—C12—F3	99.3 (9)	N1—C13—N2	121 (1)
F1—C12—F3	102.7 (9)	C14—C13—N2	120.0
F2—C12—C11	116.8 (8)	C13—C14—C15	120.0
F1—C12—C11	117.3 (9)	C14—C15—C16	120.0
F3—C12—C11	103.0 (8)	C17—C16—C15	120.0
C11—O1—Sn1	129.1 (5)	C16—C17—N2	120.0
C6—C1—C2	112.2 (6)	C17—N2—C13	120.0
C6—C1—Sn1	115.1 (4)	N1—C13'—C14'	122 (1)
C2—C1—Sn1	113.1 (4)	N1—C13'—N2'	119 (1)
C3—C2—C1	112.4 (6)	C14'—C13'—N2'	120.0
C4—C3—C2	112.8 (7)	C13'—C14'—C15'	120.0
C3—C4—C5	110.7 (7)	C16'—C15'—C14'	120.0
C4—C5—C6	109.3 (7)	C17'—C16'—C15'	120.0
C1—C6—C5	111.0 (7)	C16'—C17'—N2'	120.0
C8—C7—C8'	110.6 (9)	C17'—N2'—C13'	120.0
C8—C7—Sn1	120.5 (5)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2	0.86	1.88	2.72 (1)	162